SAND2022-3503R

R E S E A R C H

LABORATORY DIRECTED
RESEARCH & DEVELOPMENT

FY21 ANNUAL REPORT

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

All photos in this report showing individuals not wearing masks or not socially distanced from others were taken prior to the pandemic.

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SAND2022-xxxx R

Laboratory Directed Research and Development
FY21 Annual Report

From the Chief Research Officer

Sandia National Laboratories leans into the future through its Laboratory Directed Research and Development (LDRD) program. This refined and strategic mechanism allows teams to conduct innovative and exploratory research that fuel Sandia's priorities, support strategic initiatives, and address the broad range of challenging problems facing the Nation today.

The LDRD program allows Sandia to assemble experts from different fields to execute world-class science and engineering research focused on national security that are transformational in nature due to their high-risk, high-reward potential. Through leading-edge efforts, teams find new ways to leverage current capabilities and explore possibilities to amplify our country's safety and security through innovations that support nuclear deterrence capabilities, advance counterterrorism, augment defense efforts, and optimize and protect our energy production. These research projects intersect with challenges on today's world stage such as climate change, bioengineering, radioactive waste, the proliferation of nuclear weapons, and the protection of critical information and resources. The discovery research in areas such as mathematics, bioscience, computing, and pulsed power, just to name a few, will lead to long-term impacts and differentiating capabilities; their models, diagnostics and sensors will help validate methodologies and predict the behaviors of engineered and autonomous systems into the future.

Some of the Nation's most exciting innovations in 2021 have origins in LDRD investments—from highly interconnected photovoltaic cells licensed for a satellite now in orbit, to a biologically inspired electrodialysis membrane for producing fresh water from seawater, to the extraction of rare-earth metals from coal ash. Sandia scientists and engineers are supporting the missions of today and tomorrow by creating innovations for deep space, deep waters, or deep within earth.

A critical component of our LDRD program is workforce development. Sandia's internal LDRD processes and NNSA guidance allow our highly talented scientists and engineers to further develop their technical acumen by submitting proposals and performing high-end research that span foundational disciplines to more applied missions. The LDRD program also fosters a technical talent pipeline for the Laboratories by allowing university students to engage in Sandia's R&D and learn how they can contribute to the Nation. It also provides an avenue for postdoctoral students to collaborate with Sandia's teams and utilize the Labs' world-class facilities in support of NNSA priorities.

I am proud of Sandia's LDRD program and all the significant achievements it helps to facilitate. As long as the world has questions and challenges, Sandia's best and brightest will step forward to help provide the answers and solutions.

Susan Seestrom

Associate Laboratories Director & Chief Research Officer
Advanced Science and Technology

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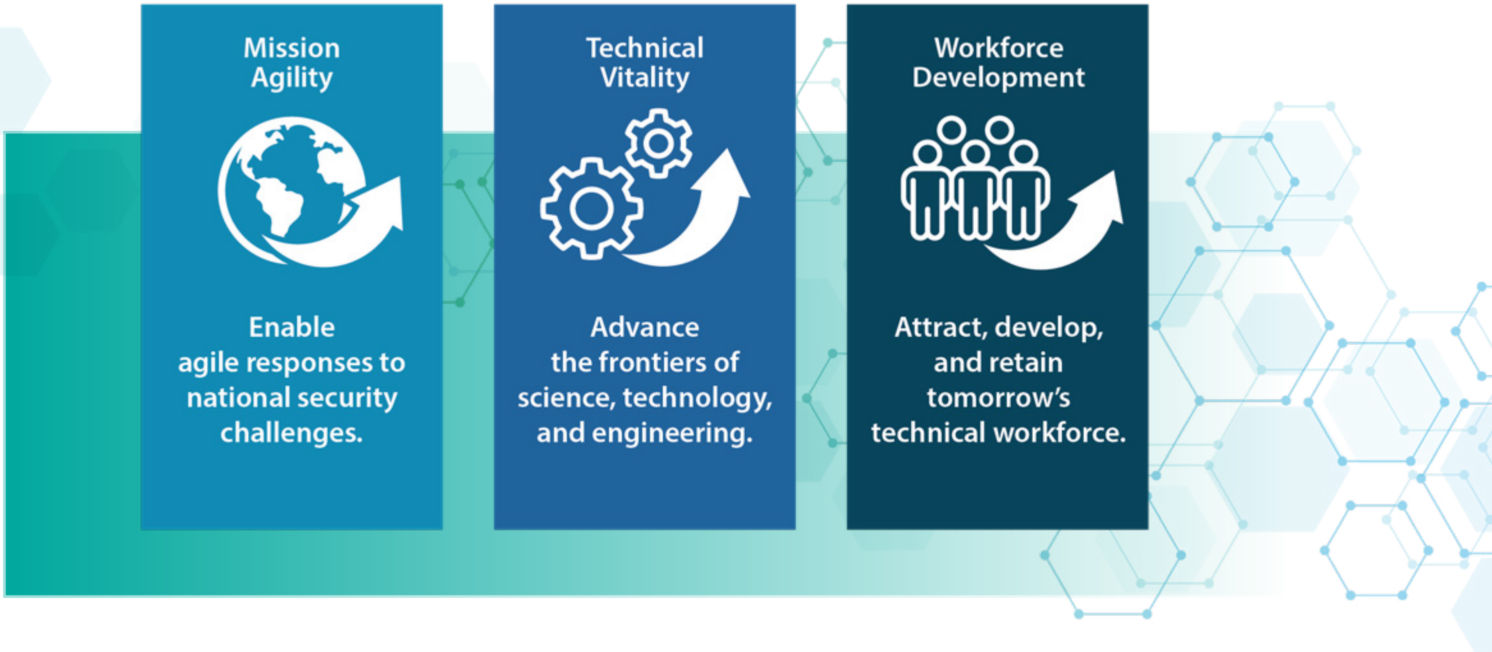
LDRD PROGRAM OVERVIEW

Sandia is a federally funded research and development center (FFRDC) dedicated to developing and applying advanced science and engineering capabilities to mitigate national security threats. This is accomplished through the exceptional staff leading research at the Labs and partnering with universities and companies.

Sandia's LDRD program funds foundational, leading-edge discretionary research projects that cultivate and utilize core science, technology, and engineering (ST&E) capabilities. Per Congressional intent (P.L. 101-510) and Department of Energy (DOE) guidance (DOE Order 413.2C, Chg 1), Sandia's LDRD program is crucial to maintaining the nation's scientific and technical vitality and enhancing the Labs' ability to address future mission needs.

LDRD Program Objectives

Sandia's LDRD program objectives align with DOE Order 413.2C and National Nuclear Security Administration (NNSA) guidance. The Mission Agility and Technical Vitality objectives are supported by the Workforce Development objective, which is a critical element to affect, grow, and leverage the technical experts needed to execute R&D projects.



Sandia's LDRD Program Structure

Sandia's LDRD investments are structured around three Program Areas further broken down into Investment Areas (IAs). Each IA responsible for discipline- or mission-based research priorities set by Sandia's leadership. The LDRD program structure aligns LDRD investments with Sandia strategy and future national security mission needs.

LDRD Investment Area Roles

Research Foundations: Research Foundations (RF) steward discipline-based science, technology, and engineering competencies that address the extensive national security challenges within Sandia's mission space. Each RF stewards differentiating or unique capabilities in one of seven critical areas.

- Bioscience
- Computing and Information Sciences
- Earth Science
- Engineering Sciences
- Materials Science
- Nanodevices and Microsystems
- Radiation, Electrical, and High Energy Density Science

Mission Foundations: Sandia oversees five major portfolios that address national security mission challenges. Mission Foundations (MF) align with the portfolios and conduct the applied research needed to develop capabilities and demonstrate solutions.

- Nuclear Deterrence
- National Security Programs
- Global Security
- Energy & Homeland Security
- Advanced Science & Technology

Strategic Initiatives: Strategic Initiatives (SI) promote strategic collaborations and CRO/Labs-directed initiatives. SI include Grand Challenge projects to solve major research challenges that require large multidisciplinary teams; Mission Campaign IAs to move ST&E intentionally from idea to mission impact; Exploratory Express to execute short-term projects of strategic importance; and New Ideas to pioneer fundamental R&D to discover game-changing breakthroughs. These initiatives also support strategic academic collaborations (111 in FY2021) and both the Harry S. Truman and Jill Hruby Postdoctoral Distinguished Fellowships.

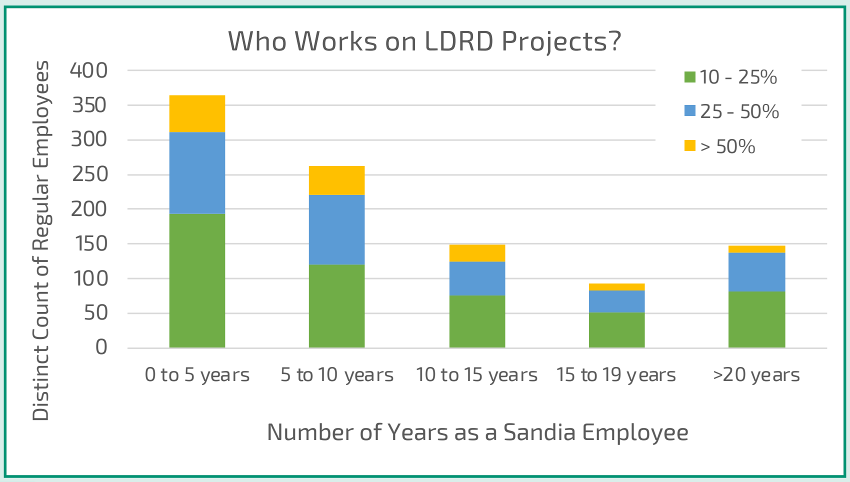
LDRD PROGRAM VALUE

Performance Indicators

While the FY2021 LDRD program represented only about 5.2% of Sandia's total costs, the metrics shown below highlight how LDRD has a much greater relative impact on key performance indicators (KPI) and metrics for the Labs. The bar graph illustrates the large percentage of early career staff, postdocs, and students engaged in the LDRD program compared to the overall eligible population, thus validating LDRD's important role in attracting, developing, and retaining a world-class workforce to meet our most challenging national security needs.

FY 2021 LDRD Program Statistics

$202.3M	$389K	493	245
Total Program Cost (not including PM costs)	Median Project Size	Total LDRD Projects	New Projects in FY20



LDRD-Supported Postdocs	196	46% of Sandia total
LDRD-Supported Postdoc to Staff Conversions	32	52% of Sandia total
Refereed Publications	366	26% of Sandia total
Technical Advances	123	40% of Sandia total
Patents Issued	63	53% of Sandia total
Copyrights	35	21% of Sandia total
R&D 100 Awards	5	56% of Sandia total

> . . . validating LDRD's important role in attracting, developing, and retaining a world-class workforce to meet our most challenging national security needs.

LONG-TERM METRICS

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 are updated annually. As expected, the data may vary from year to year so long-term running totals will be included and updated every 5 years.

Background

Applying continuous improvement, representatives from each LDRD program at the NNSA laboratories (Sandia, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory) 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 to be utilized by each NNSA LDRD laboratory, and acknowledged that individual laboratories may choose to report other long-term indicators that fit their unique missions and capabilities.

Alignment with LDRD Objectives

The KPI for LDRD, including numerical KPIs in the form of metrics and qualitative KPIs in the form of project highlights, illustrates the long-term payoffs/success of the program in meeting its three objectives: Technical Vitality, Mission Agility, and Workforce Development. Because KPIs crosscut the three objectives, this report will not provide a 1:1 mapping.

Importance of Qualitative Data

Developing numerical indicators for R&D program success is widely recognized as difficult. The NNSA LDRD metrics working group developed numerical success indicators for both Technical Vitality and Workforce Development. Project highlights or "success stories" capture the successes in Mission Agility and some aspects of the other two LDRD objectives not well represented by numerical metrics.

ROOTED IN LDRD

...having "LDRD roots" means one or more previous LDRD projects had a critical influence on the development.

Tracing impact back to LDRD

Throughout this section, you will see references to "LDRD roots." LDRD mentors and principal investigators (PI) often discuss what it means for an accomplishment to have LDRD roots. A simple case might involve an idea for an invention that 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 quickly. 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 a current LDRD project relies on an earlier LDRD accomplishment, then it is considered to have "roots" in the prior LDRD project. Other relevant definitions for metrics are included in the sections to follow.

THE INDICATORS

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 affiliated laboratory. The NNSA laboratories consider American Physical Society (APS) Fellowships as the exemplar award because physicists naturally link with NNSA's core stockpile stewardship mission, and APS Fellowship is awarded based on scientific merit and impact over an extended period of time.

As a premier engineering and science laboratory, Sandia produces relatively fewer APS fellows when compared to the NNSA physics laboratories. Of the two APS fellows elected in the past three years, both had LDRD experience. Over the past ten years, over 81% of Sandia's APS fellows have had LDRD experience.

LDRD and American Physical Society Fellows at Sandia National Laboratories

	Single Years			Five Years		To Date*
	FY19	**FY120**	**FY21**	**FY11-15**	**FY16-20**	**FY11-21**
Total Awards	2	0	0	12	10	22
Awards with LDRD Roots	2	N/A	N/A	9	9	18
% with LDRD Roots	100%	N/A	N/A	75%	90%	81%
Average Years from First LDRD Experience	12.0	N/A	N/A	14.7	13.0	13.8

**Initial year to date: Each NNSA laboratory has chosen the appropriate lookback period to ensure data integrity.*

Other Professional Societies

In addition to APS awardees, researchers at Sandia have been elected as Fellows to numerous other prestigious scientific and engineering societies, with the greatest number elected to the societies listed below. Since 2011, 42 individuals have been elected Fellow to one professional society (excluding APS). Four individuals have been elected Fellow to two professional societies, and 80% of Fellows had LDRD experience during their Sandia careers.

- American Association for the Advancement of Science
- American Institute of Aeronautics and Astronautics
- American Society of Mechanical Engineers
- Institute of Electrical and Electronics Engineers
- Society for Industrial and Applied Mathematics

R&D 100 Awards

Another 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 in either the standard category or special awards have "LDRD roots." Often, because of the long development time from an LDRD idea to practical implementation, the staff who work on an award-winning technology product may not be the same researchers who initiated 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.

Since 1976, Sandia has won 135 R&D 100 awards, illustrating the Labs' contributions in developing products and technologies with the potential to change industries and improve the world. Over the past three years, 54% of Sandia's R&D 100 winning contributions have been rooted in LDRD; over the past 16 years, over 69% have come from LDRD. FY2021 winners from Sandia are described in depth in the Workforce Development section of this report.

LDRD and R&D 100 Awards Earned by Sandia National Laboratories

Counts in the metrics below include standard R&D 100 awards and special recognition awards, as well as awards led by other organizations where Sandia was a key partner.

	Single Years			Five Years		To Date*
	FY19	**FY20**	**FY21**	**FY11-15**	**FY16-20**	**FY06-21**
Total Awards	8	7	9	20	32	82
Awards with LDRD Roots	4	4	5	15	22	57
% with LDRD Roots	50%	57%	56%	75%	69%	69%
Average Years from First LDRD Investment	3.8	8	4.6	5	5.6	5

**Initial year to date: Each NNSA laboratory has chosen the appropriate lookback period to ensure data integrity.*

Sandia won a 2021 R&D 100 Award and a Silver Corporate Social Responsibility Award for developing a reusable and rapidly producible N95 respirator for medical applications in the RAPTR N95 project.

Top 2%

A relevant indicator of career advancement in an ST&E field is the recognition of individuals as distinguished members of the technical staff, known as Senior Scientists/Engineers at Sandia, Fellows at Los Alamos National Laboratory, and Distinguished Members of the Technical Staff at Lawrence Livermore National Laboratory.

The shorthand name used here, "Top 2%," comes from the intent at each laboratory to limit membership to the top 1% or 2% of scientific and technical staff. Typically nominated and screened by a committee, the Top 2% are recognized for something similar to a lifetime achievement, in this case, for contribution to the mission of each laboratory.

Each year at Sandia, a small number of staff are appointed to the rank of Senior Scientist/Engineer, an honor based on exceptional leadership and consistently outstanding contributions to Sandia's national security missions. In FY2021, four out of the eight staff promoted to Senior Scientist/Engineer were involved in the LDRD program as a PI or team member during their careers. Since FY2011, 71% of Sandia's Top 2% have LDRD roots.

LDRD and Top 2% Technical Staff at Sandia National Laboratories

	Single Years			Five Years		To Date*
	FY19	**FY20**	**FY21**	**FY11-15**	**FY16-20**	**FY11-21**
Total Awards	11	16	8	26	46	81
Awards with LDRD Roots	11	15	4	15	38	58
% with LDRD Roots	100%	93%	50%	57%	82%	71%
Average Years from First LDRD Experience	19.1	20.0	12.1	10.4	18.7	16.3

*Initial year to date: Each NNSA laboratory has chosen the appropriate lookback period to ensure data integrity.

Typically nominated and screened by a committee, the Top 2% are recognized for something similar to a lifetime achievement, in this case, for contribution to the mission of each laboratory.

Newly Promoted Senior Scientist Highlights

Gregory Tipton

Dr. Gregory Tipton led the creation of the integrated engineering sciences analysis and experimental capabilities that transformed the nuclear deterrence enterprise qualification methods and also contributed to LDRD projects focused on nuclear weapons surety. He currently provides technical leadership to the Engineering Sciences Research Foundation (ESRF), which manages the Engineering Sciences LDRD portfolio and oversees the mentoring of new PIs in this area. Of his contributions to the LDRD program, Tipton says –

> *"Being a part of the ESRF allows me to see the breadth of technical work going on at the laboratories. It also enables me to help guide early career researchers, while helping to align research and development (R&D) to critical mission areas."*

Stephanie Hansen

Dr. Stephanie Hansen, a world leader in atomic physics and x-ray spectroscopy modeling and Fellow of the American Physical Society, has applied her expertise to a broad range of research areas, including inertial confinement fusion, radiation effects sciences, high energy density physics, and astrophysics. Hansen has led numerous LDRD projects at Sandia. Reflecting on her experience with LDRD, she noted –

> *"In my years at Sandia, I've always tried to be engaged with at least one LDRD project. I see LDRD as the lifeblood of the laboratories, giving oxygen to the creative, generative science that helps us keep pace with a dynamic world. In many cases, these past LDRDs explored new ideas that became the foundation of today's programmatic work while keeping scientists engaged with and excited about their work."*

Fellow Highlights

Sandia also reserves a special recognition for an elite group of individuals—Sandia Fellows—recognized for careers of significant technical accomplishment for the Labs and for the nation. In Sandia's history, only 15 individuals have held this title. In FY2021, six of these Fellows were on staff, and all six had been involved with LDRD in their careers. The LDRD Program's Strategic Partnerships pillar funds a set of projects selected and managed by Sandia Fellows. The Fellow projects enable the Labs' most stellar R&D staff to mentor promising staff as they pursue leading-edge, potentially high-impact R&D. Three Fellows projects are featured in this year's Annual Report:

Kathy Simonson, Sandia Fellow

Dr. Katherine Simonson is a Laboratories Fellow in Sandia's Global Security division. She has served as Sandia's project lead or PI for a wide range of research, development, and transition programs in airborne and space-based intelligence, surveillance, and reconnaissance (ISR). Her teams developed numerous statistical algorithms that enable robust, real-time processing and exploitation of data from a diverse collection of sensors and platforms. Many of the techniques she developed for automated and semi-automated data exploitation are employed in operational ISR programs, enabling system operators to rapidly identify, interpret, and act on signatures of interest. Kathy has a long history with LDRD, leading and contributing to numerous projects since 1998. Simonson reflects on the role of LDRD in her career:

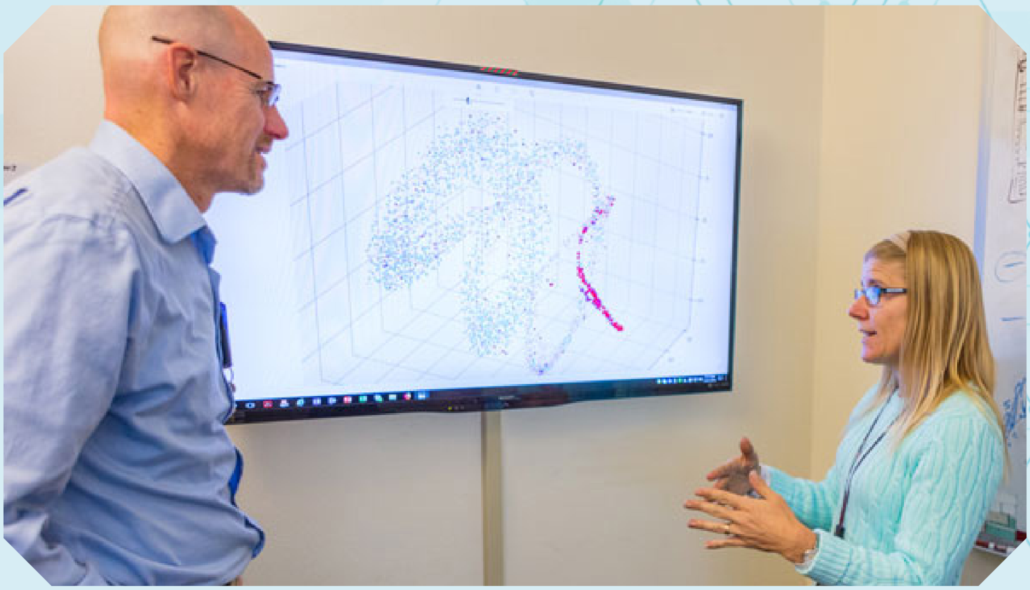
"LDRD has been pivotal in my career at Sandia! Three of the projects for which I served as PI have resulted in significant enhancements to mission performance for deployed, operational systems. In each case, the LDRD research was motivated by a realization that new research could ultimately open the door to new system capabilities with great benefit to the national security enterprise. Our teams took the work from mathematical derivations with pencil and paper through proof of concept (under LDRD funding) and on to operational transition (under sponsor funding). These were the most satisfying experiences of my career at Sandia. And each of these developments was generalizable enough that they continue to be applied in novel applications unforeseen at the time that the LDRD work was underway."

Simonson is also a champion and mentor for early career PIs and those new to the LDRD process. She helped stand up Research Clubs at Sandia, which assists new researchers in honing their skills as they submit their ideas to the LDRD program. She is currently overseeing one Fellow's project on novel detection mechanisms assess aerosol-cloud interactions. Regarding the genesis and outcome of the project, Simonson explained, "The project resulted from a brainstorming session involving

- Novel detection mechanisms assess aerosol-cloud interactions
- Impacting future nuclear deterrence products through new unique discriminators
- Ultra-high-resolution electron scattering apparatus enables advanced studies of electron interactions with gas molecules and temporal evolution of plasmas

nine early- and mid-career Sandians that I knew and respected. They came from five different divisions and mostly did not know one another. I asked them to think about research they would like to collaborate on that involved three elements: rigorous mathematics and statistics, modern computer science, and application to at least one mission area where the team had passion. They were left to decide on a PI, a project to propose, and a research plan. I loved watching the core team of five researchers come together to build a project that was compelling from a technical standpoint, and highly relevant to the climate challenge we are all facing. I love to see the team members continuing to collaborate on a range of interesting and impactful research projects."

Read more about Simonson's promotion to the esteemed rank of Sandia Fellow.



Computer scientist Jenny Galasso discusses her Exploratory Express LDRD research proposal data with fellow computer scientist Kurt Larson, a "coach" in a Sandia research club. (Photo by Nicholas Kerekes)

SHORT-TERM METRICS

Intellectual Property

Patents

Number of U.S. and foreign patents issued in a given FY.

	FY17	FY18	FY19	FY20	FY21
Sandia Patents	157	148	159	131	120
LDRD-Supported*	86	76	76	67	63
% Due to LDRD	55%	51%	48%	51%	53%

**LDRD-supported patents: Patents issued that would not exist if not for initial work funded by LDRD.*

Copyrights

Number of copyrights created in a given FY.

	FY17	FY18	FY19	FY20	FY21
Sandia Copyrights	101	107	104	163	169
LDRD-Supported*	25	17	25	40	35
% Due to LDRD	24%	15%	24%	24%	21%

**LDRD-supported copyrights: Copyrights issued that would not exist if not for initial work funded by LDRD.*

Invention Disclosures

Number of declarations and initial records of an invention (a new device, method, or process developed from study and experimentation).

	FY17	FY18	FY19	FY20	FY21
Sandia Disclosures	296	260	252	320	309
LDRD-Supported*	125	112	102	121	123
% Due to LDRD	42%	43%	40%	37%	40%

**LDRD-supported disclosures: Disclosures issued that would not exist if not for initial work funded by LDRD.*

Peer-reviewed Publications

Number of peer-reviewed publications, as a function of publication year.

	FY17	FY18	FY19	FY20	FY21*
Sandia Publications	1251	1170	1399	1299	N/A
LDRD-Supported **	293	363	366	343	N/A
% Due to LDRD	23%	31%	26%	26%	N/A

**Sandia reports publications as a lagging metric, so FY20 data will be reported in FY21.*

***LDRD-supported publications: Publications that would not exist if not for initial work funded by LDRD.*

Science and Engineering Talent Pipeline

Student Interns Supported by LDRD (>10%)

Number of graduate and undergraduate students working full- or part-time for the Labs, who charged at least 10% time to LDRD.

	FY17	FY18	FY19	FY20	FY21
Grad Students	71	82	106	127	139
Undergrad Students	98	104	115	100	84
Sandia R&D students	**542**	**614**	**733**	**722**	**711**
% due to LDRD	**31%**	**30%**	**30%**	**31%**	**31%**

Postdoctoral Researcher Support

Number of postdoctoral researchers working full- or part-time for the Labs.

	FY17	FY18	FY19	FY20	FY21
Sandia Postdocs	316	302	388	350	428
LDRD-Supported >10%*	132	133	148	163	196
% Due to LDRD	42%	44%	38%	46%	46%

**LDRD-supported postdoctoral researchers: Postdoctoral researchers charging at least 10% time to LDRD.*

Postdoctoral Researcher Conversions

Number of conversions from postdoctoral researcher to a member of the staff.

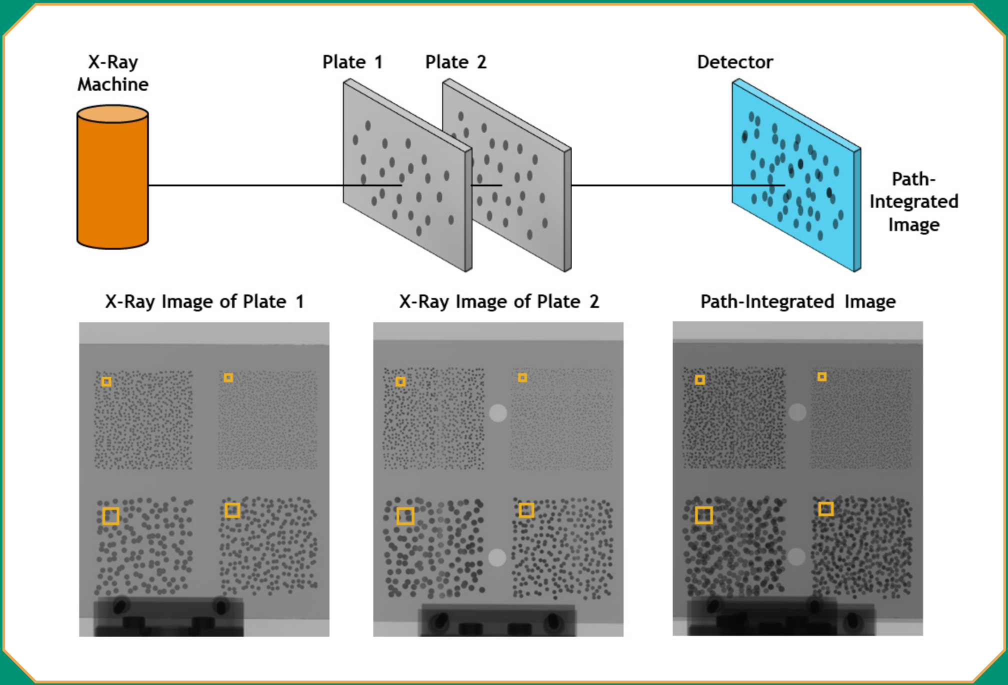
	FY17	FY18	FY19	FY20	FY21
Sandia Conversions	47	53	68	47	61
LDRD-Supported >10%*	22	25	34	25	32
% Due to LDRD	47%	47%	50%	53%	52%

**LDRD-supported conversions: Conversion of postdoctoral researchers who charged at least 10% time to LDRD in the fiscal year preceding the conversion.*

LDRD IMPACT STORY:

Digital Image Correlation: Pushing experimental innovation in data collection and model validation

Digital image correlation (DIC) is a measurement technique that allows us to "see" how materials behave, particularly under circumstances that are typically hard to measure experimentally. For example, DIC has been used at Sandia to understand how explosive devices come apart and how much destruction they cause (so that damage can be mitigated), or how a test-weapon behaves when it slams into a target. Such knowledge can then be used to validate and improve models, ultimately helping gain new insight into complex physical processes. At a high level, DIC is a tracking method that leverages high-speed photography (millions of frames per second) to compare pairs of images. Typically, an object of interest is coated with a speckled pattern that is tracked over time to ascertain how the object behaves. DIC algorithms analyze the pattern movement to measure displacement, velocity, and strain of the object. It may sound straightforward, but many factors, from the camera setup to the choice of the speckle pattern, can affect the results.



Schematic (top) and experimental x-ray images (bottom) of multiple DIC patterned planes generating a single path-integrated x-ray image. Through novel data algorithms, each plane can be separated to discern independent motion, simultaneously.

Sandia was an early adopter of DIC in 2005, as scientists were looking for better ways to validate and improve models unique to Sandia's national security missions, particularly in the areas of material deformation and explosive dynamics. Over the next decade, Sandia leveraged and enhanced the technique, including integrating uncertainty quantification into the approach—an important addition to ensure measurements made with DIC at Sandia so they could be considered traceable per the National Institute of Standards and Technology (NIST)—ultimately developing the first NIST traceable measurement for DIC. Sandia became a founding member of the DIC Society in 2015, helping to standardize the technique across the field, and actively leads efforts to train and certify DIC users on the technique, with courses being attended by scientists with Sandia, other NNSA labs, and the DoD. Sandia leads on the DIC Challenge, providing images and analysis for DIC code comparisons and improvement for users around the world.

At Sandia, LDRD advanced the state-of-the-art of DIC by both applying the technique to new domains and developing new techniques altogether. LDRD investments have:

- Improved how material models and material properties are determined via optimized test specimen design, novel inverse techniques, and full-field displacement data from DIC.
- Enabled the development and first-time demonstration of high-speed X-ray DIC in a harsh aerodynamic environment, thus improving measurements of the response of critical components to dynamic environments.
- Led the first successful demonstration of many advanced imaging diagnostics within post-detonation environments, improving models that help researchers understand fragment and fireball dynamics. Impacts from the capability development are broad. For example, DoD Joint Live Fire is adopting DIC for model validation for munitions models, and full-field model validation is now used on many non-nuclear weapons components.
- Helped nurture early career talent in the engineering sciences at Sandia. For example, early career researcher Caroline Winters contributed to numerous DIC LDRD research projects at Sandia. Winters says, “As a PI of an Exploratory Express LDRD project during my postdoc appointment and then reprising the role of PI for a full Engineering Sciences LDRD a year after transitioning to staff, LDRD has been pivotal to defining my technical path at Sandia. Through both the sponsored programming and the generous time given by the LDRD Investment Area team members, I have accelerated my technical writing, innovation, project management, and networking internal and external to Sandia.”

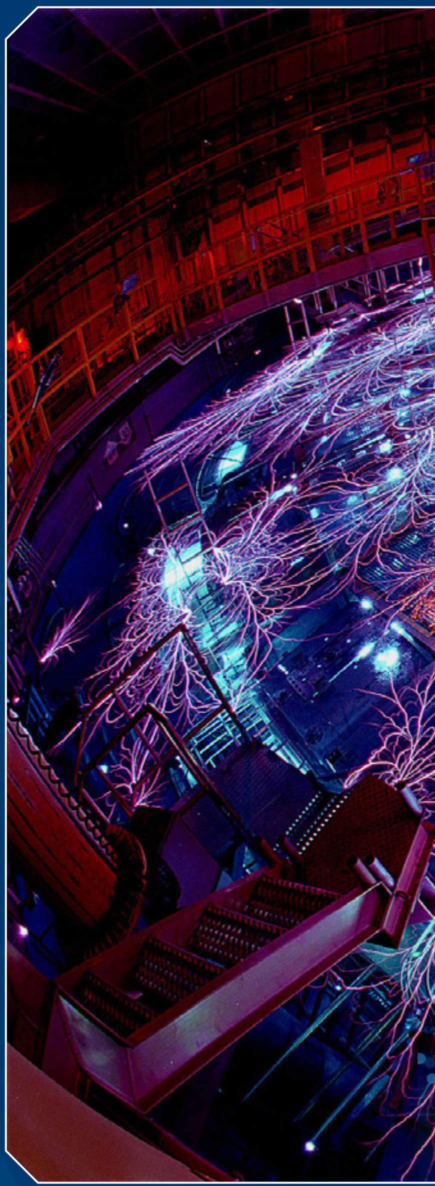
Caroline Winters

Winters is developing new DIC techniques as she leads an LDRD project that started in 2021. The work is investigating how to provide a “full” time-resolved and 3D picture of a test article undergoing combined, thermal-mechanical environments. Since tests are often conducted in occluded environments, like sooty pool fires, seeing in with X-rays is key to measuring strain, deformation, and temperature. Multi-planar X-ray DIC—an effort led by early career LDRD researchers Elizabeth Jones and Ben Halls—has extended the information we can infer from a single X-ray image. Specifically, we can now measure strain in multiple planes of motion, simultaneously, through both innovative patterning and novel data processing algorithms.”

LDRD IMPACT STORY:

Z machine: *The world's most powerful and efficient laboratory radiation source*

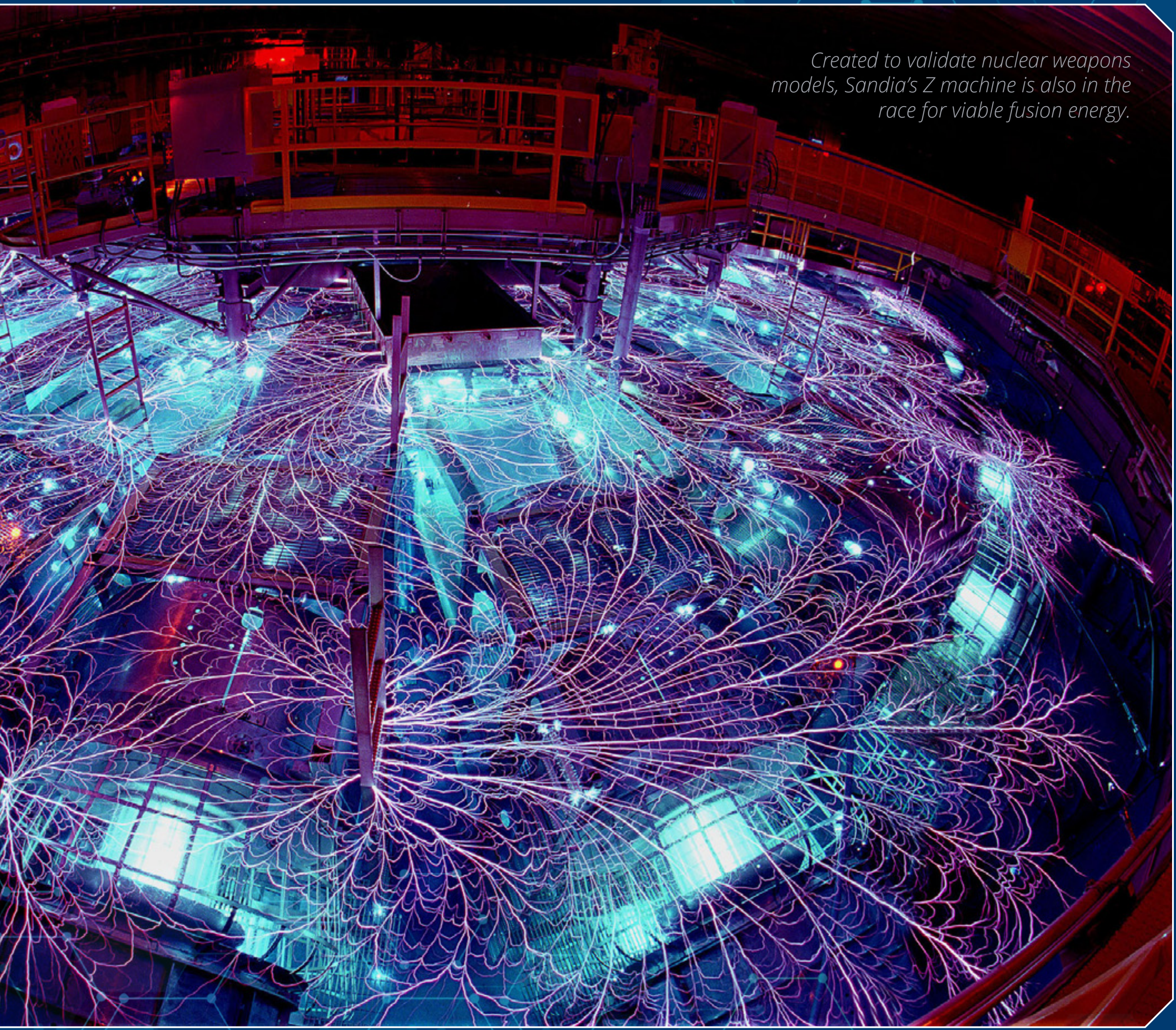
Sandia's Z machine uses high magnetic fields associated with high electrical currents to produce high temperatures, high pressures, and powerful X-rays for research in high energy density (HED) science. The Z machine, a part of Sandia's Pulsed Power program, creates conditions found nowhere else on Earth. Having a laboratory-based high-yield fusion capability within the nuclear weapons complex creates an experimental platform for assuring the U.S. nuclear weapons stockpile will perform far into the future.



Sandia's Z machine creates HED conditions, or radiation/neutron outputs, that provide data and experience to the modeling and design community in dynamic material properties, nuclear survivability and radiation effects, and inertial confinement fusion. Since the yield from the majority of the nation's nuclear weapons is generated when conditions within the explosive package are in the HED state, proficiency in HED science must remain a core technical competency for the foreseeable future.

Since 2005, LDRD investments have helped advance new HED platforms, which subsequently impacted DOE programs and enabled NNSA milestones. LDRD-funded HED research spanned topics such as advanced fusion concepts, hostile environments, dynamic temperature measurements, high pressure/pre-compression cells for planetary and stellar science, stochastic shock in advanced materials, and certifiable additive manufacturing techniques.

LDRD continues to play a key role in looking towards the next generation of pulsed power. The Assured Survivability and Agility with Pulsed Power (ASAP) LDRD Mission Campaign is a set of targeted investments spanning FY20-FY26 focused on enabling critical testing capabilities, providing validation data for national security threats, and qualification assessments for conventional and nuclear systems in hostile environments. ASAP R&D is expected to help inform the design for a next generation pulsed power facility providing ten times the energy of the current Z machine. This new facility, when realized, could address several key issues in weapon science, dynamic materials, effects modeling, and fusion research not possible at existing NNSA facilities.

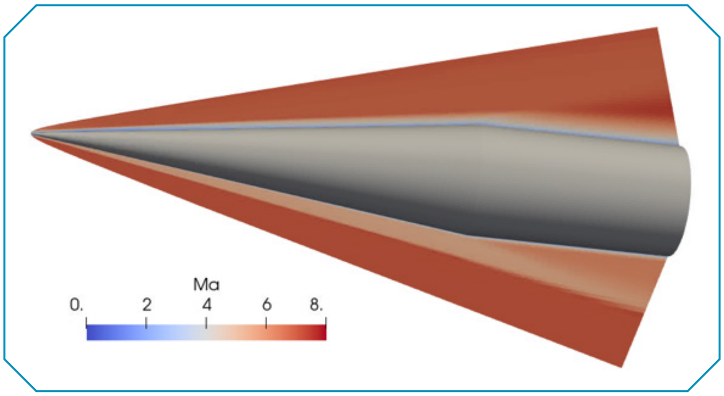


Created to validate nuclear weapons models, Sandia's Z machine is also in the race for viable fusion energy.

Project Highlights – Mission Agility

Sandia's LDRD program is organized around three themes: mission agility, technical vitality, and workforce development. Mission agility and technical vitality are closely related but differentiated by the technical readiness levels (TRL) of the research outcomes. The research outcomes in the accomplishments below have a higher TRL and could impact Sandia's mission work more quickly.

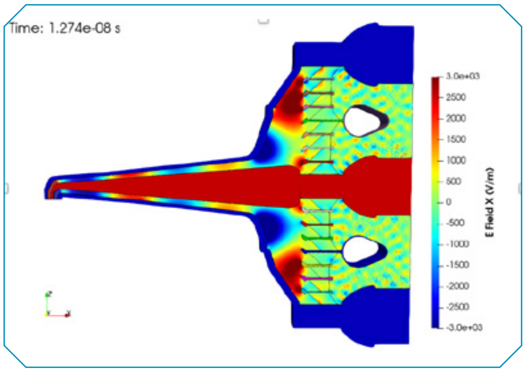
Unless otherwise noted, these highlights are for projects that ended in FY21.



A grid-tailored ROM with three input parameters for 3D flight vehicle geometries accurately computed the flow field and also improved axial force and wall heat flux accuracy over a data-driven surrogate model.

Reducing the costs associated with high-fidelity aerothermal simulations of hypersonic vehicles.
Thermal protection system designers rely heavily on high-fidelity computational simulation tools for the design and analysis of high-speed aerospace engineering applications due to the expense and difficulty of flight tests and experiments. Because necessary fine-grid resolution makes the computational fluid dynamics models expensive, analysts primarily use low-fidelity or surrogate models when simulations at many different flight conditions or designs are required. In this Autonomy for Hypersonics LDRD Mission Campaign project, researchers explored an alternative approach where projection-based reduced-order models (ROM) were used to approximate the computationally infeasible high-fidelity model. By applying cutting-edge ROM techniques, specifically the Petrov-Galerkin ROM equipped with hyper-reduction, the team demonstrated the ability to significantly reduce simulation costs while retaining high levels of accuracy in computed quantities of interest on a range of aerothermal problems related to national security. (PI: Pat Blonigan)

Improving accuracy of neural network algorithms.
Decreasing the risk for tailored hardware solutions in hypersonic flight system applications is essential. By using conventional and low-size/weight/power (SWaP) analog neural accelerator hardware, this LDRD project research team significantly improved accuracy of neural network algorithms. By comparing the energy and delay of analog-to-digital conversion (ADC) schemes, the team proposed a more energy-efficient ADC, enabling them to develop a detailed accelerator architecture model. By modeling the feasibility of implementing modern neural algorithms in current and future onboard systems where SWaP is constrained, system architects will be able to evaluate more hardware-conscious decisions. (PI: Matt Marinella)

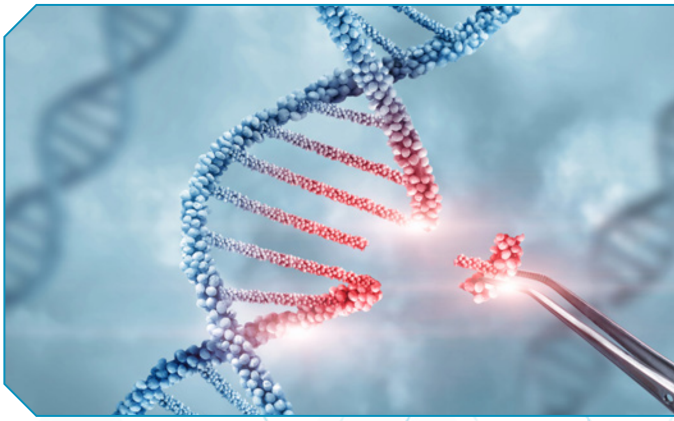


An EMPIRE-enabled simulation shows how transverse magnetic wave perturbation drives the lowest level magnetically insulated transmission line of the Saturn accelerator.

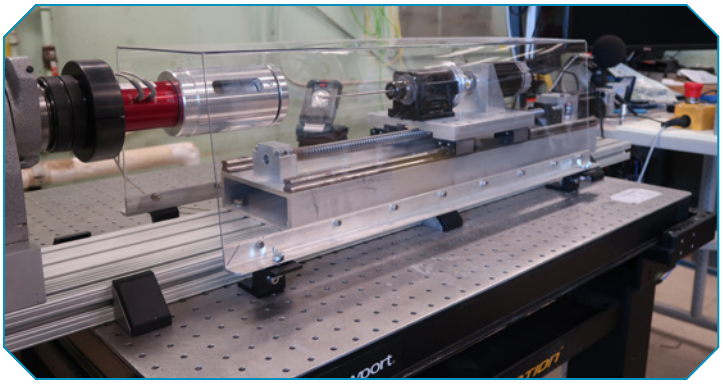
Coupling power flow to target simulations in support of next generation pulsed power facilities.

A one-year project under the Assured Survivability and Agility with Pulsed Power Mission Campaign explored problem reduction techniques for powerflow calculations in large pulsed power facilities to both improve time to solution and enable the characterization of electromagnetic drive in powerflow calculations. This work expanded the transmission line coupling capability in the ElectroMagnetic Plasma in Realistic Environments (EMPIRE) modeling and design tool—developed under the Plasma Science and Engineering Grand Challenge LDRD (FY18-FY20)—to include representations of Transverse Magnetic (TM) waves. TM waves, a generalization of the fundamental Transverse Electromagnetic (TEM) mode previously simulated, can represent pulse asymmetry in the system. In addition to a higher fidelity representation of waves in transmission line models, the team applied the theory developed during the LDRD to produce new synthetic diagnostics that allow analysts to quantitatively assess the regularity of the electromagnetic fields in a powerflow simulation. Using the new capabilities, the team evaluated the pulse regularization of the driver used in the Saturn accelerator. With such prototype calculations, it will be possible to evaluate the science-based design plans for the next generation pulsed power facilities at Sandia. (PI: Duncan McGregor)

Data science for detection of genome editing.



The current explosion of advances in gene editing technology and public accessibility to these techniques pose potential biosecurity threats. To accurately assess the risk to national security, bioengineering threats must be clearly distinguishable from natural genome variation, or edits. This LDRD project focused on a gap for detecting edits without prior information of the most likely regions in the genome where the edit effects will occur. The team employed three specific classes of algorithms: (1) decision-tree learners to identify subtle patterns and signatures that indicate an edit, (2) two complementary architectures of Deep Neural Networks learners to classify edit versus non-edit regions and learn grammatical patterns indicative of edit versus non-edit regions in next generation deep sequencing DNA reads, and (3) novel Anomaly Detection algorithms to characterize edit versus non-edit regions. Using large data sets from various genome editing experiments, the team built a data-processing pipeline to handle raw data file formats and provide genomic noise counts, and ultimately created features now used in machine learning algorithms. Results show significant evidence of success in detecting targeted edits in the human genome. The developed capabilities will provide both decision support for the national security community in assessing potential biosecurity threat risks and possible consequences and options for mitigation and/or forensic investigation. (PI: Stephen Verzi)



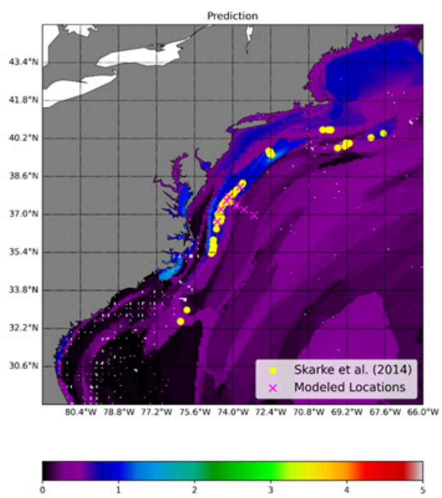
This drilling testbed collected force and torque data, which helped to develop the material transition detection algorithm for the microhole drilling system.

Supporting aging wellbore infrastructure through precise micro drilling.

By developing a revolutionary, remote, precision measurement capability, this team is enabling direct wellbore integrity assessment and supporting the aging wellbore infrastructure both in the United States and abroad. A microhole drilling system is being pursued to allow access to the cemented annular region between the casing and the rock mass enabling direct measurements of critical factors addressing wellbore integrity. The wellbore integrity platform consists of a microhole (< 0.100”) drilling system capable of reaching arbitrarily deep into the casing/formation. The emplacement sub-system is coupled with a machine-learning based leak detection algorithm that can localize a leak based on measured downhole data. A material transition detection algorithm will support the precision emplacement of sensors within the wellbore stack. This work, with a submitted patent application, will significantly impact the prevention of catastrophic oil and gas release events and is relevant to drilling automation and to other national security applications. (PI: Jiann Su)

Forecasting marine sediment properties.

The Arctic Ocean is one of Earth’s last frontiers. As climate change continues to expose this once frozen marine expanse, it is becoming the newest and most challenging theater of maritime operations for the military. The Navy relies on acoustic waves (sound) in the ocean to perform a variety of tasks critical to its national security mission. Sound can be altered significantly as it penetrates the seafloor and interacts with geologic structures or trapped gases before returning to the water column to propagate further. This project demonstrated the integration of geospatial machine learning prediction and sediment thermodynamic/physical modeling to create continuous, high-resolution, probabilistic maps of geoacoustic and geomechanical seafloor sediment properties even when existing observations of the seafloor are sparse. This new technique incorporated software developed in partnership with the University of Texas at Austin (UT Austin) and will be able to produce more reliable estimates of Arctic seafloor properties to support Arctic Naval operations relying on sonar performance and seabed strength, improve understanding of permafrost-associated natural gas hydrate resources, and constrain models of shallow tomographic structure important for nuclear treaty compliance monitoring/detection. (PI: Jennifer Frederick)



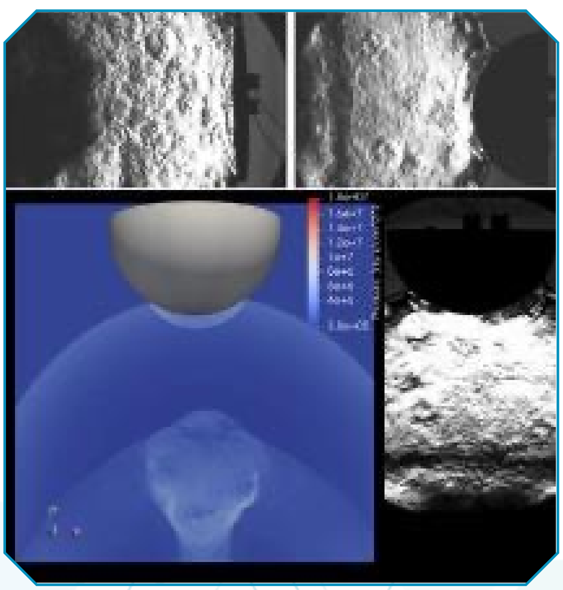
Output maps from the U.S. Naval Research Laboratory’s Global Predictive Seabed Model over the area 29°N–45°N and 82°W–66°W. Locations with known total organic carbon (TOC) values are marked by small white dots. Methane seeps (large yellow dots) identified by Skarke et al. (2014) are also plotted and support the increased TOC prediction between (35.4°N, 75.0°W) and (39.0°N, 72.0°W). Modeled gas hydrate locations were identified through models developed by UT Austin and are marked with a magenta X.

Predicting polymer foam deformation leads to accurate modeling for Sandia missions.
Many national security applications use polymer foam in transportation, necessitating accurate, predictive modeling capabilities. The three large-deformation constitutive models for flexible polymer foams resulting from this LDRD project are unified across foam densities and based on microstructural and macroscopic data and solid polymer physics. The models vary in maturity: the most mature model, density-as-an-input, is now available for nuclear deterrence use; the anisotropic quasi-linear visco-elastic model incorporating foam anisotropy and solid polymer physics models require some implementation; while the data-driven machine-learned model is the least ready for technical use. In addition to the models, this project discovered the relationship between the evolution of microstructural descriptors and macroscopic deformation and created an extensive data set of large-deformation testing data for a variety of transportation foams, including in situ X-ray computed tomography during deformation at both Sandia and Argonne's Advanced Photon Source. As a result of this work, the team submitted a patent filing and a technical advance for a high-force computed tomography-compatible load frame. The density-as-an-input model is currently being used to predict abnormal mechanical crash environments. The experimental approach led to material characterization and validation testing for numerous programs, and the models, associated data-science tools, and overall approach transformed Sandia's ability to predict polymer foam deformation. (PI: Sharlotte Kramer)

An experimental test system is mounted on the centrifuge arm prior to combined environments testing at the Sandia National Laboratories Superfuge/Centrifuge Complex in Albuquerque, New Mexico. (Photo by Byron Demosthenous)

Revolutionizing mechanical part design through a unique computational engineering design tool. Mechanical part designers and analysts are currently burdened by a traditional design-then-simulate iterative process that is extremely costly, time consuming, sub-optimal, and error prone. To address this, a research team developed a novel capability for solving inverse, topology optimization and optimal design problems where the physics is governed by nonlinear solid mechanics with contact and friction. Machine-learning based reduced-order modeling techniques were developed by Georgia Tech to complement the design optimization. In addition to enabling improved engineering designs, this computational tool significantly accelerates and improves the way mechanical part design is performed, which will help the national security enterprise respond more quickly to changing design requirements. (PI: Michael Tupek)

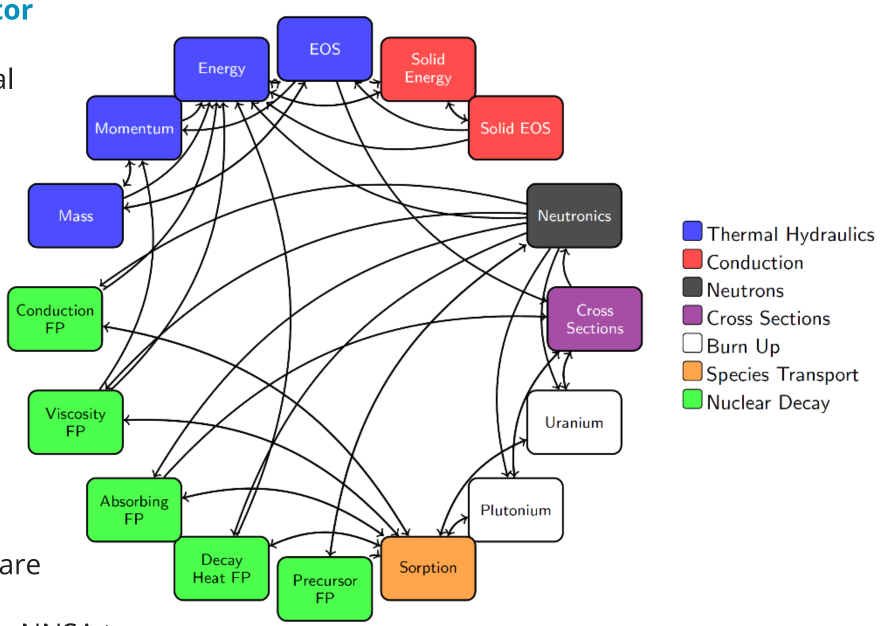
Proof of concept provides foundation for future testing of reentry devices. Sandia currently cannot fully test reentry vehicles in a complex and combined representative environment. This LDRD project tightly integrated experiments with high-fidelity simulations to provide proof-of-concept for a new test capability. The high-risk, high-reward idea introduced a tailored explosive shock loading to Sandia's Superfuge facility to enhance its combined inertial and vibration environments with a hostile blast. New Mexico Tech, an academic partner, conducted blast induced shock loading experiments with the assistance of graduate student, James Reeves, under the supervision of his professor, Dr. Michael Hargather. These experiments enabled a modest modeling/simulation/testing plus validation and verification effort. The successful combined environment test capability that could result from this proof-of-concept will drastically increase the agility of design, development, and qualification activities, and strengthen the nation's overall engineering capabilities. (PI: Timothy Miller)



(Top) Schlieren images showing a 1-gram-pentaerythritol tetranitrate blast on a 6-inch plate (left) and on a 6-inch hemisphere (right). (Bottom) Zapotec simulation and Schlieren video side-by-side 180 microseconds after detonation.

Predicting behavior of molten salt reactor facilities before final design.

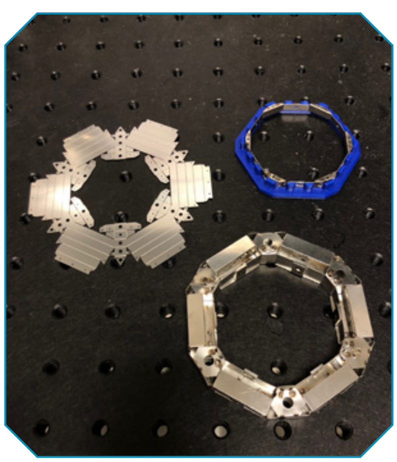
One challenge of using land-based, thermal reactors with uranium fuel is the complex coupling between the neutronics and thermal hydraulics due to chemical changes caused by fission products in the molten salt, which is both the fuel and the coolant. Although many promising capabilities for liquid-fueled molten salt reactors (MSR) exist, researchers face limited experience operating these designs for generating electricity, a lack of high-quality validation experiments, and a lack of knowledge of the long-term behavior of new fuels. This LDRD project produced a simulation software tool to predict the behavior of these MSRs before designs are finalized that will enable NNSA to define new monitoring processes and measurement equipment before this new class of nuclear reactors is deployed internationally. (PI: Vincent Mousseau)



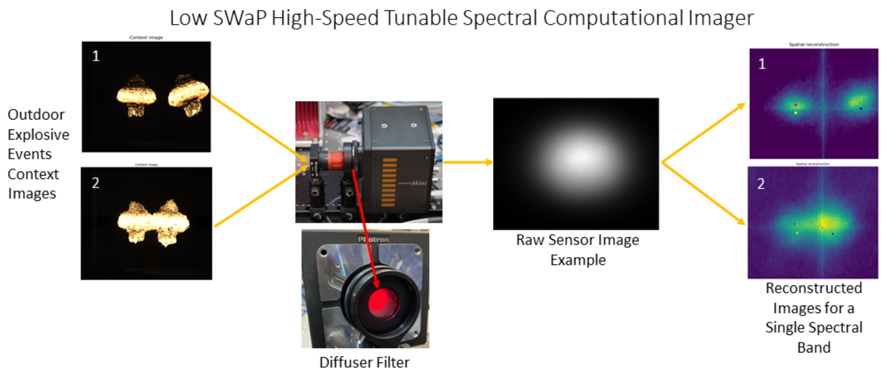
This diagram represents the complexity of molten salt reactors, showing traditional physics codes by color and nonlinear coupling between physics as arrows.

Extremely lightweight structures made from folded and 3D-printed metal.

Sandia opto-mechanical engineers used origami-style folding of photo-etched and micro-welded sheet metal along with 3D-printed metal parts to create ultralightweight structures for spaceborne optical systems. Traditional light-weighting usually starts with a heavy block of material that is then cut away. Sandia uses material thinner than traditionally machined ribs and walls and folds it to create the stiff structures the design requires. Photo-etching creates the shapes and fold lines for easy assembly. Two optical systems were created with designs guided by topological optimization techniques. Both approaches realized structure weight savings of >90% and 20% diameter reduction compared to traditional space system optical design and fabrication methods. Because the price and speed of photo-etching is fairly independent of a part's complexity , these designs are both less expensive and more quickly realized than standard machined assemblies. The possibility of extreme weight savings also makes using heavier materials like steel, invar, or copper more feasible for space applications. (PI: Edward Winrow)

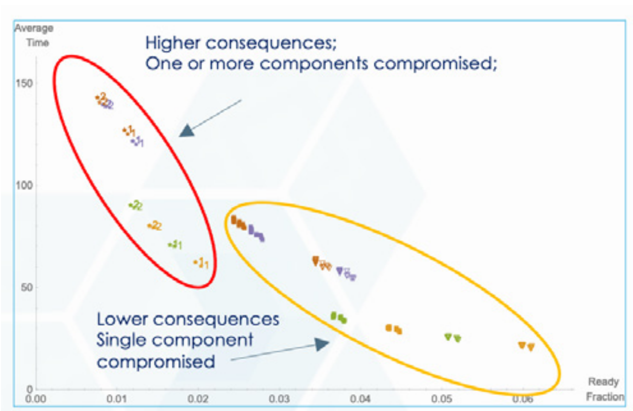


(Left) Folded and hybrid 3D-printed ultralight optical structures. (Right) Folded and unfolded lens subcell components.



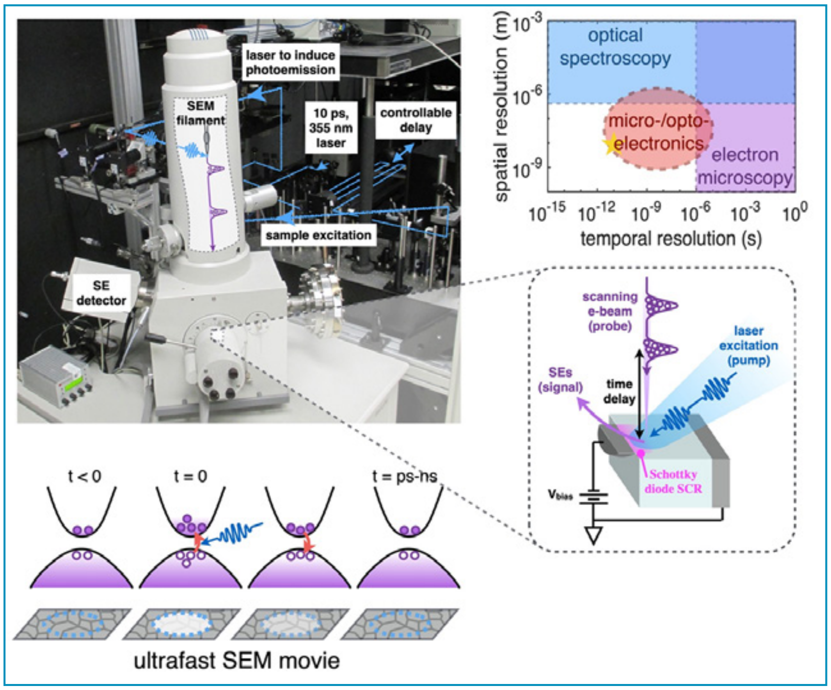
Sandia's low SWaP high speed tunable spectral computational imager helps to determine an explosive event's composition and configuration.

Low SWaP tunable hyperspectral video imager helps analyze explosions. Explosive events consist of rapidly varying spatial, spectral, and temporal information that produce a key signature to determine an explosive event's composition and configuration. Ideal measurement of explosive events is performed with a single low size, weight, and power (SWaP) instrument, which is capable of high spatial resolution, high-speed temporal sampling, and fine spectral resolution. This 4D dataset, also called a datacube, is not measurable with a single traditional 2D imaging system and requires compressive and computational optical methods. This LDRD project team designed, built, and tested a low SWaP diffuser-based high-speed spectral computational optical imaging system. The low SWaP spectral imager was successfully tested in a lab-based setting and during outdoor explosive testing. The team also developed image reconstruction methods, both traditional and machine learning, to reconstruct the spatial and spectral scene with high fidelity. Sandia partnered with New Mexico Tech to develop and build a prototype multichannel spectral imager as a complementary instrument to Sandia's imager. This project showed that computational optical methods can enable measurement of critical optical signatures for Sandia and NNSA's non-proliferation missions. (PI: John VanderLaan)



Each data point represents a combination of command and control experiment, scanning/detection experiment, and attacker/defender strategy. Defender's goal is to push the attacker toward top left of the plot.

Quantifying the security of a cyber system. Although the national security community widely recognizes the need for evidence-based cybersecurity, cyber analysts largely rely on qualitative metrics and expert intuition. The Science and Engineering of Cybersecurity by Uncertainty Quantification and Rigorous Experimentation (SECURE) Grand Challenge laid a foundation for cyber modeling and experimentation to catalyze the use of quantitative metrics and analytical evidence to inform high-consequence national security decisions. The SECURE project produced Defender, an objective, verified, and validated process that quantifies the security of a cyber system. As a result, it is now possible to quantify return on cybersecurity investments, rigorously compare two proposed remediations, identify critical components for improving security and model fidelity, and quantify attack consequences. The project created tools to automate and orchestrate cyber experiment scenarios, solve multi-level adversarial optimization problems, and reduce the number of expensive, high fidelity runs. The LDRD team developed the ability to optimize resilience against two cyberattacks on a power grid control system, as well as methods to quantify, compare, and rank defenses to quantify the resilience of the defender system. (PI: Ali Pinar)



The scanning ultrafast microscopy tool built at Sandia and its basic operation mechanism.

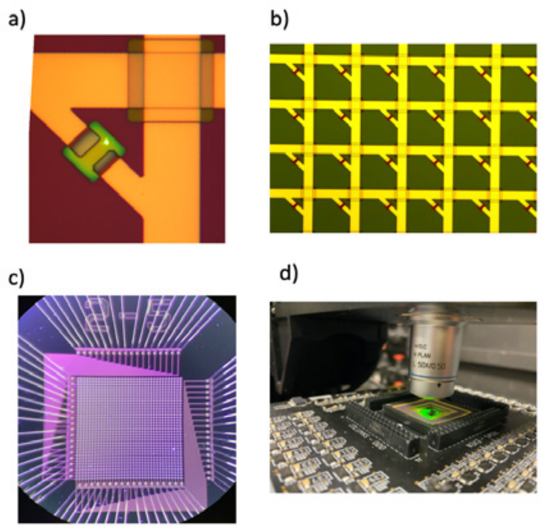
Expanding performance limits using ultrafast electron microscopy. Thermal imaging is used extensively in national security missions, so it is essential to identify the performance-limiting mechanisms in mid- to far infrared sensors. This LDRD probed photogenerated free carrier dynamics in model detector materials using scanning ultrafast electron microscopy (SUEM) to identify the mechanisms. SUEM combines ultrafast electron pulses with optical excitations in a pump-probe configuration to measure charge dynamics in semiconductors with high spatial and temporal resolution and without the need for microfabrication. A SUEM tool was constructed (one of only two in the world) and used to examine several semiconductor systems relevant to detectors. A new contrast mechanism potentially useful for next-generation chip fabrication was discovered, which will enable ultrafast probing of defects and contaminants at deeply buried oxide/semiconductor interfaces. (PI: A. Alec Talin)

Moving toward modernized strategic radiation-hardened microelectronics technology. Enabling Sandia to field a sub-100-nm strategically radiation hardened (SRH) CMOS technology would vastly improve the effectiveness of critical national security mission systems, including those relevant to nuclear deterrence and non-proliferation. With that goal in mind, the research team created a novel metal oxide semiconductor (MOS) capacitor architecture, demonstrated a functional n-MOS field-effect transistor with a metal gate process, developed techniques to probe electrically active interface traps, and designed a simulation methodology for resistor-capacitor hardening of devices and circuits. By identifying scientific solutions for engineering problems, researchers successfully highlighted a new path for SRH technology that can improve speed and computing power without sacrificing Sandia's integrated circuits' world-class performance in harsh environments. (PI: Mike King)

Sandia launched a suborbital rocket from NASA's launch range at Wallops Flight Facility in Virginia. (Photo by Lee Wingfield, NASA Wallops Flight Facility)

Optical and electronic control of titanium suboxide memory devices for strategically radiation-hardened environments.

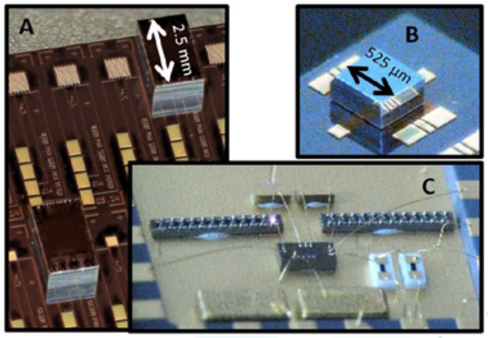
Many mission applications operate in extreme environments that subject computing components to challenges such as radiation-induced noise and power collapse. This team investigated emerging non-volatile memory and communication architectures with radiation hardness. Titanium oxides provide insulating, semiconducting, and metallic phases relevant to memory devices, and recent discoveries of reversible photo-induced phase transitions could make these attractive candidates for all-optical computational architectures. Memory arrays, fabricated at Sandia's MESA semiconductor facility, were found to be robust to 500 kRad(Si) in total ionizing dose experiments. Further experimentation is needed to uncover the physical mechanisms underpinning the observed optically induced phase transitions. (PI: Elliot Fuller)



Device arrays (a) titanium suboxide resistive junction in a crossbar array, (b) small section of the crossbar with visible row and column leads, (c) crossbar chip wire bonded into a chip carrier, and (d) chip carrier integrated into a printed circuit board used for measuring the resistance of single junctions or for electrical programming of single junctions. The 50X microscope objective focusing green laser light seen at the junction in (d) is also depicted in (a).

Heterogeneous integration enables miniaturizing and increased performance in next generation systems.

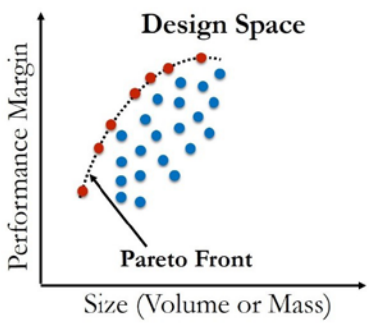
Sandia's vision for heterogeneous integration (HI) is to facilitate future microsystems comprised of disparate technologies with different materials, devices, and suppliers. To that end, LDRD researchers explored the integration of silicon-based electronics with compound semiconductor photonics in future optoelectronic microsystems by leveraging externally-sourced state-of-the-art silicon electronics, Sandia's radiation-hardened silicon electronic technologies, and Sandia's custom photonic technologies. To support short interconnects and accommodate differences in materials and processes, the project explored a scalable integration path in which different technologies were fabricated and then integrated as individual die. This approach provides the potential for trusted, robust, high-performance microsystems combining complex electronic functions with optoelectronics having rich bandgap engineering. These developments will lead to miniaturizing and increasing the performance of future communication, radar, and data processing functions in next-generation systems. (PI: Chris Nordquist)



(A) Two 2.5 × 1.5 mm² chiplets assembled into a silicon interposer using flip-chip gold thermocompression bonding with bump pitches of 25 µm and 55 µm. (B) A 525 x 435 µm² foundry-fabricated silicon RF integrated circuit amplifier flip-chipped onto a silicon interposer with bump pitch of 100 µm. (C) A wire-bonded assembly consisting of silicon electronics and compound semiconductor lasers and photodiodes for electrical-optical conversion.

Bridging modern power concepts into weapons systems.

To enhance the nation's ability to iterate and optimize systems used in select space and defense applications, this LDRD team investigated the use of optimization tools in the design of power conversion and distribution architectures. Researchers studied the deployment of power conversion components and circuits for specific use cases, subject to constraints on volume, weight, and extreme environment specifications. By computing the benefits of select power architectures, and evaluating these in trade-spaces, these approaches will help teams identify the best design for a given application or set of applications and quantify the performance limits based on existing or forthcoming technologies.

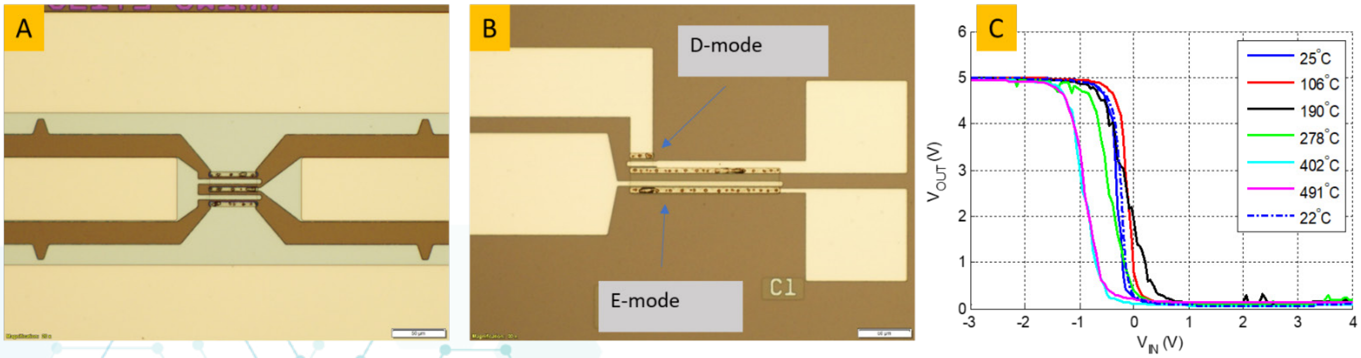


Optimizations can also be applied across several mission scenarios to identify power architectures that offer the best mission agility. This optimization work utilized and extended the capabilities of the Sandia-developed Whole System Trades Analysis Tool. Beginning in FY22, this tool with extended capabilities will be adapted for use in designing power distribution systems for a high-consequence military application. (PI: Jason Neely)

The Pareto Optimal Front includes the set of non-dominated designs in a design space; the Performance Metrics for Power Architectures may include Size, Electrical Performance, Cost, Environmental Resilience, and Upgradeability.

Digital logic gates for extreme environment applications.

Ultra-wide bandgap (UWBG) aluminum-rich gallium nitride (AlGaN) transistors and high electron mobility transistor (HEMT) logic gates may be candidates for use in extreme environments, particularly ones with high temperatures (up to 500°C) and radiation. Because of the UWBG of AlGaN, these semiconductors offer potential immunity to environmentally harsh conditions where conventional semiconductors cannot operate, including automotive, aerospace, military, petroleum, and geothermal well applications. The key results were a demonstration of AlGaN inverters operating from room temperature to approximately 500°C and GaN SRAM operating from room temperature to 300°C. Academic partner, Georgia Tech, developed a Finite Element Method (FEM) model which compared different thermal management solutions specific to AlGaN HEMTs, and those findings are already contributing to new designs for other AlGaN projects at Sandia. For applications where environmental shielding is unavailable, ultra-wide bandgap AlGaN's superior electrical performance at elevated temperatures and high intrinsic material radiation tolerance can be exploited to insert digital logic directly into extreme environments. This project's work has laid a foundation to support more advanced high-temperature circuitry maturation in the future. (PI: Brianna Klein)



(A) AlGaN high electron mobility transistor, (B) inverter with combined enhancement- and depletion-mode transistors, and (C) inverter electrical performance over temperature with devices tested from 25°C to 491°C.

Impacting future nuclear deterrence products through new unique discriminators.

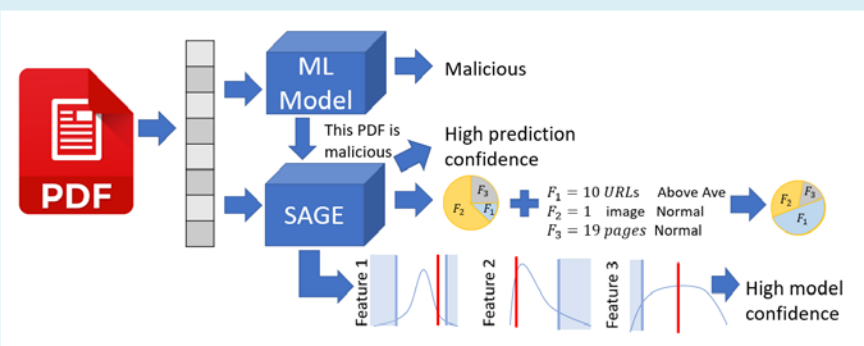
A new unique signal (UQS) discriminator could replace the current all-mechanical discriminator and increase the ease of integration and reduce time-to-field for nuclear deterrence surety systems. This LDRD project team's near-term goal was to define requirements and explore technology, design, and architecture options (proof-of-concept prototypes) for a new discriminator that would maintain or improve surety (safety, security, reliability). Building on those successes, the expected outcome of this ongoing project is a prototype UQS discriminator design with the enhanced agility to have significant national security impact by lowering system lifetime costs and reducing time-to-field for new systems. (PI: Paul Galambos)

Extending the capability of machine learning for use in radioisotope identification of gamma spectra.

Successful machine-learning (ML)-based radioisotope identification (RIID) will significantly impact the nation's ability to perform real-time, autonomous RIID on deployed detectors and provide additional capabilities to analysts. In pursuit of this goal, researchers created a Python-based software package (PyRIID) that enables users to rapidly create a radioisotope-targeting ML model based on signatures observed with their detector(s) and then use that model to perform RIID in real-time. Note that the most efficient way to build models requires a well-crafted detector response function, for which GADRAS (Gamma Detector Response and Analysis Software) is recommended. With this base technology established, the next step is to continue building trust through demonstrations of ML-based RIID effectiveness in multiple global security applications. (PI: Tyler Morrow)

Sensitivity analysis-guided explainability for machine learning.

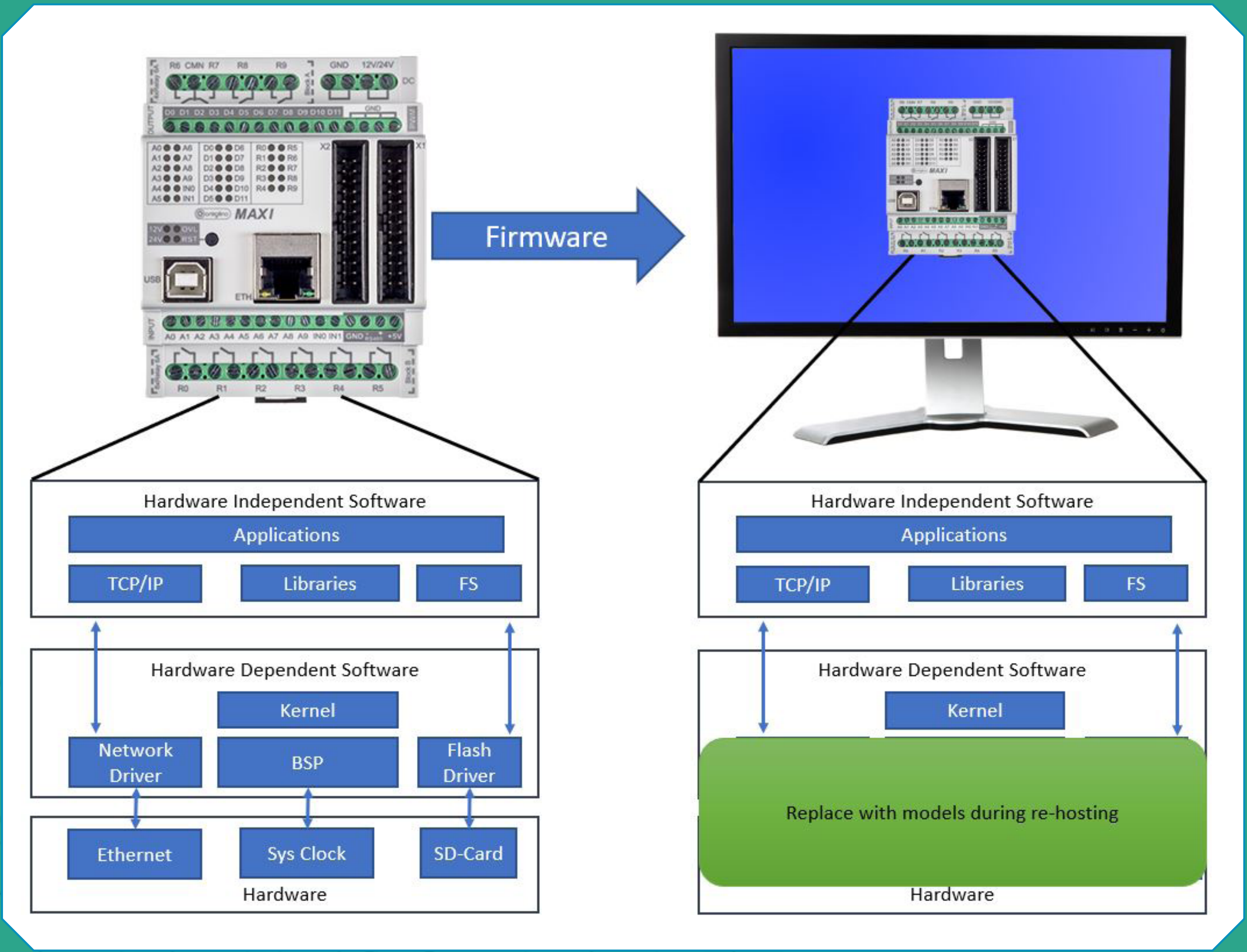
Despite the potential of machine learning (ML) models to address the efficient analysis of increasing amounts of data, ML algorithms are not fully leveraged in many high consequence national security domains because their output cannot be sufficiently validated and trusted. This research investigated the quality and impact of explanations for ML models using sensitivity analysis and user studies, and exposed significant gaps in explainable ML that should be examined further. Using sensitivity analysis methods to quantitatively assess the quality of explanations revealed that most state-of-the-art explainable ML methods explain the ML model with low fidelity. The low fidelity explanations are due to simplifying assumptions (e.g., independent features and linear approximations) made by explainable ML methods. The analyses from this LDRD provides a foundation for trusting conditions explanations. It also explains how to identify and address gaps, and significantly improve both the fidelity of explanations and the usage of the model outputs in deployed settings. This research also highlighted the need for more disciplines to be represented in the teams supporting the effort, including computer science, human cognition, mathematics, and domain experts where the ML model will be deployed. (PI: Michael Smith)



SAGE: Sensitivity Analysis Guided Explainability (SAGE). Idealized information for validating the output of an ML model capturing model uncertainty, prediction uncertainty, and explaining the decision process.

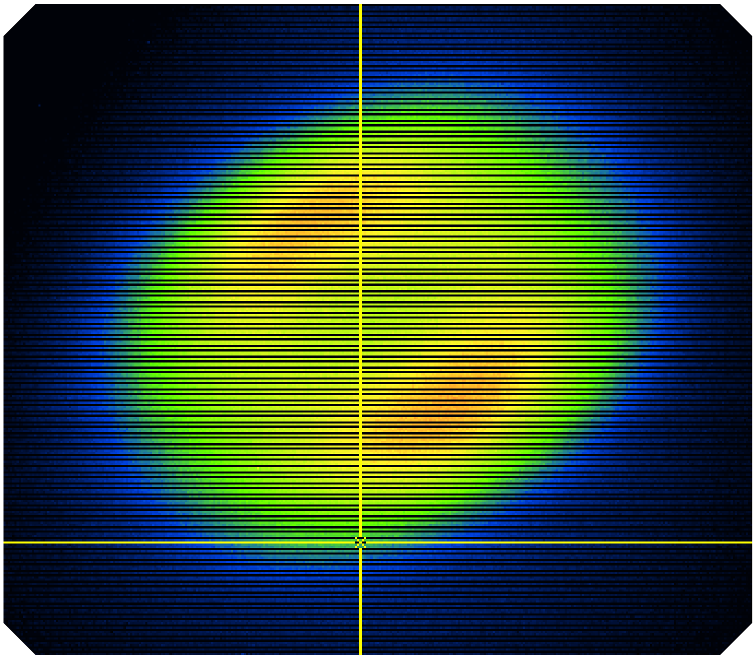
Scalable firmware re-hosting.

Embedded systems that execute low-level software (i.e., firmware) control our vehicles, airplanes, traffic signals, critical components in the power grid, and many other systems including the Internet of Things. Because these systems are increasingly targeted by cyber-attackers, the U.S. needs to be able to assess for vulnerabilities and understand their impact within the system context. Modeling systems at the high fidelity needed to understand cyber vulnerabilities and system-level consequences is challenging. Re-hosting firmware in a safe environment is complicated by the tight coupling of firmware with its hardware and requires custom emulators built for each system, a process that can take up to a year for each device. This LDRD project leveraged a technique called high-level emulation whereby low-level common application programming interface (API) functions responsible for hardware interaction are replaced during emulation with models. Any firmware using those APIs can be rapidly re-hosted and the modeled API can be reused for many devices. As a proof of concept, the research team implemented support for key functionality of the VxWorks Real Time Operating Systems, which is commonly used in critical infrastructure. The time to re-hosting the first device with serial and filesystem support was reduced from 12–18 months to only six weeks for the last device. Using this scalable way to employ firmware re-hosting, teams will be able to understand the impacts of vulnerabilities in embedded systems on the larger systems they comprise. (PI: Abraham Clements)



By employing high-level emulation in scalable firmware rehosting, significant development time is saved across embedded systems.

Polymers in extreme environments examined with novel experimental and computational tools.

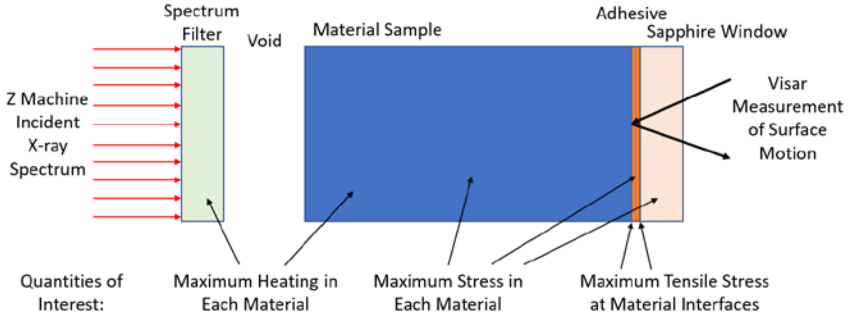


Intensity map of fluorescence from a polyethylene specimen while its surface is bombarded with electrons (region is several millimeters across).

Polymer surfaces and interfaces, common in myriad engineered systems as insulators and protective coatings, must survive extreme environments. Researchers constructed a test chamber at Sandia's Ion Beam Laboratory to bombard polymers with controlled doses of electron beam irradiation, allowing ionization and thermal effects to be studied independently, and changes in composition to be observed. Using polyethylene as a test case, the team developed computer models to account for rapid transformations arising from charge accumulation associated with X-ray or electron backscattering, photoionization, chemical decomposition, thermomechanical shock, temperature-dependent spall fracture, and phase change. These expanded capabilities for evaluating material survivability will allow a broader use of polymers and other complex materials in engineered systems. (PI: Nathan Moore)

Rapid physics-informed survivability assessments.

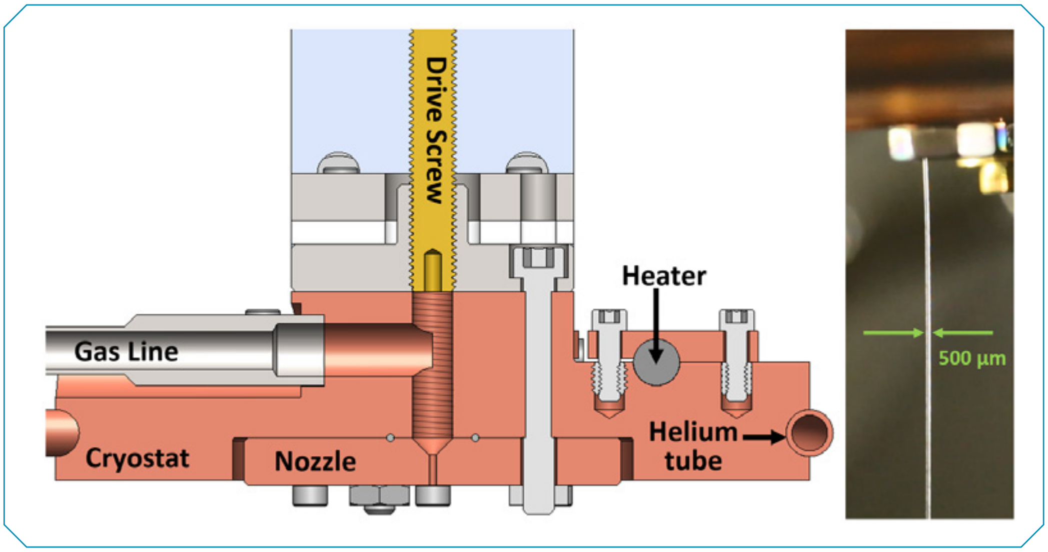
Producing methods that simplify, automate, and streamline the tasks associated with survivability assessments to facilitate agile concept exploration is an important part of mission work. This LDRD project leveraged Sandia's production codes to ensure long-term support for the underlying capabilities. The work included modeling an experiment in which a material sample is exposed to radiation at a facility such as the Z machine or the National Ignition Facility, specifically focusing on the thermal and thermo-mechanical responses of the sample. The team also evaluated the radiation environments where materials used in electrical devices subject to radiation should be tested. This method of modeling allows for assessment of detailed mechanical responses, such as velocity, stress, and strain, as well as metrics for understanding radiation response of electrical devices, such as dose, dose rate, and damage. A user interface simplifies the evaluation by providing a constrained set of options for using the underlying physics codes. Workflows automate the evaluation by coordinating input setup, executing code, transferring data transfer between codes, and processing results. Documented exemplars demonstrate the general applicability of the tools for survivability assessments. (PI: Brian Franke)



An exemplar survivability problem in which a spectrum filter and material sample are exposed to radiation at a test facility. Analysts may wish to rapidly assess the effects of variability in the spectrum, materials, and layer thicknesses.


PUSH PULL CONFIGURATION
MB MODEL C-210 EXCITERS
TWO SHAKER INPUT

New cryogenic fuel configurations for magnetically driven inertial confinement fusion targets.
There is near-term need within the Inertial Confinement Fusion (ICF) program at Sandia's Z machine for advanced cryogenic fuel configurations. This LDRD project provided three new cryogenic fuel configurations for novel ICF target concepts: (1) Deuterium ice fibers with diameters ranging from 200 to 500 µm were extruded to lengths (> 1 foot) and lifetimes (> 10 min), which exceed the needs of Z experiments. Next, thin ice layers (2) and thick ice layers (3) were grown via desublimation, where a slow flow of deuterium gas enters the target and freezes to the walls without entering the liquid phase. The team first demonstrated 10-100 µm layers of deuterium ice for metallic-wall mix mitigation. Next, millimeter(s) thick cylindrical ice shells were grown on the inner wall of cylindrical liners for future high-gain applications. The desublimation-based fills have now been used successfully on Z-ICF experiments, and a near term goal is to grow ice layers which include uniformly mixed spectroscopic dopants (e.g., krypton). The first experiments on Z to use the deuterium ice extruder technology are planned for April 2022. If a next generation petawatt-class pulsed power facility (e.g., 60-MA, 100-ns) capable of nearly double the current of Z becomes available, these and other more complex fuel geometries could be used. (PI: Thomas Awe)

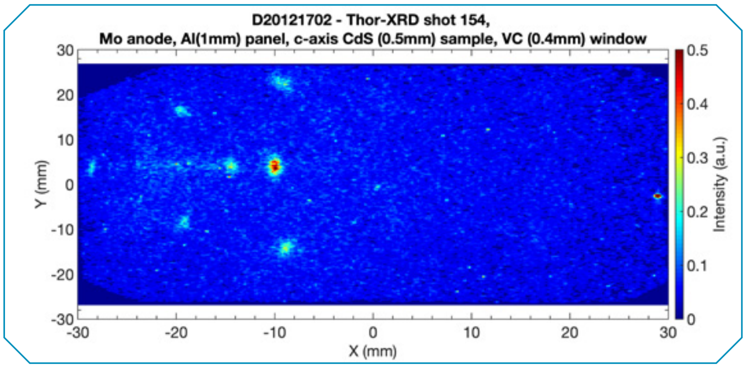


(Left) Cross-sectioned CAD rendering of a screw-driven extruder assembly. The extruder is filled via desublimation. When the extruder cavity is filled with ice, the screw is driven downward, closing off the gas-fill line. With the ice cavity isolated, further screw rotation compresses the deuterium ice through a nozzle, extruding a fiber. (Right) Image of a ~500 µm diameter ice fiber. A full description of the extruder design, operation, and performance is available.

Data-driven, radiation-aware, agile modeling approach for rapid nuclear deterrence design assessment.
This LDRD project pioneered a range of data-driven and machine learning (ML) approaches for the accelerated and automated development of fast, accurate, and predictive data-driven compact device models for normal and radiation environments, with Sandia's academic experts in ML at University of Illinois Urbana-Champaign contributing. The impacts and contributions of this pathfinder effort are manifold. First, the project established the viability of data-driven compact models for both normal and radiation environments. Second, it demonstrated that data-driven approaches can reduce development times from months to days or even hours, and in some cases can enable a fully automatic model development from data. Last, in collaboration with an ASC advanced ML project, this LDRD provided a first-of-its kind demonstration of the data-driven models and "data-to-simulation" pipeline in Sandia's production circuit simulator Xyce. These efforts paved the way for early adoption of research results by the NA-11's Aging and Lifetimes Program to develop an automated tool for nuclear deterrence core surveillance. (PI: B. Paskaleva)

X-ray diffraction for probing phase transition behavior at extreme high pressures.

Sandia's nuclear mission requires understanding the response of materials to high-pressure, including the complexities of pressure-induced solid phase transitions and important transient kinetic effects. This project developed a powerful new in-situ X-ray diffraction (XRD) diagnostic capability to capture and characterize the extreme compression states found during dynamic compression on Sandia's current (and future) pulsed-power platforms. Partners at the University of New Mexico and the Advanced Photon Source (APS) at Argonne National Laboratory aided in synthesis of well-characterized nanostructured materials and state-of-the-art static high-pressure diamond-anvil compression experiments.
(PI: J. Matthew Lane)

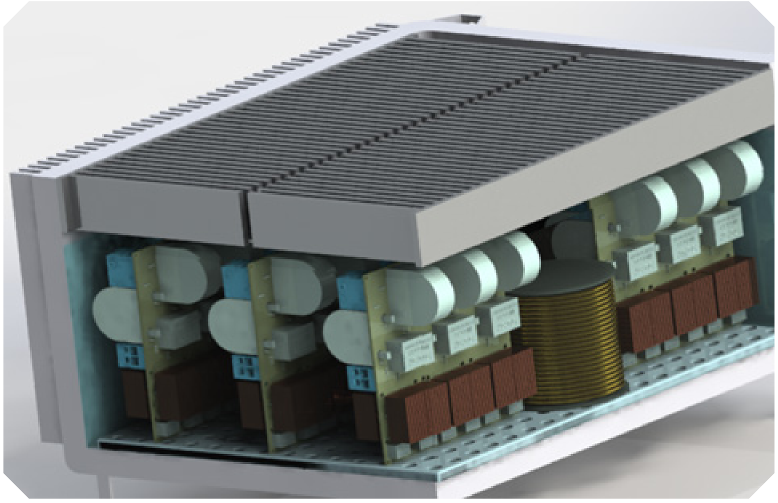


Initial ambient Wurtzite phase and dynamically compressed rock salt phase X-ray diffraction patterns from pressure-induced phase transition experiments on Thor.

Preventing widespread blackouts through Solid-State Transformer (SST) technology.

The current power system depends on thousands of generators working in unison to meet the nation's ever-increasing power demands. SSTs have been hypothesized as having the potential to prevent and/or reduce the cascading failures caused by the synchronization requirements of large AC electrical grids. Funded through the Resilient Energy Systems LDRD Mission Campaign, this research team developed the first commercially viable circuit architecture for AC–AC SSTs, Sandia's patent-pending "Low-Modulation-Index 3-phase Solid State Transformer" (LMI3-SST) technology. Extensive testing on the new technology demonstrates it to be a viable solution for making the electrical grid more resilient to power outages. Sandia filed a provisional patent for the LMI3-SST, and the technology, as reviewed by an independent analysis, already shows it to be competitive in some transformer applications.
(PI: Karina Munoz-Ramos)

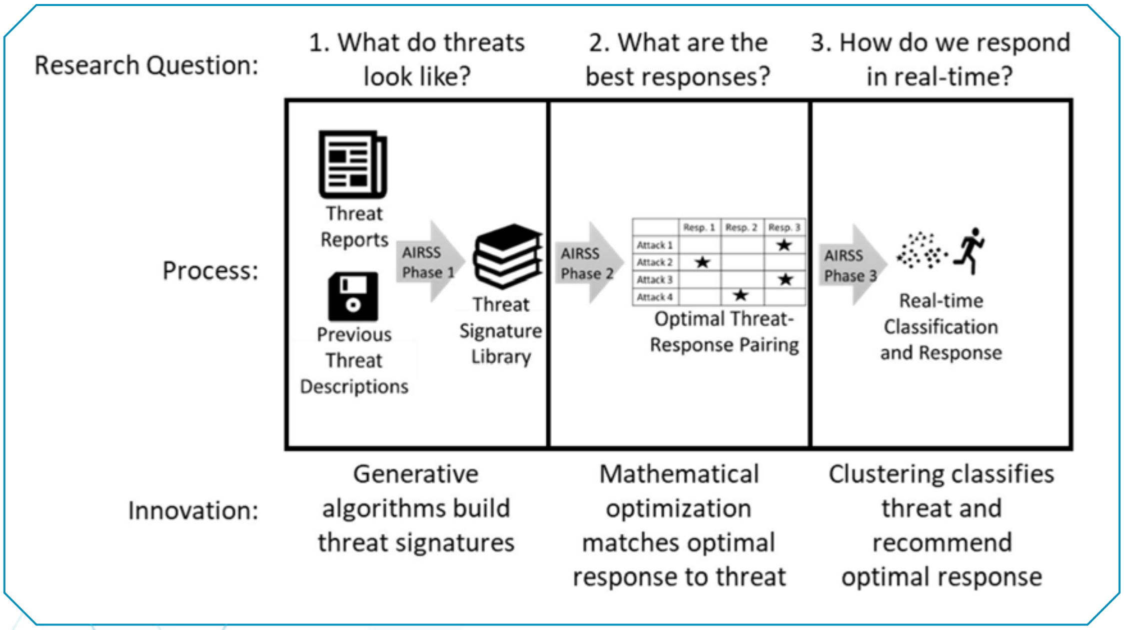
Sandia's LMI3-SST can make the electrical grid more resilient to power outages.



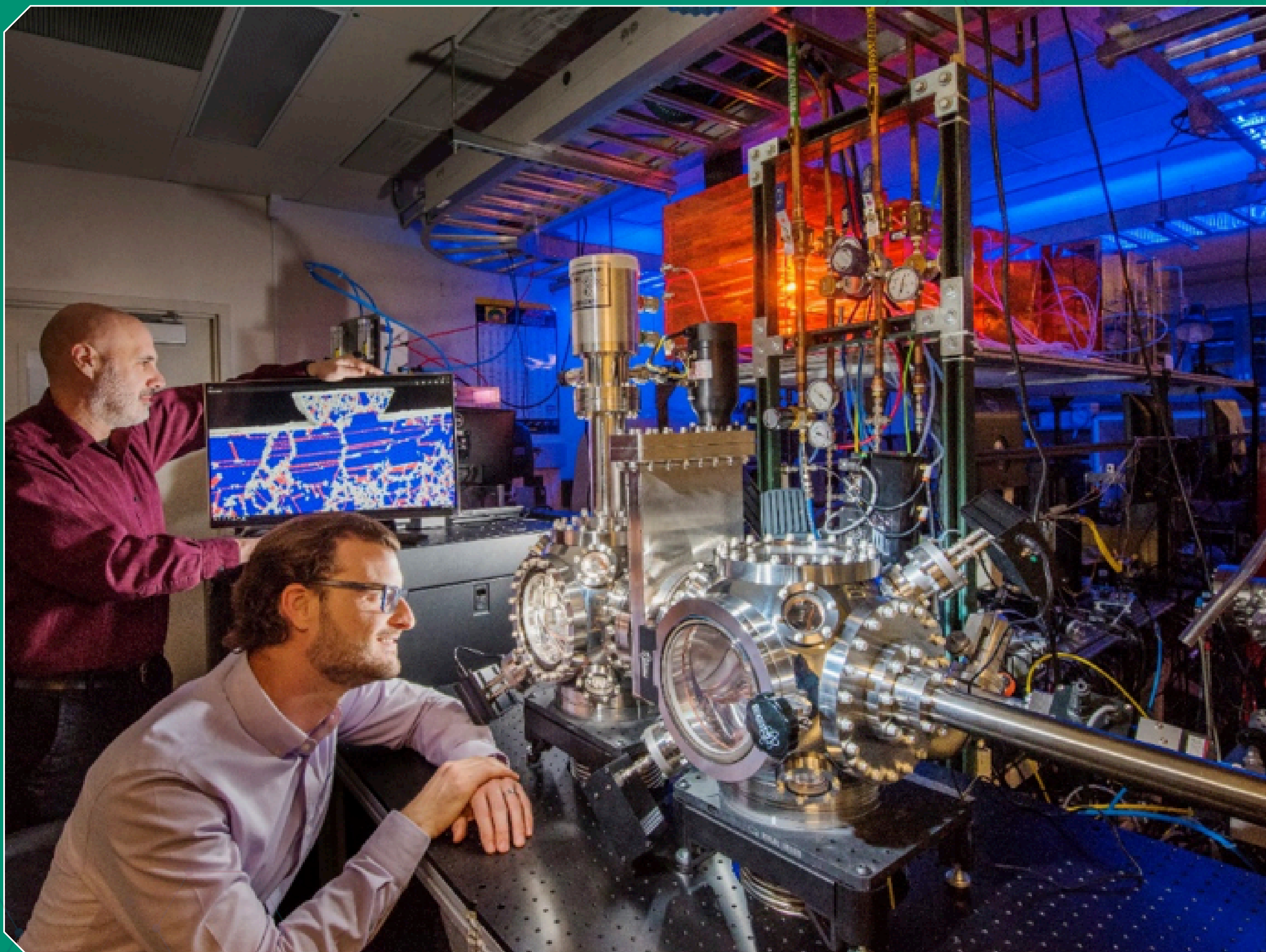
Advanced techniques for optimal power system emergency control.
A major disturbance to the electric power grid can lead to a severe power outage, leaving residential, business, or industry customers without power for extended periods of time. An outage can be exacerbated through cascading power outages caused by protective grid devices tripping power connections automatically to try maintaining dynamic stability. This effort, part of the Resilient Energy Systems LDRD Mission Campaign, focused on investigation and application of direct shooting methods for optimal control of power systems after a disturbance. Features of this framework include the options of constant, piecewise linear, and piecewise cubic basis functions, as well as a direct single-shot method using adaptive time for control action updates. Researchers used the Matlab-based nonlinear programming solver *fmincon* for optimization and used *ode15s* for numerical solutions of the stiff differential and algebraic equations. The outcome of this project will inform resilient energy systems. (PI: Bryan Arguello)

Moving target defense for space systems.
Space Policy Directive-5 Cybersecurity Principles for Space Systems describes both the cyber threat to space systems and the need for these systems to be secure and resilient against cyberattacks. Nation-state adversaries can disrupt critical infrastructure through cyberattacks targeting systems of networked, embedded computers. This project, funded by the Science and Technology Advancing Resilience for Contested Space (STARCS) LDRD Mission Campaign, developed a patented moving target defense (MTD) algorithm that adds cyber resilience to space systems by improving their ability to withstand cyberattacks. MTDs create dynamic, uncertain environments that seek to confuse the attacker and attempt to defeat cyber threats. Most proposed cyber resilience solutions focus on or require detection of threats before mitigations can be implemented, a significant technical challenge. The new MTD approach avoids this requirement while creating informational asymmetry that favors defenders over attackers. Researchers conducted three key experiments: i.e., functional, cyber resilience, and machine learning (ML), which helped quantify the benefit of the LDRD team’s approach to cyber resilience against different types of cyberattacks. Results show a 97% reduction in adversarial knowledge on a MIL-STD-1553 network. A collaboration with Purdue University using ML to defeat the MTD algorithm highlighted the strength of the algorithm by showing a small change in one of the algorithm parameters substantially decreased the success rate of the LSTM machine learning model. Further, the generalizable algorithm led to Sandia working with a small business that plans to use this technology to mitigate ransomware and disseminate MTD technology for the U.S. government. (PI: Chris Jenkins)

Adaptive intrusion response for space systems (AIRSS).
The U.S. government critically depends on space systems for government and commercial applications. As technological and financial barriers to space are decreasing, access to space is becoming more achievable, which only increases threats to the nation's space systems. As cyber threats evolve, the space community recognizes it is impossible to prevent all cyber-attacks, so cyber security measures need to be complemented with resilience technologies to overcome a spectrum of cyber-physical threats and ensure the survival of mission critical assets. The AIRSS LDRD, part of the STARCS Mission Campaign, focused on developing a set of algorithms that can, in real-time, classify cyber-attacks on space systems and identify optimal mitigation responses for defeating the threats. The research leveraged generative algorithms, clustering, and mathematical optimization to create a tool set that provides space system operators with increased situational awareness and strategies for more rapid and effective responses against cyber threats. The AIRSS toolset will integrate with other capabilities (such as advanced anomaly detection tools) to create a holistic platform for both detection and response to cyber threats. Ultimately, this research will not only will enable resilient space systems to execute their missions despite the presence of an attacker, but also extend easily to other types of cyber-physical systems. (PI: Meghan Sahakian)



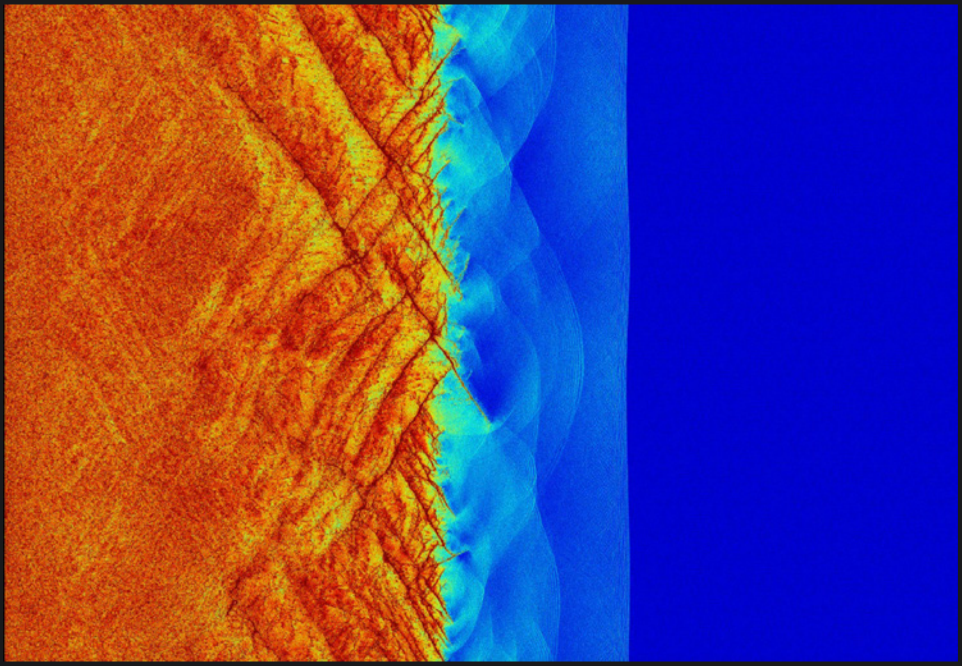
AIRSS enabling capabilities.



Sandia researchers Michael Chandross, left, and Nic Argibay show a computer simulation used to predict the unprecedented wear resistance of their platinum-gold alloy, and an environmental tribometer used to demonstrate it. (Photo by Randy Montoya)

LDRD IMPACT STORY:

Powerful Sandia machine-learning model with hardware and software improvements shortens 'run time' from year to a day



This multi-billion atom simulation of shockwave propagation into initially uncompressed diamond (blue) uses a high-accuracy SNAP model from Sandia to predict that the final state (orange) is formed by recrystallization of amorphous cracks (red) that take shape in the light blue, green and yellow compressed material. (Image with colors added)

SNAP, a supercomputer simulation model, first hit the scene in 2012 with funding from Sandia's LDRD program. But since then, what started as a proposal by researcher Aidan Thompson has grown into something supported continuously since 2017 by the DOE Exascale Computing Project, a collaborative effort of the DOE Office of Science and the NNSA.

What makes SNAP (Spectral Neighbor Analysis Potential) so valuable? SNAP rapidly predicts the behavior of billions of interacting atoms, and it has captured the melting of diamond when compressed by extreme pressures and temperatures. At several million atmospheres, the rigid carbon lattice of the hardest known substance on Earth is shown in SNAP simulations to crack, melt into amorphous carbon and then recrystallize.

The work could aid understanding of the internal structure of carbon-based exoplanets and have important implications for nuclear fusion efforts that employ capsules made of polycrystalline diamond.

A technical paper describing the simulation was selected as a finalist for the Gordon Bell prize, sponsored annually by the Association of Computing Machinery. The diamond-specific modeling, which took only a day on the Summit supercomputer (the fastest in the U.S.) at Oak Ridge National Laboratory, relied on SNAP, one of the leading machine-learning descriptions of interatomic interactions, to model and solve a very important problem, said Thompson.

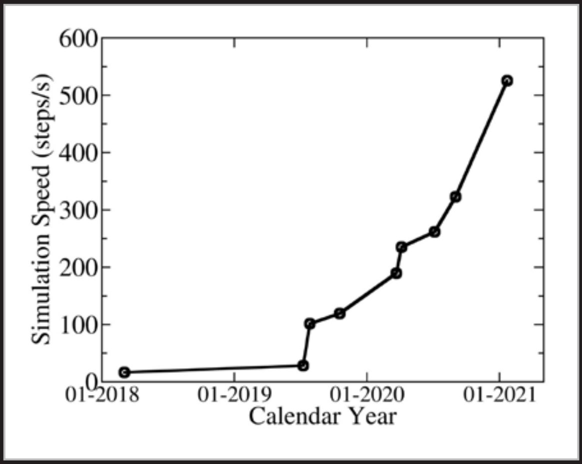
Designing novel materials and implications for giant planets

"We can now study the response of many materials under the same extreme pressures," said Thompson. "Applications include planetary science questions—for example, what kind of impact stress would have led to the formation of our moon. It also opens the door to design and manufacture of novel materials at extreme conditions. "The effect of extreme pressures and temperatures on materials also is important for devising interior models of giant planets. Powerful DOE facilities like Sandia's Z machine and Lawrence Livermore National Laboratory's National Ignition Facility can recreate near-identical conditions of these worlds in earthly experiments that offer close-up examinations of radically compressed materials. But even these uniquely powerful machines cannot pinpoint key microscopic mechanisms of change under these extreme conditions, due to limitations in diagnostics at the level of atoms. "Only computer simulations can do that," said Thompson.

An artist's conception of the magnetic fields of selected super-Earths as the Z machine, pictured at bottom, mimics the gravitational conditions on other planets. Planetary magnetic fields deter cosmic rays from destroying planetary atmospheres, making life more likely to survive. (Artist image by Eric Lundin; Z photo by Randy Montoya)

Machine-learning bridged with quantum mechanical calculations

SNAP used machine-learning and other data science techniques to train a surrogate model that faithfully reproduced the correct atomic forces. These were calculated using high-accuracy quantum mechanical calculations, which are only possible for systems containing a few hundred atoms. The surrogate model was then scaled up to predict forces and accelerations for systems containing billions of atoms. All local atomic structures that emerged in the large-scale simulations were well-represented in the small-scale training data, a necessary condition for accuracy.

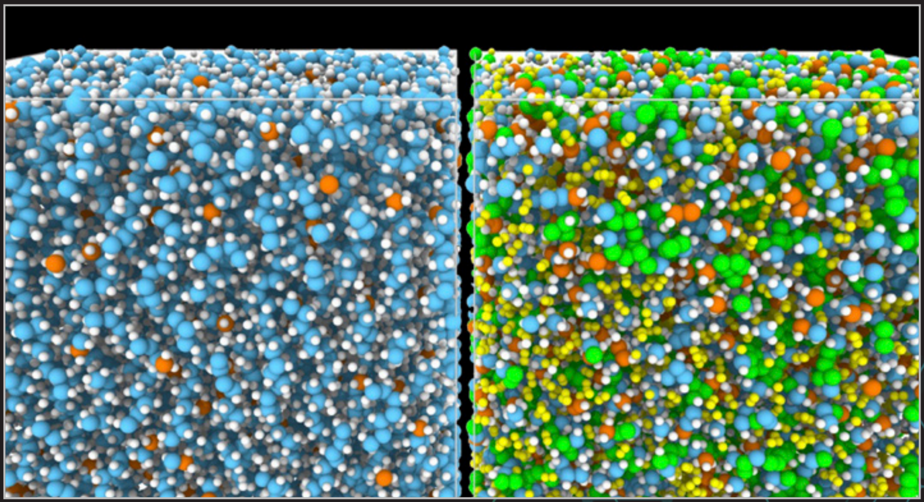


Another critical part of the final result was performance optimization of the software to run efficiently on GPU-based supercomputers like Summit, said Thompson. "Since 2018, just by improving the software, we have been able to make the SNAP code over 30 times faster, shortening the time for these kinds of simulations by 97%. At the same time, each generation of hardware is more powerful than the last. As a result, calculations that might have until recently taken an entire year can now be run in a day on Summit."

The graph demonstrates the dramatic improvement in computational speed achieved by Sandia National Laboratories' SNAP model from 2018 to 2021.

Run time shortened by 97 percent

"Since supercomputer time is expensive and highly competitive," said Thompson, "each shortening of SNAP's run time saves money and increases the usefulness of the model." Sandia researchers Stan Moore and Mitchell Wood made important contributions to the SNAP model and the dramatic performance improvements. The optimized software for running SNAP on supercomputers is available in the open source distribution of Sandia's LAMMPS molecular dynamics code. The Sandia FitSNAP software for building new SNAP models is also publicly available.



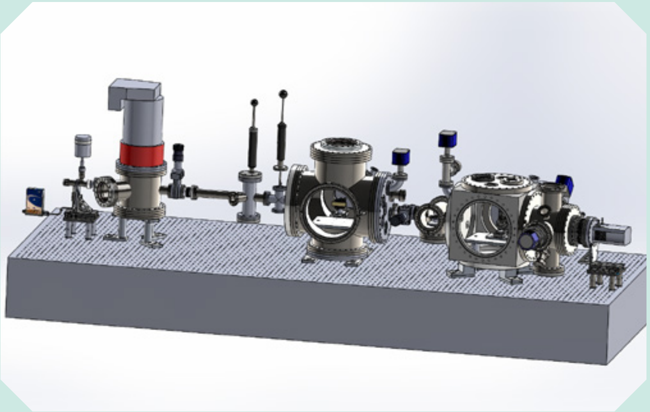
This work by Matt Lane and Nathan Moore (Sandia), aims to understand the high-rate thermal decomposition of organics by simulation of conditions comparable to recent Z machine X-ray ablation experiments.

(Generated using LAMMPS in 2018)

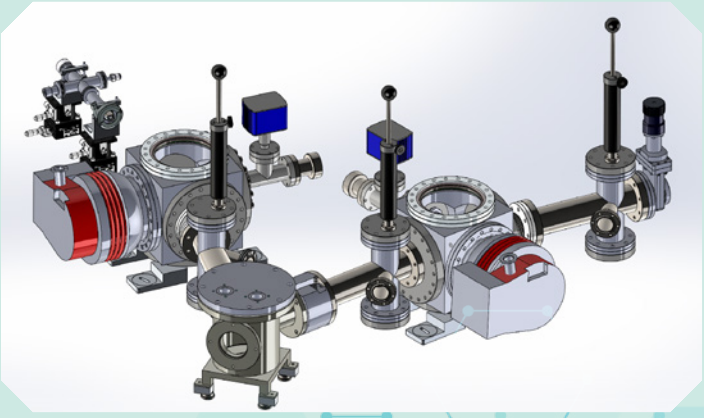
Project Highlights – Technical Vitality

LDRD is essential to maintaining the Labs' scientific vitality and Sandia, as the nation's most diverse national security laboratory, is uniquely equipped to tackle groundbreaking, interdisciplinary research. Researchers collaborate across a broad spectrum of disciplines and achieve research breakthroughs, which enables national security technology to be transferred to industry, commercialized under licensing agreements, and brought to market for the U.S. public good. The LDRD accomplishments in the technical vitality section highlight research outcomes that significantly extend knowledge in the scientific field or have the potential to provide a new capability for Sandia in the future.

Table-top XUV/VUV radiation instruments will enable study of fast chemical transformations. Sustainable energy technologies of the future will revolve around transformational new materials and chemical processes that convert energy efficiently among photons, electrons, and chemical bonds. The two new major instruments for generating high-photon energy pulses developed through this LDRD project provide the capability to perform ultrafast core-level spectroscopy, which opens avenues for studying fast chemical transformations that govern processes such as bond dissociation, charge transfer, and carrier dynamics in gas phase, solid state, and interfaces, in an element-specific way. These new extreme ultraviolet (XUV) and vacuum ultraviolet radiation (VUV) techniques and tools will benefit researchers engaging in basic energy sciences and provide the U.S. with the ability to engineer effective catalysts for essential processes such as fuel generation and chemical synthesis. (PI: Krupa Ramasesha)



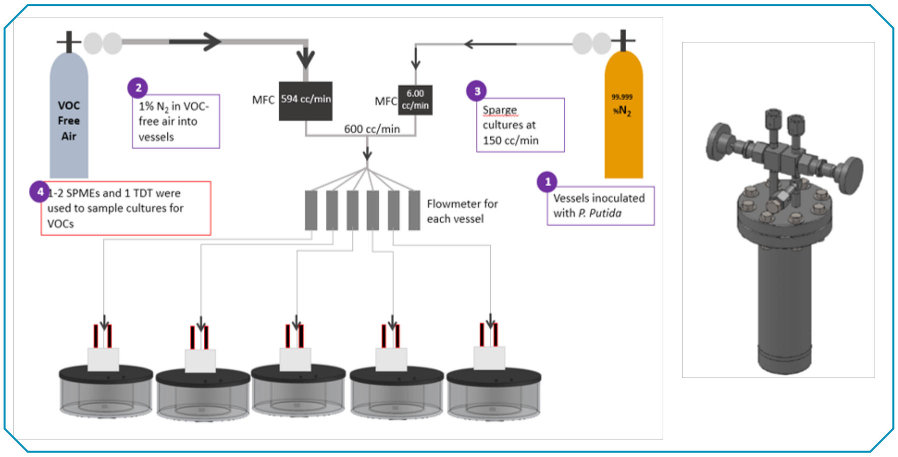
XUV apparatus.



VUV apparatus.

Developing engineered bioremediation technologies for breaking down waste.

By applying gene editing tools and metabolically engineering microorganisms, LDRD researchers determined the key enzymological parameters needed to influence the kinematic activity of polymeric degradation via enzymatic activity for bioremediation. The team leveraged material characterization methods derived from dielectric permittivity changes within polymers to understand the material structure and composition changes necessary for developing engineered bioremediation technologies. The team created innovative capabilities (a) to characterize changes in complex permittivity and (b) provide materials information regarding changes in material composition and structure, such as degree of cross-linking, the amount of solvent uptake, and changes in porosity among others. Ultimately, the research characterized kinetic reaction parameters for biodegradation, yielded understanding of metabolic by-products, and demonstrated the potential system scalability required for plastic waste bioremediation. (PI: Isaac Avina)



Biomaterial testbeds.

First step toward understanding device-aware probabilistic neural networks.

Many critical applications that involve forecasting or predictions based in high uncertainty or complex scenarios could benefit from artificial intelligence (AI) capabilities that leverage probabilistic computing. Unfortunately, research into probabilistic neural networks has proven challenging due to the computationally prohibitive nature of producing large-scale random numbers. This LDRD project investigated how algorithms using probabilities to compute could be modified to take advantage of novel microelectronics devices that produce noise through their physics. Results provided preliminary evidence that probabilistically sampling neural networks with a paradigm consistent with potential noisy devices could lead to achieving uncertainty-aware AI. Researchers observed that sampling neural networks does not significantly impair performance and that uncertainty introduced by sampling appears to match intrinsic uncertainty in data. Furthermore, it appears that these algorithms may tolerate devices whose noisy behavior is of limited precision, an important consideration for translating this approach to emerging hardware technologies. The research supports the team's supposition that co-design between AI algorithms and emerging hardware technologies may yield advanced microelectronics capabilities. (PI: Brad Aimone)

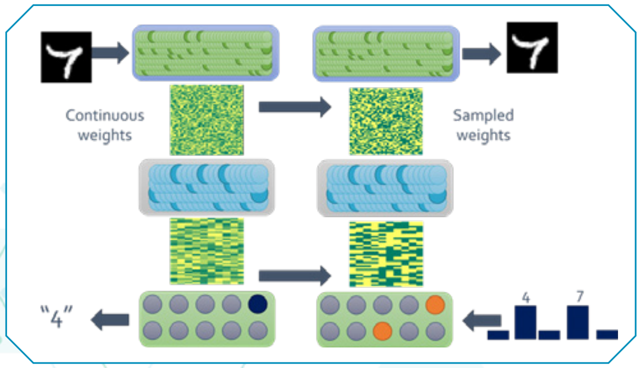
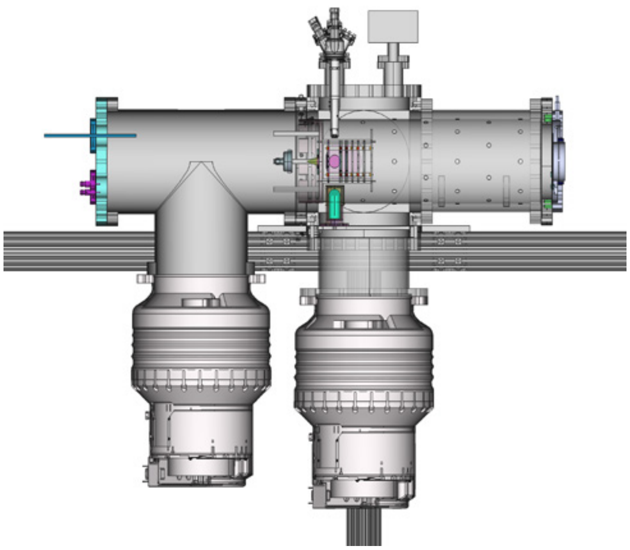


Illustration of how sampling an artificial neural network can allow uncertainty in inputs to be appropriately be recognized by an AI algorithm.

Ultra-high-resolution electron scattering apparatus advances study of electron interactions with gas molecules and temporal evolution of plasmas.

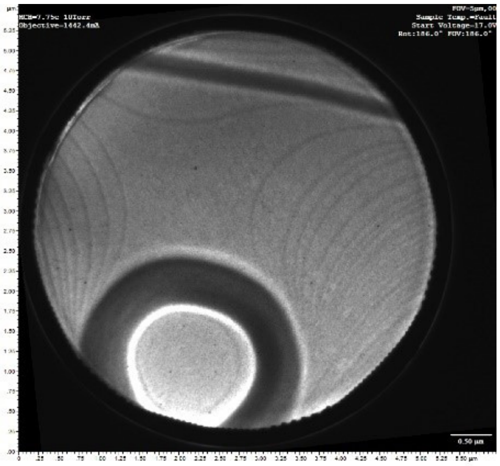
Electron scattering by atoms and molecules, a fundamental process occurring in a broad range of scientific disciplines, is integral to plasma properties. Plasmas impact a diverse field of technical applications critical to national security, and advances in understanding and modeling plasmas enable faster development of associated technology. An ultra-high-resolution electron scattering apparatus, developed by leveraging Sandia's expertise in ion/electron imaging methods, enables the study of electron-scattering processes in gas phase molecules and provides a method for studying the temporal evolution of laser-initiated plasmas. The versatile capability developed through this LDRD project will be used by multiple sponsors in applied and fundamental fields to inform predictions of plasma physics, plasma-assisted chemistry, neutron generation, and arcing. (PI: Jonathan Frank)



Cross-section view of ultra-high-resolution electron scattering apparatus.

Novel capability will enable researchers to tackle ongoing questions of gas-surface chemistry.

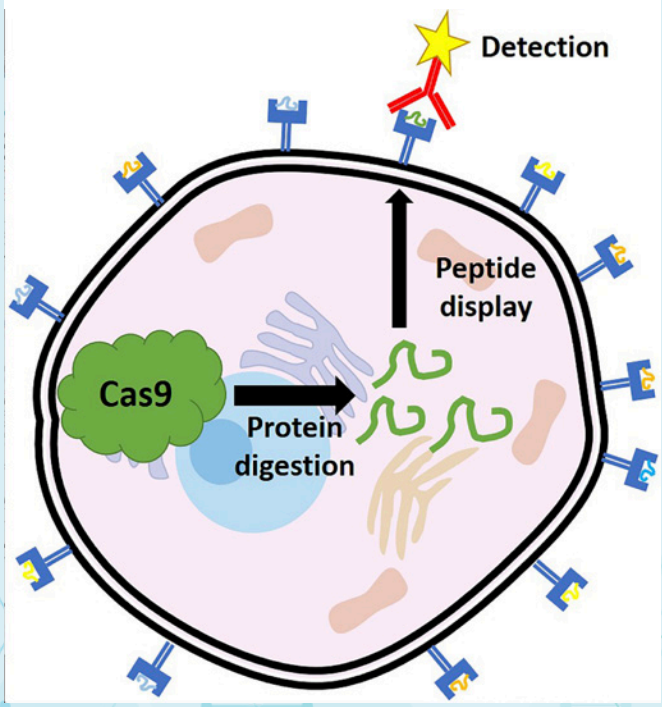
Energy efficient heterogeneous catalytic processes are key to energy applications. This LDRD project focused on developing an experimental method able to image the near-surface gas-phase with high spatial resolution. Combining the benefits of electron microscopy with selective laser ionization of important heterogeneous reaction products emitted from catalytic surfaces, this approach will provide for fundamental mechanistic insight into gas-surface chemical interaction and cooperative pathways. Researchers can use this novel, cross-cutting tool to measure maps of gas-surface exchange as it depends on the local structure and composition of the surface, elucidating the combined effects of surface activity, gas-phase transport, and gas-phase reactivity. This will lead to a more predictive capability in heterogenous catalysis and have a significant impact in basic energy and science fields. (PI: Chris Kliewer)



The development of a method for correlated operando surface/gas characterization provides a great sandbox for surface studies. Shown here is a low-energy electron microscopy image of a clean Iridium (111) surface.

Engineering the future of renewable biofuels/bioproducts through phycoviruses.
Domestic production of next generation renewable biofuels and bioproducts would enhance U.S. energy security. The team discovered that by genetically engineering a new class of viral vectors based on the ubiquitous class of viruses that naturally infect algae, a new system, capable of introducing entire metabolic pathways into algae, could be facilitated. The genetically tractable algal species Tetraselmis striata, known to be easily infected with an isolated virus, is emerging as a potential biotechnology strain and selected as the project's algal/viral model system. A novel DNA virus, TsV-N1, that infects T. striata has been isolated with a much smaller genome (30 kB) than most algal viruses, so the team engineered a specialized transducing virus from the TsV-N1 viral chassis to transfer specific, defined DNA fragments with the virus to the host upon infection. Georgia Tech, one of Sandia's academic partners, was instrumental in identifying a potential chemical compound that can protect algae from deleterious species and prevent pond crashes. These compounds represent several "lead targets" for the engineering of resistance into microalgal production strains through the types of mechanisms that Sandia is developing. Progress made in the first year of this three-year project already represents a significant advance in the ability to rapidly create wholescale genetic changes in microalgae—an important first step toward production of critical renewable biofuels. (PI: Todd Lane)

New antibody capable of detecting genome editors.
CRISPR-based genome editing, most commonly using Cas9, revolutionized biomedical research and is poised to revolutionize medical treatment, with human clinical trials having begun in 2016. Current tools available for detection of Cas9 focus on bulk detection. No current technology can rapidly detect Cas9 expression within individual live cells. This LDRD project harnessed the naturally occurring antigen-presenting properties of mammalian cells to develop tools to detect intracellular Cas9 and resulted in a detailed understanding of how CRISPR is delivered to and used in humans, both experimentally and in silico methods to understand and predict the cellular immune response to Cas9, and the development of the first antibody capable of detecting immune presentation of Cas9 peptides or other genome editors. The tools developed through this project enable (1) rapid prediction and understanding of immune response to foreign proteins and (2) the development of detection reagents for foreign intracellular proteins that apply broadly to understanding and enhancing genome editing and combating intracellular infections. (PI: Kimberly Butler)



Method to detect intracellular Cas9 utilizing the native mammalian cell antigen presentation.

Multiple applications to benefit from distributed-in-time techniques for optimization at extreme scales (DITTO-X).

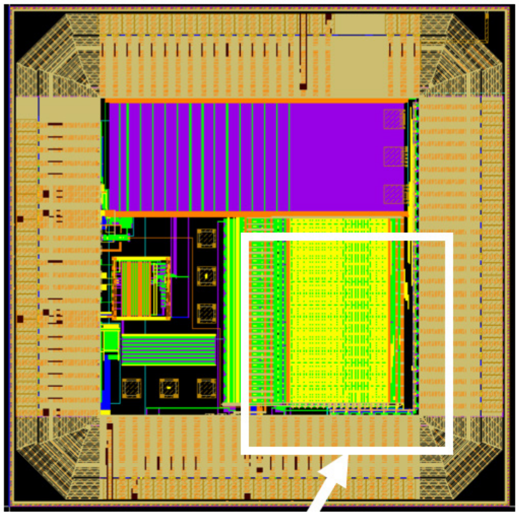
Pioneering *parallelization across the time dimension* as a transformative computational technique for parameter estimation, design optimization and control of engineered systems driven by long-time scale dynamics was at the heart of this LDRD project. The research team developed new optimization algorithms and software geared toward extreme-scale computing, enabling the solution of critical optimization problems in power grid, pulsed power, and reentry applications. Speed-ups of 10x to 360x have been demonstrated. (PI: Denis Ridzal)

Analyzing complex datasets through quantum manifold learning.

Manifold learning, the task of understanding the geometric structure of a dataset, is a critical tool for reducing the dimensionality of large, complex datasets and making interpretation and analysis tractable. This research team developed a new theoretical framework and associated software tools for manifold learning on large datasets using quantum dynamical processes. While developing the algorithm, which exploited the properties of propagating quantum wavepackets, researchers connected the disparate fields of quantum dynamics and data analysis and revealed the intimate relationship between discretization induced by sampling and quantum uncertainty. The convergence and accuracy properties of their algorithm was proven and illustrated on several datasets, including an analysis of adherence to social distancing measures during the COVID-19 pandemic. (PI: Mohan Sarovar)

Increasing computing performance through high-precision sparse and dense analog matrix multiplication.

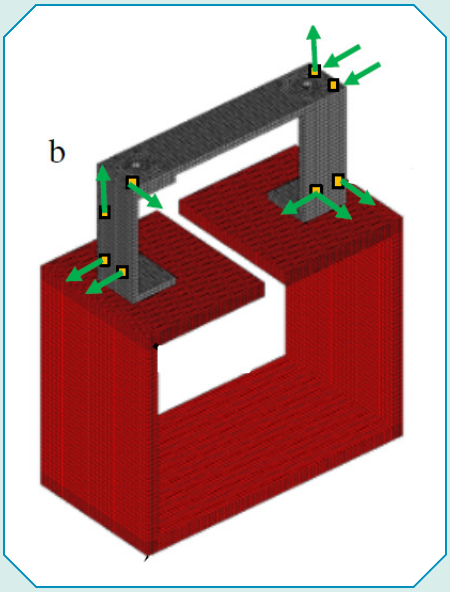
Co-designing the hardware architecture and the corresponding algorithms, researchers developed several novel analog linear algebra accelerators that could revolutionize computing by enabling orders of magnitude reduction in computation energy and time for matrix operations. Using crossbar memories accelerates both sparse and dense matrix multiplication and matrix inversion/solution. These matrix operations are critical for any large-scale simulation, including those for electromagnetics, climate, material science, structural mechanics, and fusion energy. Accelerating matrix multiplication will also accelerate neural networks and other data processing algorithms critical for cyber analytics, image processing, and more. This project has shown increased performance of greater than 100x over digital architectures for both high performance computing and high throughput data analytics. (PI: Sapan Agarwal)



32x32 Analog Solver Array

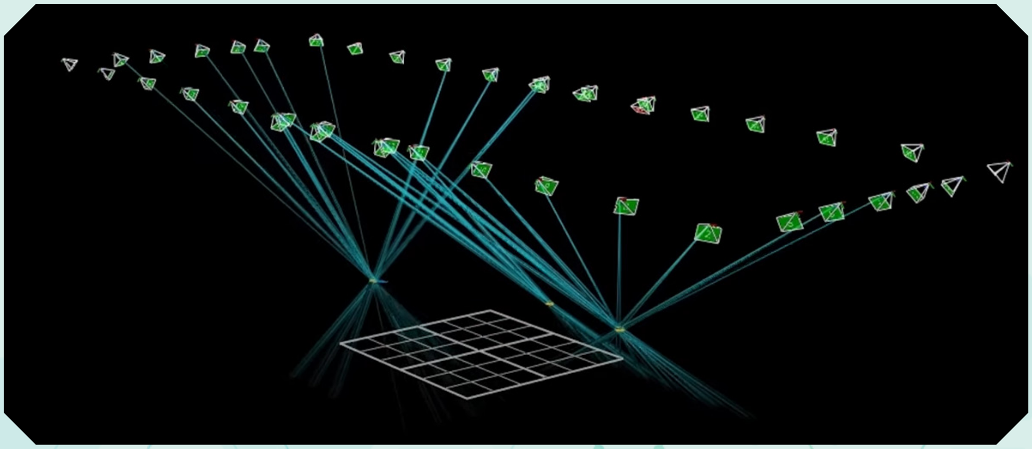
Example of analog pre-conditioning solver array fabricated using Global Foundries 45 nm silicon on insulator process.

Risk-adaptive experimental design for high-consequence systems.
Credible assessment of high-consequence systems requires the fusion of simulation and experimental data. Currently, the nuclear weapons qualification process is data-starved and based on experimentation and engineering judgment with some simulation guidance. Each aspect is conducted independently without statistical mapping, leading to exaggerated margins and over-designed components. This LDRD team developed an automated and goal-oriented framework to facilitate the rapid online design of experiments that target conservative measures of prediction uncertainty. Their approach minimizes the tail average of the prediction variance to produce certifiable and realistic margins that are robust to data corruption and noise. Researchers also developed specialized algorithms to solve such design problems, yielding a 200-fold reduction in computational effort. (PI: Drew Kouri)



Optimally placed accelerometer locations (green arrows) on a BARC ground-based test as determined using risk-adapted experimental design.

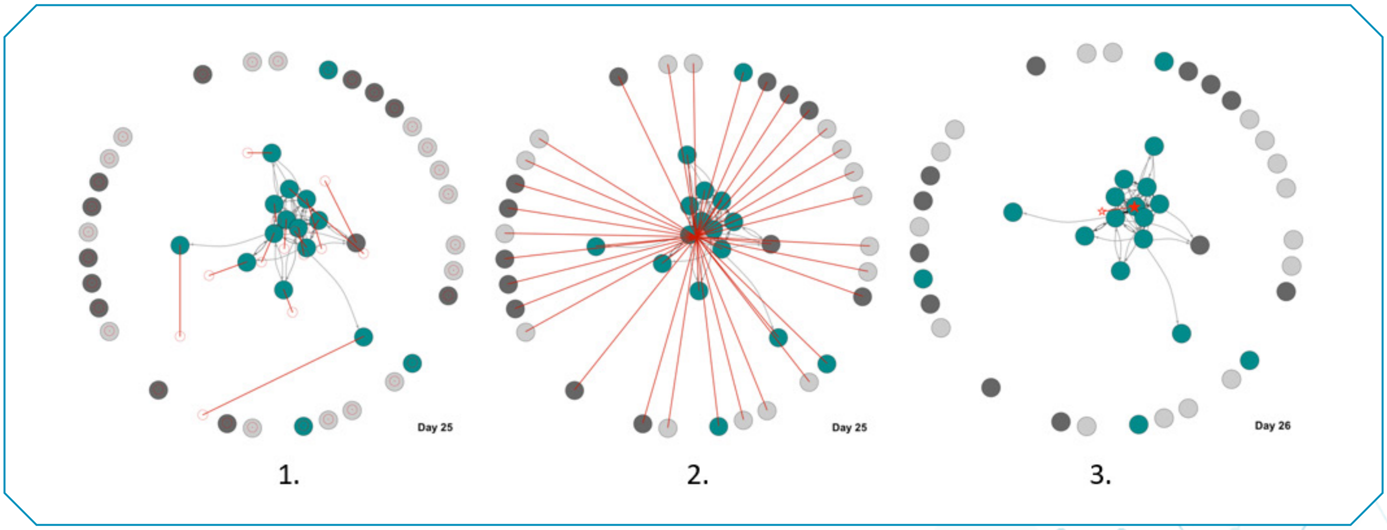
Adapting secure multiparty computation to support machine learning in radio frequency sensor networks.
This LDRD project team developed theoretical and practical foundations for secure and intelligent decentralized networks of low-power sensors that communicate via radio frequency. These networks are resilient to the random failure of a small fraction of nodes, remain secure even if an adversary captures a small subset of nodes, and are capable of basic machine learning. This new privacy-preserving machine-learning capability will help address national security priorities such as physical security and nuclear command, control, and communications. (PI: Jonathan Berry)



Privacy-preserving machine learning is demonstrated on a large network of autonomous drones at the AutonomyNM Robotics Lab.

Assessing cognitive impacts of errors from machine learning and deep learning models on human cognitive performance.
Researchers characterized the impact of errors from machine learning and deep learning algorithms on human cognitive performance in visual search and identification tasks. The results support a systems-engineering approach to implementating these algorithms by quantifying the impact of different types, rates, and visual implementation (e.g., explainability or confidence metrics) of errors and providing evidence-based recommendations for integrating machine learning and deep learning with human decision making within analytical systems. The research focused on common visual tasks (search and identification in still images) and produced results that will generalize across multiple national security domains, including international nuclear safeguards, physical protection, intelligence, homeland security, and nuclear weapons manufacturing/engineering. (PI: Zoe Gastelum)

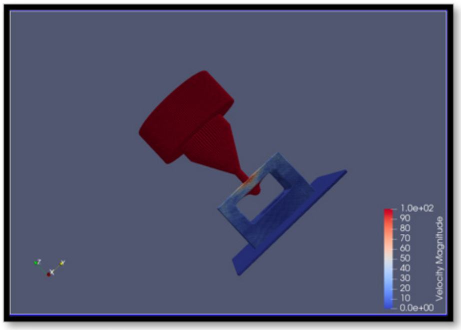
Anticipating group dynamics through emergent recursive multiscale interaction.
Understanding group emergence can improve our ability to anticipate and understand how group dynamics can be influenced in national security applications. Particularly impactful is the new theory on the multiscale, fractal-like nature of the emergence of groups, including recursive interactions between scales that resulted from this LDRD project. This work, supported through collaborations with professors Yuguo Chen at University of Illinois Urbana-Champaign and Abdullah Mueen at the University of New Mexico, will be important to NNSA and the DoD. (PI: Asmeret Naugle)



Group dynamics modeled using new communication vibration theory: (1) Movement of members between days; (2) changes in the average distance between group centroid and members between days; and (3) movement of centroid of group members relative to non-members.

ASCeND project provides mathematical tools to discretize models.

Nonlocal models, which describe a system via integral operators acting over a finite length scale, provide a unique ability to describe mechanics of interest to DOE, but face technical hurdles that prevent broader adoption. The ASymptotically Compatible strong form foundations for Nonlocal Discretization (ASCeND) project developed mathematical tools for discretizing these models that preserve notions of asymptotic compatibility, whereby the solution will recover classical theory as a nonlocal parameter is reduced to zero. Guided by this objective, the team developed mathematics that maximize impact to mission exemplars related to ductile fracture and energy storage devices fracture. (PI: Nat Trask)



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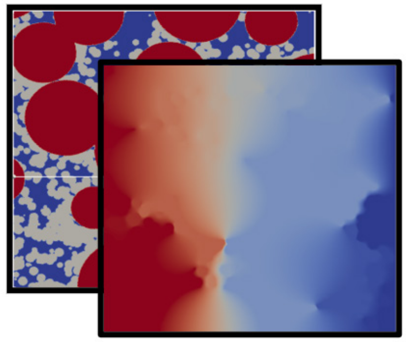
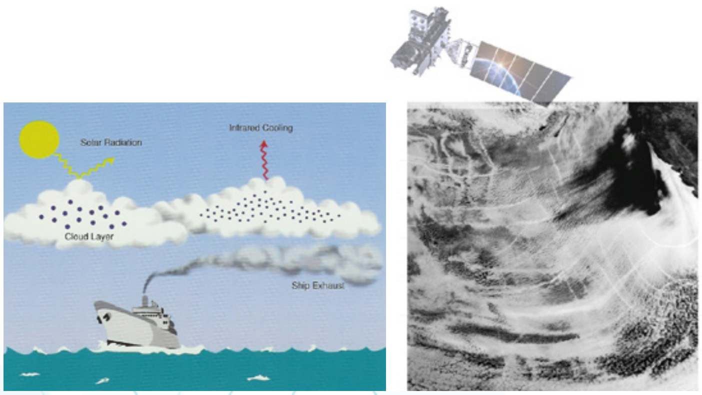


2.

Exemplar problems: (1) Large deformation ductile fracture. (2) Transport induced brittle fracture and lithiation-induced failure of Li-ion batteries.

Novel detection mechanisms assess aerosol-cloud interactions.

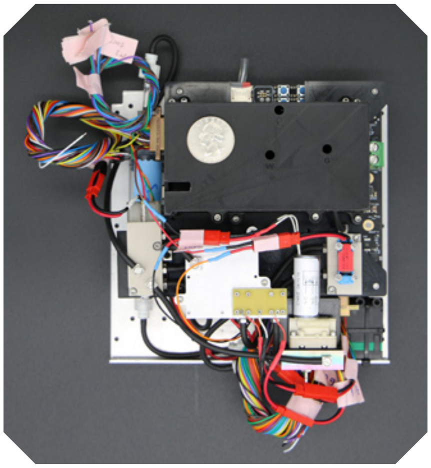
Ship tracks are quasi-linear cloud patterns produced from the interaction of ship emissions with low boundary-layer clouds. They are visible throughout the diurnal cycle in satellite images from space-borne assets like the Advanced Baseline Imagers aboard the National Oceanic and Atmospheric Administration (NOAA) Geostationary Operational Environmental Satellites (GOES). Complex atmospheric dynamics, however, often make it difficult to identify and characterize the formation and evolution of tracks. Ship tracks could increase a cloud's albedo and reduce the impact of global warming. Thus, it is important to study these patterns not only to better understand the complex atmospheric interactions between aerosols and clouds to improve climate models, but also to examine the efficacy of climate interventions, such as marine cloud brightening. During this LDRD project, the team developed novel data-driven techniques that advance our ability to assess the effects of ship emissions on marine environments and the risks of future marine cloud brightening efforts. The three main innovative technical contributions include a method to track aerosol injections using optical flow, a stochastic simulation model for track formations, and an automated detection algorithm for efficient identification of ship tracks in large datasets. (PI: Lyndsay Shand)



(Left) Ship tracks in action. (Right) Ship tracks as seen in NOAA GOES-17 imagery.

A synthetic opioid detector technology.

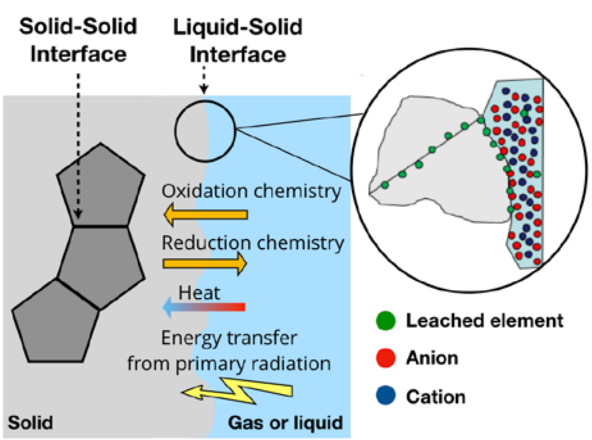
Synthetic opioids such as Fentanyl and its analogs are a toxic drug class that readily cause harm, present detection challenges, and are illegally imported into the United States in large quantities. Producers rapidly proliferate altered chemical structures to increase drug potency and make detection attempts more difficult. The Sandia research team developed a method to detect this class of compounds, independent of their altered chemical structure, by thermally-fragmenting them at high temperatures and identifying the common chemical products that emerge. After understanding how these fentanyl analogs decompose, the team developed the capability to separate and detect these decomposition products even in complex chemical mixtures. They designed a prototype portable detector, consisting of a microfabricated pyrolyzer, a two-dimensional micro gas chromatograph, and a miniature ion mobility spectrometer, to identify these compounds in the field. Matured versions of this technology may support law enforcement and border patrol agents to intercept these deadly drug compounds. The LDRD team prototyped this unique "platform" technology for the detection of synthetic opioids, but future work could readily adapt the technology for the detection of additional compounds of national security and law enforcement concern. (PI: Matthew Moorman)



This prototype portable device created by Sandia can detect synthetic opioids by thermally-fragmenting them and detecting the decomposed chemical products that emerge.

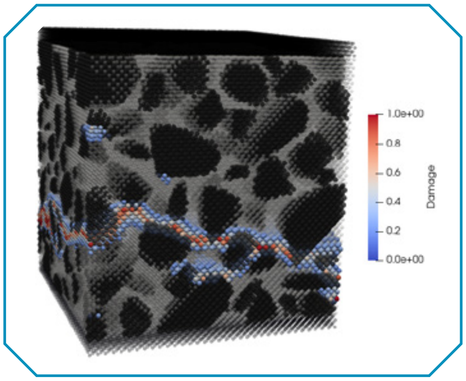
Addressing aging mechanisms in harsh environments.

In Molten Salt Reactor (MSR) environments, corrosion- and radiation-induced degradation occurs at the material-salt interfaces. To address the issue, the project team used a multi-resolution characterization capability that combines unique experimental characterization techniques and novel multi-physics computational models. One aspect of the LDRD was conducted in conjunction with Georgia Tech (GT), which performed combinatorial molten-salt corrosion experiments. This research led to many peer-reviewed manuscripts, including publication in *Corrosion Science*, *Acta Materialia*, *Scripta Materialia*, and *Applied Surface Science*. Owing to the importance of surface chemistry in corrosion processes, Sandia's collaboration with GT advanced fundamental understanding of how surface properties are modified by the presence of impurities near alloys surfaces, which will lead to the deployment of current and development of novel alloys that can be used in the next generation of nuclear reactors. Overall, the project addressed the challenges of materials aging by systematically characterizing the coupling effects of molten salts, high temperature, and irradiation on corrosion performance. (PI: Remi Dingreville)



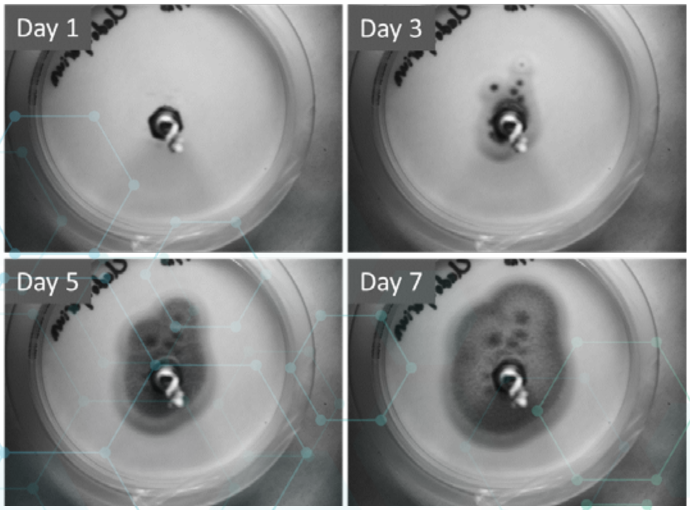
Because researchers now understand how impurities near alloy surfaces modify surface properties, advanced materials can be designed specifically to withstand the corrosion and radiation-degradation found in harsh environments.

Predicting stability of infrastructure following disasters.
Environmentally assisted brittle fracture in infrastructure (bridges, dams, tunnels) can occur following man-made threats or natural disasters. For accurate prediction of catastrophic failure and collapse, integrated multiphysics modeling requires the incorporation of environmental impacts into modeling efforts. Through this LDRD project, the team developed new modeling capabilities for evaluating multiphase phenomena in cement-based materials in energy and infrastructure applications. They also developed a chemo-mechanical model for cement fracture, identified sources of uncertainty in cement degradation and concrete fracture, and created six new capabilities for modeling brittle fracture in open-source code, Peridigm. Academic collaborations with University of Colorado Boulder, the University of New Mexico, and Purdue University provided evaluation of concrete fracture in gravity dam structures and the degradation and clay composition on evolving cement fracture. A funded strategic initiative on decarbonization of cement manufacturing incorporated the work; DOE Earthshot included content on the project; and a white paper was authored for the U.S. Army Corp of Engineers. (PI: Jessica Rimsza)



Peridynamic simulation of concrete fracture under tension with cracks forming in the mortar between the solid aggregates.

Evaluating metabolic energy for black molds.
Melanin-containing fungi (black molds) can thrive under extreme environmental conditions such as the high radiation levels inside the former Chernobyl reactors. These fungi have been hypothesized to use gamma radiation as an energy source (radiotrophism), but the literature has not clearly addressed which energies of the electromagnetic spectrum, if any, positively affect the growth of fungi. This LDRD team sought to assess the existence of radiotrophism in this class of fungi, as it could have broad scientific implications and provide novel approaches for radiation measurement, monitoring and managing nuclear and radiological materials, dosimetry, and environmental remediation. The project evaluated a range of electromagnetic energies using a technical approach that coupled analyses from optical engineering, nuclear engineering, and fungal biology, but the data did not establish evidence supporting radiotrophic behavior in the dose regime used by the team. (The regime was representative of gamma emissions from fission products and would signal applicability for global security and nonproliferation.) Future work to expand on these findings and evaluate other signals may enable significant new solutions to national security challenges. (PI: Jesse Bland)



The image series shows the melanized fungi Cladosporium cladosporioides grown under gamma irradiation over seven days. The hexagonal shape in the center is a 352 microcurie cesium-137 source. The experiment found no evidence of radiotrophism for this fungi and dose regime.

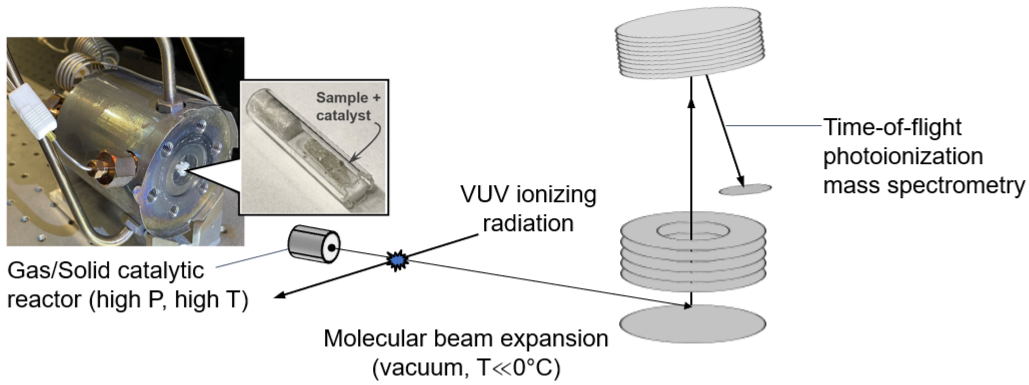
Sandia researchers create a platform for discovering, designing and engineering novel antibody countermeasures for emerging viruses, including SARS-CoV-2.

Saliva mimicking medium for use in viral studies.

The global outbreak of SARS-CoV-2 has emphasized the need for a deeper understanding of infectivity, spread, and treatment of airborne viruses. With convergently evolved structural similarities to viral pathogens, tailless phages are an ideal surrogate for studying respiratory pathogenic viruses. Phages are highly tractable, allowing investigations to proceed quickly and at the lowest biosafety level. However, the aerosolization of enveloped SARS-CoV-2 surrogate phi6 usually results in a ~3 $\log_{10}$ reduction in viability, limiting its usefulness as a surrogate for aerosolized coronavirus in "real world" contexts. Recent work has shown that saliva or artificial saliva greatly improves the stability of viruses in aerosols and microdroplets relative to standard dilution/storage buffers, like an SM buffer. The LDRD team investigated whether media could be formulated that preserves the viability of airborne phi6. A supplement has been identified that dose-dependently stabilizes phi6 to nearly zero losses in the aerosol testbed and outperforms commercially formulated artificial saliva. These data suggest that the saliva mimetic media may facilitate a lower-cost alternative to artificial saliva for future airborne virus studies. (PIs: Bryce Ricken and Jesse Cahill)

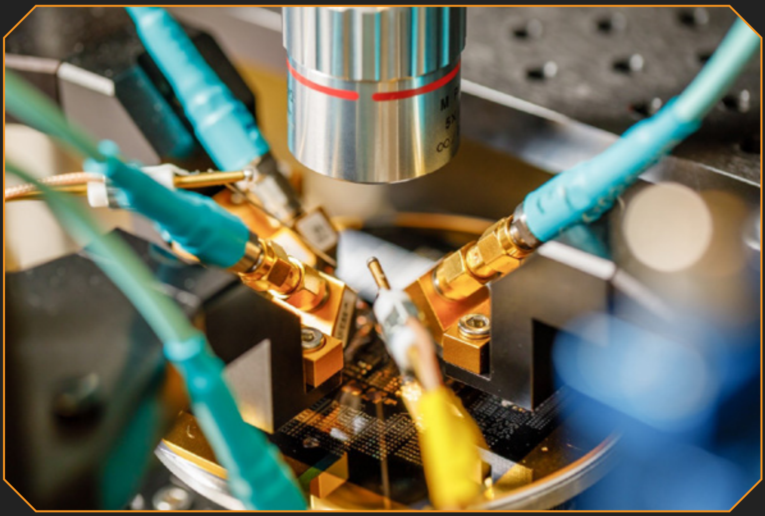
New approach for fundamental mechanism discovery in polymer upcycling.

A deep mechanistic understanding of complex multi-phase processes is critical to rational, physics-based co-design of advanced new polymers, catalysts, and depolymerization/repolymerization chemistries. This LDRD project investigated the use of detailed chemical analysis of the gas flow above a reacting catalyst to provide insight into catalytic depolymerization reactions. Gas-phase chemical species were detected by vacuum-ultraviolet (VUV) photoionization mass spectrometry (PIMS)—a high-throughput method that can distinguish among chemical isomers with the same molecular formula and is equally sensitive to stable products and short-lived reactive radicals. In the first of two proof-of-principle demonstrations, the team quantified methyl radical intermediates and observed selective C-C bond activation in small aliphatic hydrocarbons, which are model oligomers of polyethylene plastics. In the second demonstration, researchers revealed the dominance of singly-unsaturated, methylated alkene products in the deconstruction of high-density polyethylene (HDPE). This work, performed in collaboration with Johns Hopkins and UC-Davis researchers, opens the door to detailed mechanistic studies of depolymerization and shows the power of cutting-edge gas-phase analysis tools to investigate complex multi-phase processes. (PI: Leonid Sheps)



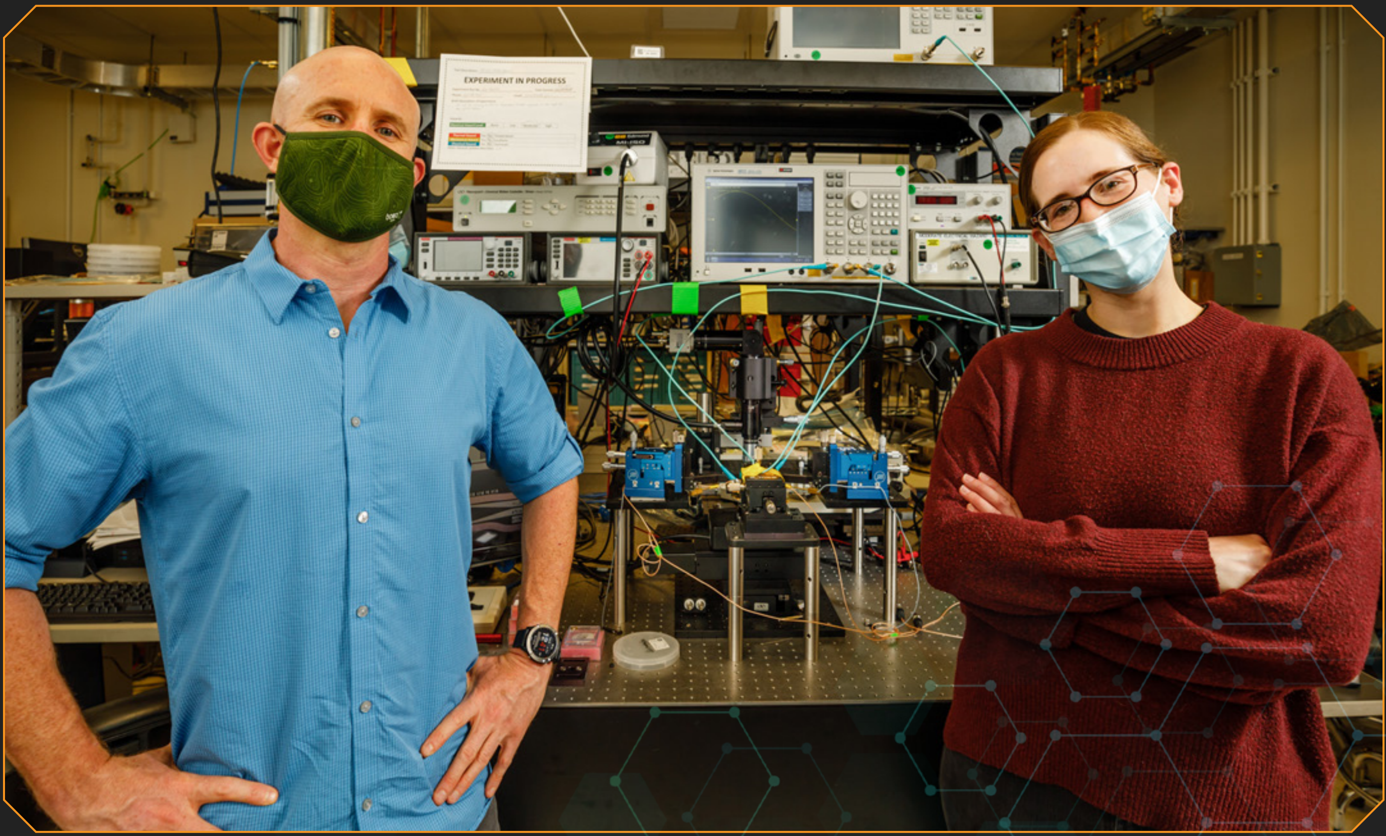
Synchrotron-VUV PIMS analysis of gas flow over a solid catalyst/polymer yields detailed isomer-resolved product distribution in the deconstruction of HDPE.

New radiofrequency acoustic wave mixer to enable all-acoustic signal processors. Within the national security arena, several applications require compact devices that can operate with low power consumption in congested spectral environments. Through this one-year LDRD project, the team developed a radiofrequency acoustic wave mixer device by experimentally investigating the fundamental nonlinear electron-phonon interaction in a heterogeneously integrated compound semiconductor on a piezoelectric material platform. The successful demonstration of an acoustic frequency conversion with high efficiency completed a final technological hurdle to enable all-acoustic, and therefore, ultra-compact radiofrequency signal processors. (PI: Lisa Hackett)



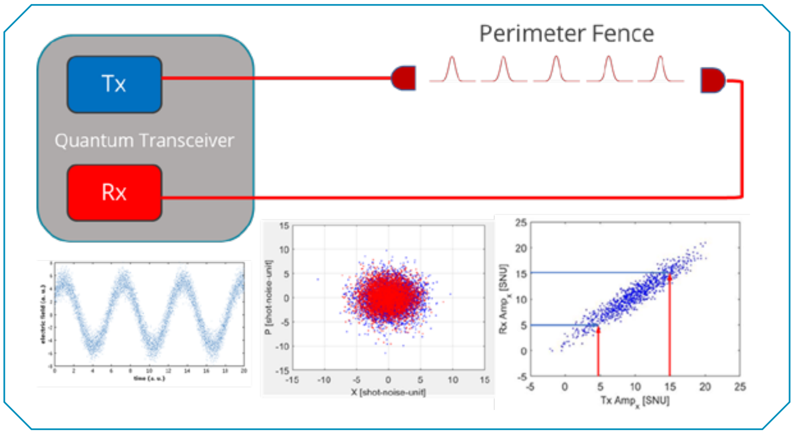
The successful radiofrequency acoustic wave mixer device developed during this LDRD project is a significant step toward enabling ultra-compact radiofrequency signal processors. (Photo by Bret Latter)

Scientists Matt Eichenfield, left, and Lisa Hackett led the team at Sandia that created the world's smallest and best acoustic amplifier. (Photo by Bret Latter)



Quantum-secure optical fence for physical security.

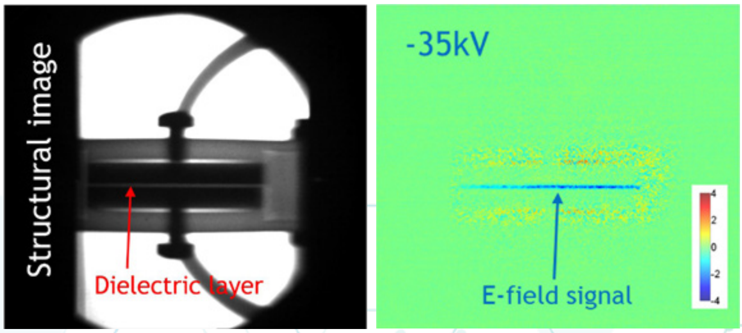
A proof-of-concept quantum sensor for perimeter monitoring of critical facilities was developed to enhance detection of sophisticated spoofing attacks. Standard intrusion systems often encode streams of light pulses to monitor and prevent security breaches around facilities, but in principle, advanced attacks can be used to create holes in these security systems. To address this gap, researchers investigated a quantum intrusion sensor using coherent states as quantum probes and leveraging the Uncertainty Principle and No Cloning Theorem. Shot-noise-limited detection of encoded quantum probes and hypothesis test analysis enabled researchers to establish statistical quantum correlations for high sensitivity detection, a novel capability that could bolster physical protection systems for high-consequence assets. (PI: Junji Urayama)



(Top) Schematic of quantum transceiver and optical fiber configured for perimeter monitoring. (Bottom) Coherent state measurements used as quantum probes and their statistical correlations.

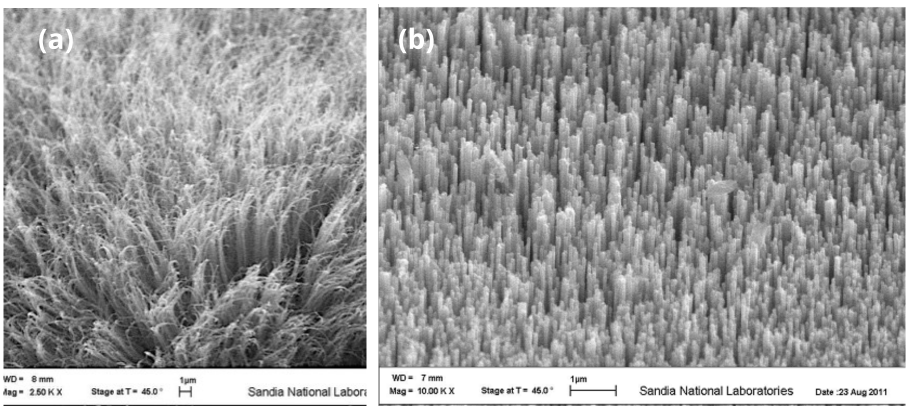
Sensing what cannot be seen through advanced neutron imaging technology.

A global first, this novel metrology can determine the charge/voltage state of shielded electronics—something not achievable by any existing detection technologies. By using electrically neutral, but highly penetrative neutrons to interact with the associated electric fields (E-fields) produced by the charged/energized electronics inside a conductive enclosure, the researchers obtained E-field imaging signals to absolutely determine the voltage/charge state. The highly penetrative neutron beam used by this new technology can directly "visualize" static or dynamic electro-magnetic fields, especially the electrostatic field produced by electronics. This successful development will greatly benefit to the applications of weapon security, national security, and global security. (PI: Yuan-Yu Jau)



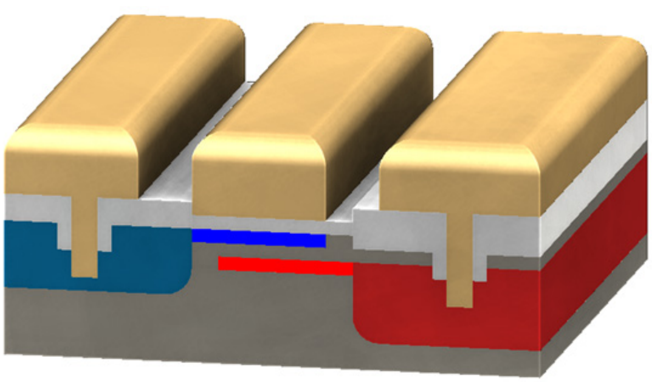
(Left) A normal neutron transmission image of an electric-field sample. (Right) Image of electric field in the dielectric layer of the sample with "Jet" color scheme. Inside the sample, the voltage across the electrodes is -35 kV, which leads to a negative signal in the blue-color region.

Dissipating advanced satellite systems heat load with a new thermal interface material.
The problematic heat load from advanced satellite systems with focal-plane array sensors, central processing units, and graphics processing units continues to increase. Existing thermal interface materials (TIM) limit operational performance and/or require high power cryocoolers to achieve desired operating temperatures. With thermal conductivities potentially 10x greater than metals, arrays of vertically-aligned carbon nanotubes (CNT) could greatly reduce thermal resistances. This LDRD project team built on previous LDRD projects and focused on growing high quality, vertically aligned CNTs in high packing fractions on thermally-conductive substrates to optimize overall TIM conductivity. Sandia also collaborated with Georgia Tech and Carbice™ to measure the thermal cooling properties from CNT arrays they developed on a thermally-conductive adhesive substrates approved for use by NASA. Considering the superior CNT quality and array geometry of Sandia's materials, researchers anticipate even greater advantages for CNT-TIM applications. (PI: Mike Siegal)



(a) Vertically-aligned CNT array grown via nanopore template method resulting in > 40% volumetric fill factor. (b) Nanowires dried in supercritical CO_2 to prevent agglomeration.

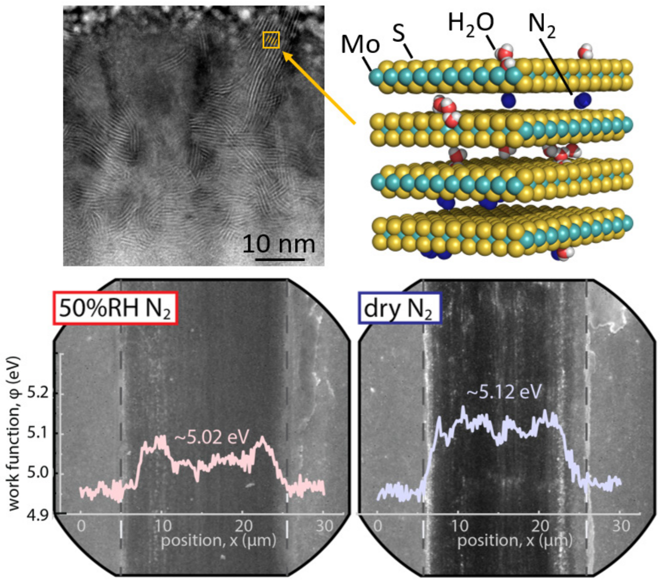
Using atomic precision advanced manufacturing to unlock computing hardware functionality.
Unlocking inaccessible computing hardware functionality is the focus of the Far-reaching Application, Implication, and Realization of Digital Electronics at the Atomic Limit (FAIR DEAL) Grand Challenge project. The LDRD team developed the science and technology required to use atomic precision advanced manufacturing (APAM) to meet their objective. APAM uses surface chemistry to introduce dopants into silicon at a density that exceeds the solid solubility limit and with sub-nanometer precision, and this technique may be used to improve the energy efficiency of microelectronics by leveraging new physical effects. The team fabricated the first complicated transistor devices based on APAM that works at room temperature and also expanded the applicability of APAM by developing an APAM acceptor chemistry, an APAM oxide chemistry, a route to image reversal, and two paths to high throughput fabrication. A foundational achievement came through direct integration of APAM with complimentary metal-oxide semiconductor (CMOS) and identifying a near-term application in improving state-of-the-art CMOS metal-semiconductor contacts. (PI: Shashank Misra)



Tunnel field effect transistors are predicted to improve the energy efficiency of microelectronics by 10x, which APAM is helping to realize in practice.

Next generation strategically radiation hard computing.
Modern smartphones using state-of-the-art complementary metal oxide semiconductor (CMOS) can execute teraflops while consuming only a few watts. However, strategically radiation hardened (SRH) embedded CMOS technologies are constrained to much older technology nodes, with the most scaled SRH process technologies being about 150 nm (with 90 nm under development). This represents a gap of about seven generations between SRH and modern CMOS. (Modern CMOS has a performance advantage of 100 to 1000 times that of SRH CMOS.) Sandia's Secure, Efficient, Extreme Computing (SEEEC) Grand Challenge project is addressing this performance gap by combining high performing SOTA CMOS with SRH CMOS. SEEEC integrated an SRH supervisor chip with advanced, high-performance commercially fabricated integrated circuits. This required the creation of a new modelling framework for the SEEEC architecture with a high-fidelity multi-scale model of radiation effects in modern scaled CMOS. Multiple radiation environments are under investigation; models are experimentally informed using test structures including single transistors, gates, larger blocks (e.g., arithmetic logic unit), full processor cores, and caches. SEEEC is providing a path to achieve state of the art computing performance in strategically radiation hard systems and has inspired a larger framework on advanced hybrid architectures. (PI: Matt Marinella)

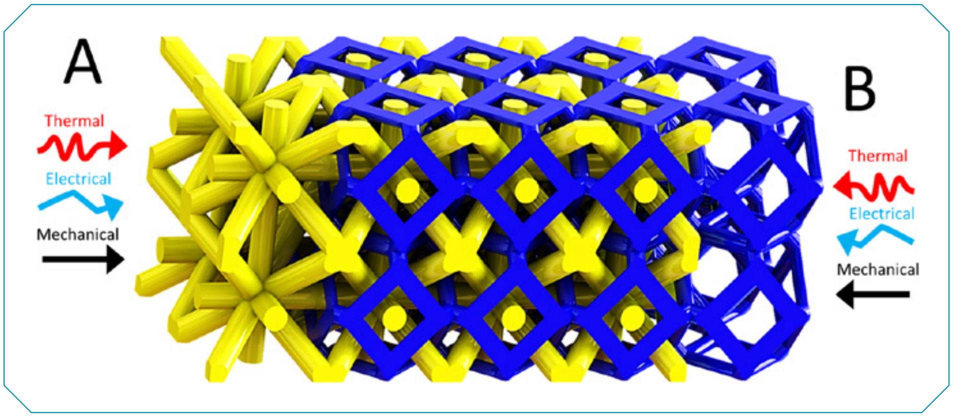
Fundamental mechanisms of friction evolution in lamellar solids.
A variety of precision electromechanical devices in commercial aerospace and Sandia mission applications require critical solid lubricants because frictional performance changes during operation and storage in reactive atmospheres, thus restricting usage and limiting device designs. This LDRD project focused on understanding the atomic scale processes responsible for the evolution of friction coefficient in 2D lamellar materials. Recent research on molecular electronics motivated the first use of 'work function' to provide insights on atomic structure and defect content of worn surfaces and, with molecular dynamics simulations, showed that water increases the friction coefficient exhibited by MoS_2 (an exemplar lubricant) through disrupting the shear-induced restructuring of the surface into large, ordered lamellae. Sandia partnered with Florida A&M-Florida State University's College of Engineering, which developed a novel way to look at transfer films resulting from contact of lamellar solids. The resulting understanding will inform the design of tailored nanocomposites that suppress aging mechanisms and significantly improve reliability and performance of solid lubricants. (PI: Michael Dugger)



Work function (bottom) of MoS_2 wear tracks showing structure modification of surface lamellae (top left) due to environment. Atomistic simulations of MoS_2 (upper right) show water clustering at S vacancies.

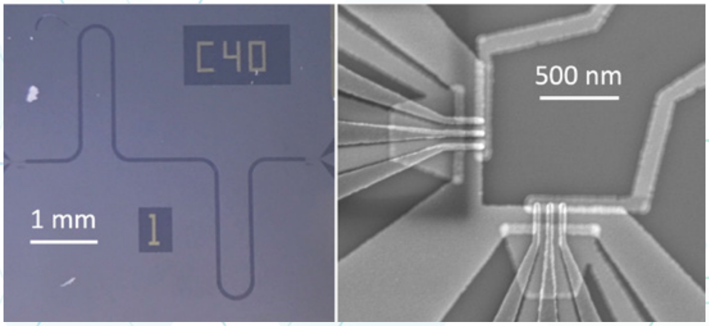
The Experimental Impact Mechanics Lab at Sandia allows engineers to test the strength and impact properties of any solid natural or manmade material on the planet. Mechanical engineer Bo Song, shown here, makes adjustments to the Drop-Hopkinson Bar — the only one of its kind in the world. (Photo by Bret Latter)

Developing novel structural metamaterials to mitigate harsh environments.
Sandia components must survive in harsh environments, including shock, crush, thermal, vibration, radiation, etc. In use for several decades, metamaterials, otherwise known as lattice materials, have origins in metallic honeycombs. Through additive manufacturing technologies, far more sophisticated geometries are now possible. The LDRD project team focused on three theme areas: (1) inventing, building, and testing completely new lattice architectures that possess unique abilities to mitigate harsh structural environments; (2) employing gradient-based optimization strategies to enable generative design of architectures tailored to meet specific requirements; and (3) understanding the role of manufacturing defects on the performance of these as-printed lattices. This project led to two filed patents and eleven published journal articles, including the most recent one in Materials & Design. In parallel, Texas A&M University, a Sandia academic partner, developed the capability to print such lattices in a nickel-titanium shape memory alloy with precise compositional control necessary to maximize the functional benefits of these alloys. Ben Young, a doctoral student on this project, will join Sandia in 2022 as a postdoctoral appointee. To date, this project has spawned several new efforts, including a funded collaboration with the Air Force. (PI: Brad Boyce)



The novel interpenetrating lattice metamaterial controls the transmission of thermal, electrical, or mechanical energy through surface interactions between two interwoven constituent sublattices ("A" and "B," represented in yellow and blue). This patented design, with its unusual but useful properties, is described in a recent Additive Manufacturing article.

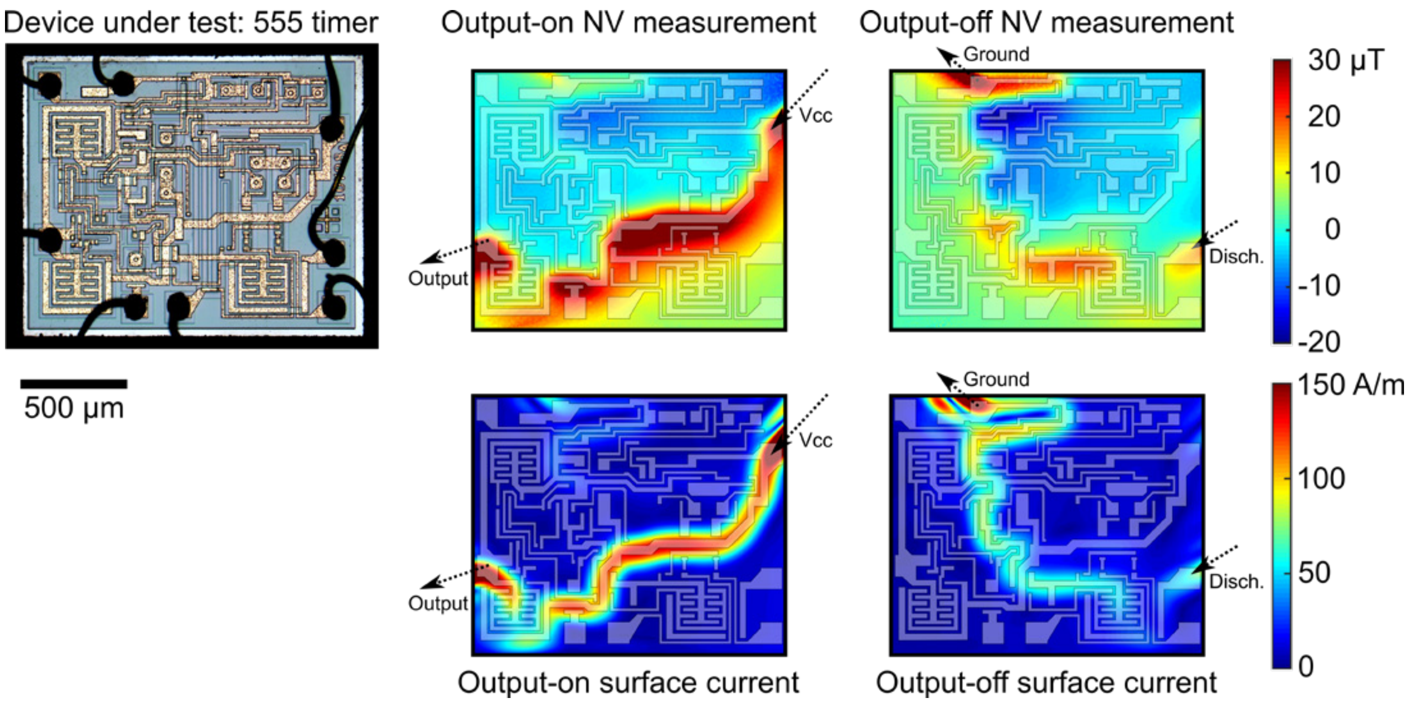
Leveraging spin-orbit coupling in heterostructures for quantum information transfer.
Coherent distribution of information will be required for many future applications that take advantage of quantum phenomena. The information in hybrid systems will need to be transferred between hardware elements that process quantum information in physically different ways. For this LDRD project, researchers developed the fundamental building blocks of one potential distribution node in the solid-state. The team investigated the unique properties of single-hole-spin qubits in germanium (Ge) and silicon/germanium (SiGe) quantum dots and the potential to couple hole spins to photons trapped in a superconducting resonator through intrinsic spin-orbit coupling. The work highlights a compelling path forward for quantum information distribution between heterogeneous quantum elements that can benefit national security applications relying on quantum networks. (PI: Dwight Luhman)



An image of superconducting resonator (left) and a lithographic quantum dot device in Ge/SiGe (right) fabricated as part of the project. Note the difference in length scales between the two quantum technologies.

Using defects in diamonds to protect against counterfeiting and assess the behavior of electronic devices.

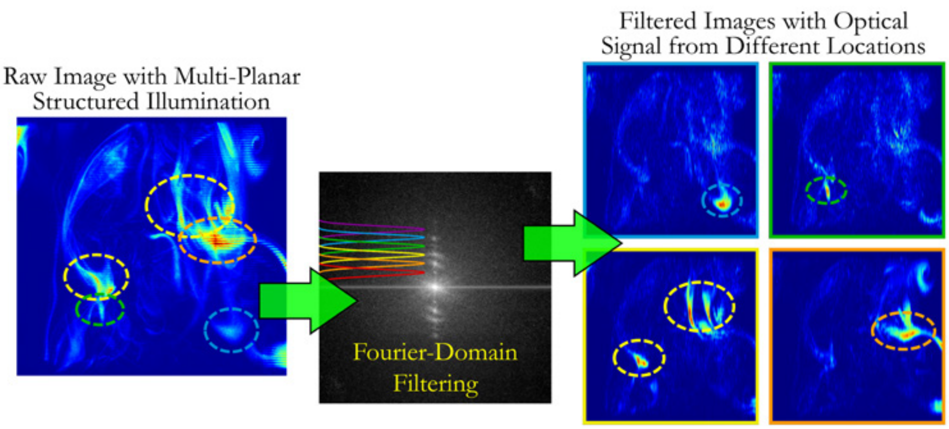
Nitrogen-vacancy (NV) defect centers are magnetically-sensitive fluorescent defects that are used for quantum magnetic sensing in basic and applied sciences. When used to image magnetic fields from sources external to diamond, NV magnetic imagers offer room-temperature operation, micrometer-scale spatial resolution, a small sample-sensor distance (as small as a few nanometers), and parallel multi-pixel readout over a few-millimeter field of view. In this project, LDRD researchers used an NV magnetic imaging apparatus to optically image magnetic fields and yielded quantitative information about the field magnitude, direction, polarization, and relative phase with wide frequency range (DC to 100 GHz), micron resolution, and a few-millimeter field-of-view. This research demonstrated a new way to quickly read out micron-scale "magnetic fingerprints" (to protect against counterfeiting) and to magnetically interrogate the internal currents and behaviors of integrated circuits (to probe what electronic devices are doing internally). Going forward, the goal is to advance NV magnetic imaging such that it is a useful tool for real-world national security applications, including imaging the fields from microelectronics and antennas, ion chip traps, and nanostructured devices and materials. (PI: Pauli Kehayias)



Using a surface layer of magnetically-sensitive nitrogen-vacancy centers in diamond, researchers imaged the magnetic fields from the currents in a commercial 555 timer integrated circuit (top left) when the device is in different internal states (output-on and output-off). After measuring the magnetic field maps with high spatial resolution (top row), they reconstructed the surface current densities (bottom row), allowing the team to probe the internal current paths and assess the behavior of the device.

Instantaneous 3D temperature measurements via ultrafast laser spectroscopy with structured light.

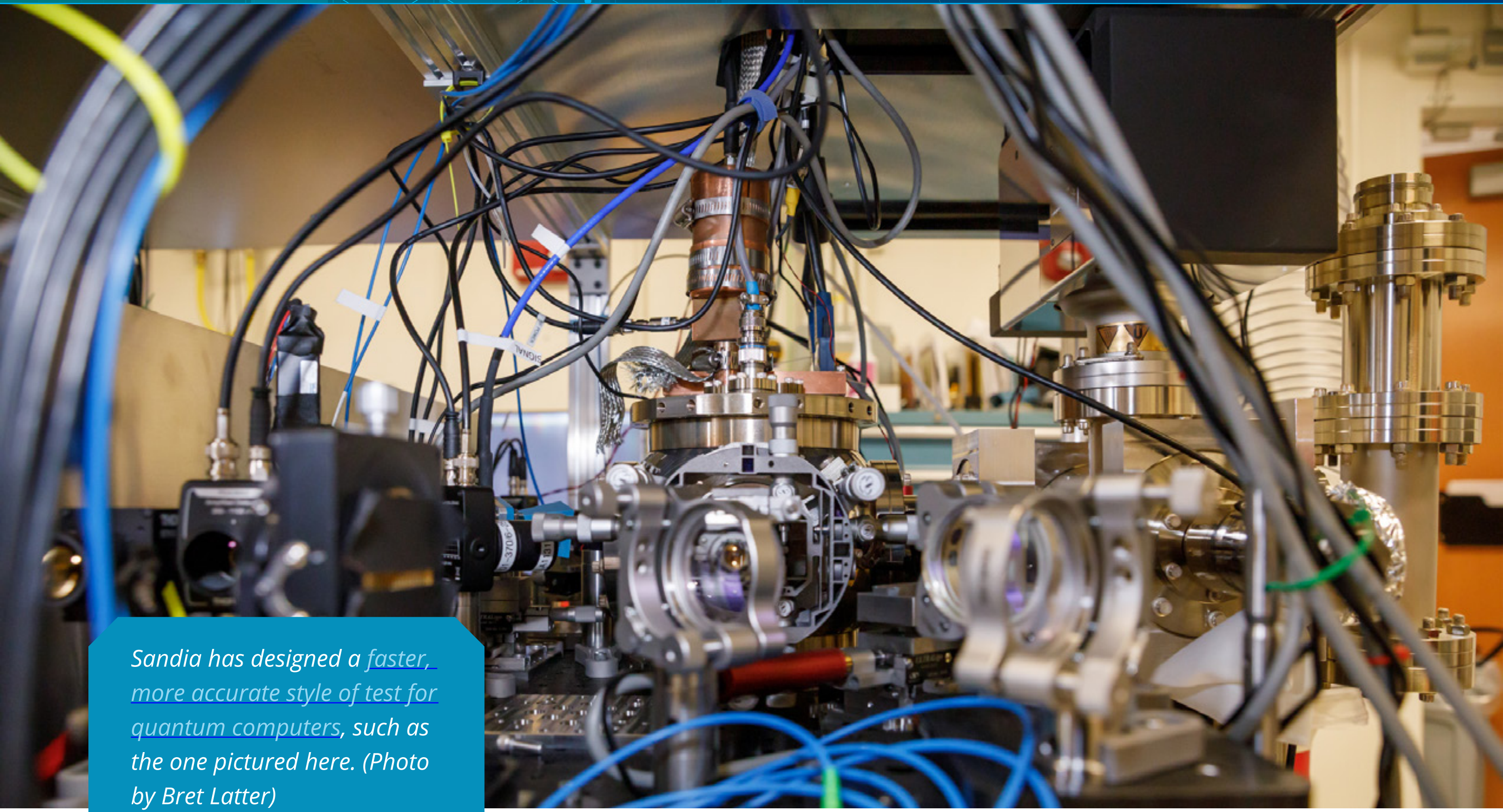
Optical measurements can provide accurate data in hostile environments where physical probes are not feasible but are typically performed at a point or along a line. This project combined various optical diagnostic techniques with principles of structured illumination to provide enhanced dimensionality. In this research, structured illumination involved the use of modulated intensity patterns, which were used to distinguish optical signals from different spatial locations and from background optical signals much as a lock-in amplifier filters signals in the time domain. This technology was demonstrated for multi-planar particulate concentration measurements in turbulent flames with a single laser and a single camera and was applied to distinguish laser-induced fluorescence signals from intense background radiation in detonation fireballs. Additionally, emission spectroscopy from multiple 1D measurement locations was demonstrated with a single set of detection optics and camera. These measurement techniques will be transformative for future studies in heat transfer and fluid dynamics where multi-dimensional data will aid in understanding complex phenomena. (PI: Daniel Richardson)



Simultaneous measurements from six different planes are performed with a single camera using structured illumination and Fourier-domain filtering.

Impacting the nanotherapeutics community via zeolitic imidazolate frameworks.

This LDRD project investigated the relevance of zeolitic imidazolate frameworks (ZIFs) as a materials platform responsive to intracellular pH in the biologically relevant range (5.2-7.4). Rationally designed nanomaterials responsive in this range contribute to emergent intracellular pathogen treatment. Endosomal trapping is one of the greatest barriers to the development of nanomaterial-based therapeutic delivery, since it leads to the destruction of the nanomaterial and cargo. Researchers first investigated how the structural features and chemical functionality in ZIFs are impacted by change in pH and how ZIFs respond to the intracellular environment. Based on their findings, they successfully synthesized a variety of size tunable ZIF nanoparticles with distinct topologies and chemical functionalities. To facilitate rapid and comparable assessment of endosomal release through endosomal pore formation or endosomal rupture, the team developed quantitative imaging strategies for endosomal interactions and assessed the importance of coatings to the cellular interactions of ZIFs with mammalian cells. This project generated relevant new capabilities in nanoscience through both nanomaterials and novel endosomal imagining modalities development. Further, it produced a generalizable and quantifiable method to understand endosomal interactions of nanomaterials, which will greatly impact the nanotherapeutics community. This research will enable novel technologies for the delivery of advanced therapeutics needed to counter biothreat agents. (PI: Dorina Gallis)



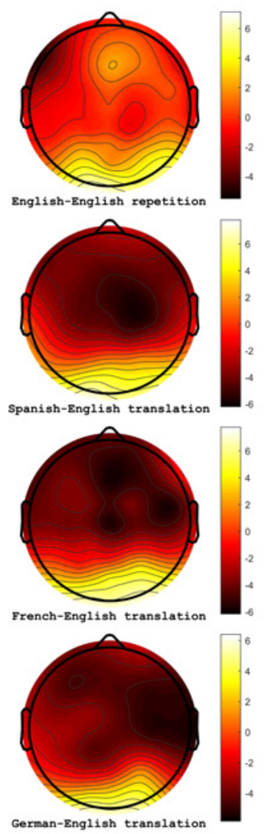
Sandia has designed a faster, more accurate style of test for quantum computers, such as the one pictured here. (Photo by Bret Latter)

A fast-cycle charge noise measurement for better qubits.

The spins of electrons localized in quantum dots are prime candidates for quantum bits (qubits) in a solid-state quantum computer. Quantum dots are fabricated using standard semiconductor fabrication techniques on silicon substrates. However, defects such as charge traps and dangling bonds are always present at materials interfaces and are also introduced during many fabrication steps. Defects cause charge noise leading to qubit decoherence. Characterization of this noise, traditionally performed with qubits themselves, is accurate but slow, hindering progress towards better devices. Through this LDRD project, researchers developed a noise spectroscopy technique to measure charge noise based on superconducting resonators. The technique leverages the high-quality factor resonators possible with superconductors, achieving sensitivity to noise in the stock material used to fabricate a qubit at the ultra-low temperatures and power levels encountered in qubit research. It also permits rapid testing of qubit fabrication processes. This research is expected to benefit not only spin-based quantum dot qubits, but also superconductor-based qubits such as the transmon (PI: Rupert Lewis)

Realizing high temperature superconductivity near ambient conditions in metal hydrides. Sandia is working to realize materials that exhibit superconductivity near ambient conditions. Superconducting materials exhibit zero electrical resistance, a property that would enable low-loss power transmission and revolutionize any electrical technology. Existing superconductors exhibit zero resistance only at very low temperatures, or at high temperatures but very high pressures. These limitations eliminate any benefit of zero resistance, so very few applications of superconductors have been realized. To solve this problem, researchers are developing ways to reduce the pressure required to realize high temperature superconductivity in the metal hydrides. Metal hydrides that contain large amounts of hydrogen, such as LaH_{10}, exhibit superconductivity near 270 K, the freezing point of water, at high pressures. The LDRD team sought ways to lower the formation pressure for LaH_{10} by modifying the lanthanum metal precursor to accept more hydrogen at lower pressures. Sandia's superconducting hydride team discovered that ball milling improves the reactivity of lanthanum, likely by promoting damage sites that improve hydrogen absorption. The goal is to reach sufficiently high hydrogen content that will promote superconductivity near room temperature. This project has stimulated collaboration between Lawrence Livermore National Laboratory, Argonne National Laboratory, and academic partners at California State University Northridge. (PI: Peter Sharma)

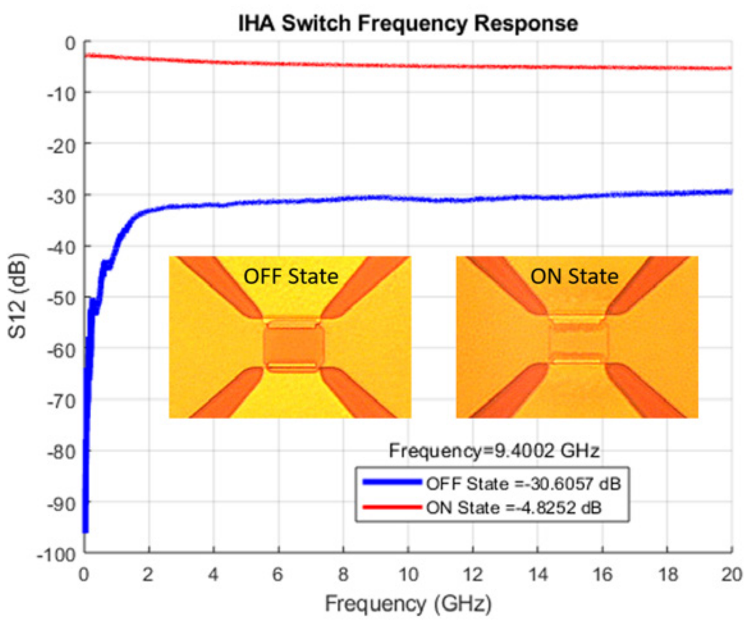
Developing methods for modeling and making predictions about individual differences in human cognition. Understanding individual cognitive differences is important for maximizing human and human-system performance. To predict how specific individuals will perform or process information, researchers asked, "Can we train a model to make predictions about which people understand which languages?" Language processing was selected because of the well-characterized differences in neural processing that occur when people are presented with linguistic stimuli they either do or do not understand. Sandia researchers and academic partners at the University of Illinois at Urbana-Champaign conducted a series of experiments to collect participants' behavioral and neural responses to words in many languages. In one experiment, participants viewed words in English and Spanish and were asked to press one button if a word contained five letters or fewer and another button if the word contained six letters or more. Another experiment used electroencephalography (EEG) to record participants' brain activity while reading words in English, Spanish, French, and German. Researchers used machine learning methods to model the resulting data in both experiments. Both models achieved high accuracy in predicting which participants understood which languages, with the best performance achieved by the EEG-based model. The new methods developed for this project can be applied in several research areas to better understand individual differences in cognitive processing. The project also laid the groundwork to develop new methods for characterizing cognitive performance in applied settings and developing individualized approaches to improving human performance. (PI: Laura Matzen)



These scalp maps show the electrical activity of a monolingual English speaker's brain from 350-450 milliseconds after reading a word. The EEG shows a different pattern of brain activity in response to pairs of English words than for word pairs in other languages. Modeling this response across many individuals can be used to make predictions about the language proficiency of new participants.

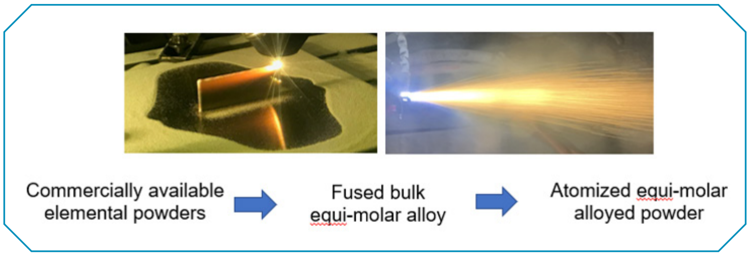
Machine learning for correlated intelligence.
Developing and characterizing the capability of machine learning (ML) algorithms in the electro-optical (EO) imaging space is vital for correlated intelligence applications. Correlated intelligence discovers coincidence in multiple modalities (radioisotope, electro-optical, radio frequency, synthetic aperture radar, etc.). The research team used commercial open source data sets to develop several ML algorithms for detecting objects in overhead imagery. An automated, distributed benchmarking framework was used to evaluate performance. Successful implementation of ML for overhead imagery, combined with automated benchmarking and continuous improvement frameworks, is a critical part of deploying effective, real-time, correlated intelligence applications. The use of continuous improvement, automated benchmarking methods attracted a number of externally funded projects across the Department of Defense. (PI: Emily Moore)

Germanium telluride chalcogenide switches for radio frequency (RF) applications.
RF systems are used across the gamut of national security applications, so any device that improves SWaP (size, weight, and power) and signal quality would have a high impact on current national security goals for improved communication systems and communication technology supremacy. This LDRD project team developed prototype germanium telluride switches that can allow for highly reconfigurable systems, including antennas, communications, optical systems, phased arrays, and synthetic aperture radar. The demonstration of the successful germanium telluride RF switches showcased a critical element necessary for a single chip RF communication system. (PI: Gwendolyn Hummel)



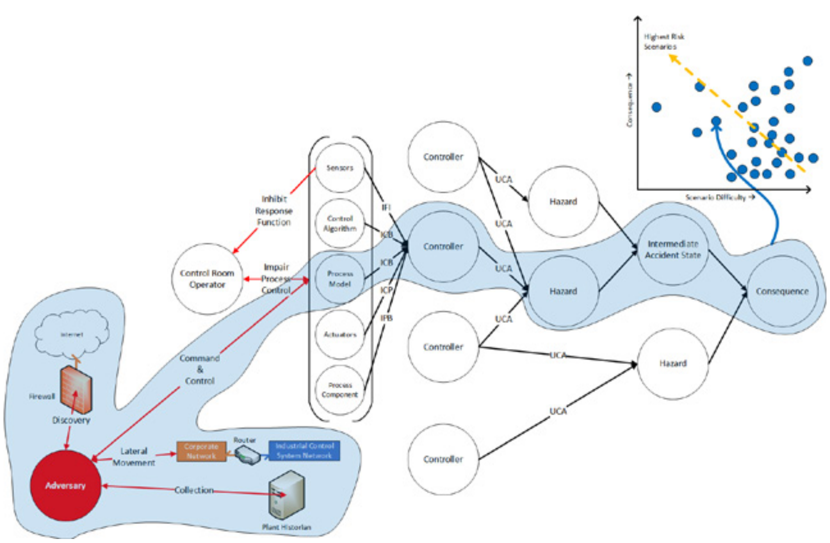
Indirect heating device with 6.0 micrometer gap. S-parameter measurement with insets showing optical images before (OFF state) and after (ON state) heating process; dB values were taken at displayed frequency.

Using additive manufacturing to rapidly develop specialized alloys for spray processing. Plasma spray is a useful advanced manufacturing process for depositing thick coatings of various materials with unique structure-property relationships. However, a primary roadblock to the successful integration of spray coatings, especially for complex or custom high-performance refractory-based alloys, is the limited available options for starting feedstock materials. In this LDRD project, researchers used a novel high-throughput metal additive manufacturing approach to rapidly create refractory-based high entropy alloy feedstock for thermal spray applications intended for downstream use in plasma spray processing applications. The success of this method readily expands the feedstock and alloy options available for use in plasma spray processing, enabling researchers to make custom alloys from elemental feedstock. (PI: Shaun Whetten)



The process used by the LDRD team to create refractory-based high entropy alloy feedstock for thermal spray applications.

Developing integrated cybersecurity safety and security models for energy systems. Protecting the electric grid is crucial to national security. This project, part of the Resilient Energy Systems LDRD Mission Campaign, investigated a new cyber security capability that integrated advanced hazards analysis, risk assessment, safety, and cyber security models into a risk-based approach for cybersecurity resilience. This methodology used the causal logic model Systems-Theoretic Process Analysis (STPA) to link digital control susceptibilities to facility hazards and consequences. The resulting STPA causal analysis provided a systematic approach for constructing Bayesian Networks (BN) to model consequence-based security scenarios in higher fidelity. As a stand-alone new capability, this approach illustrates how cyber-based attacks relate to industrial hazards and provided a way to incorporate industrial process design into security analysis. When combined with risk-informed management methodologies, this STPA/BN-based approach offers a comprehensive risk-informed cybersecurity analysis that allows decision-makers to prioritize based on understanding the potential system-level risks. When combined with well-known cyber security methods (e.g., MITRE's ATT&CK framework), the approach could allow for predicting the difficulty of an attack—forming the basis of more justifiable and efficient designs to protect the electric grid and associated energy systems. (PI: Andrew Clark)



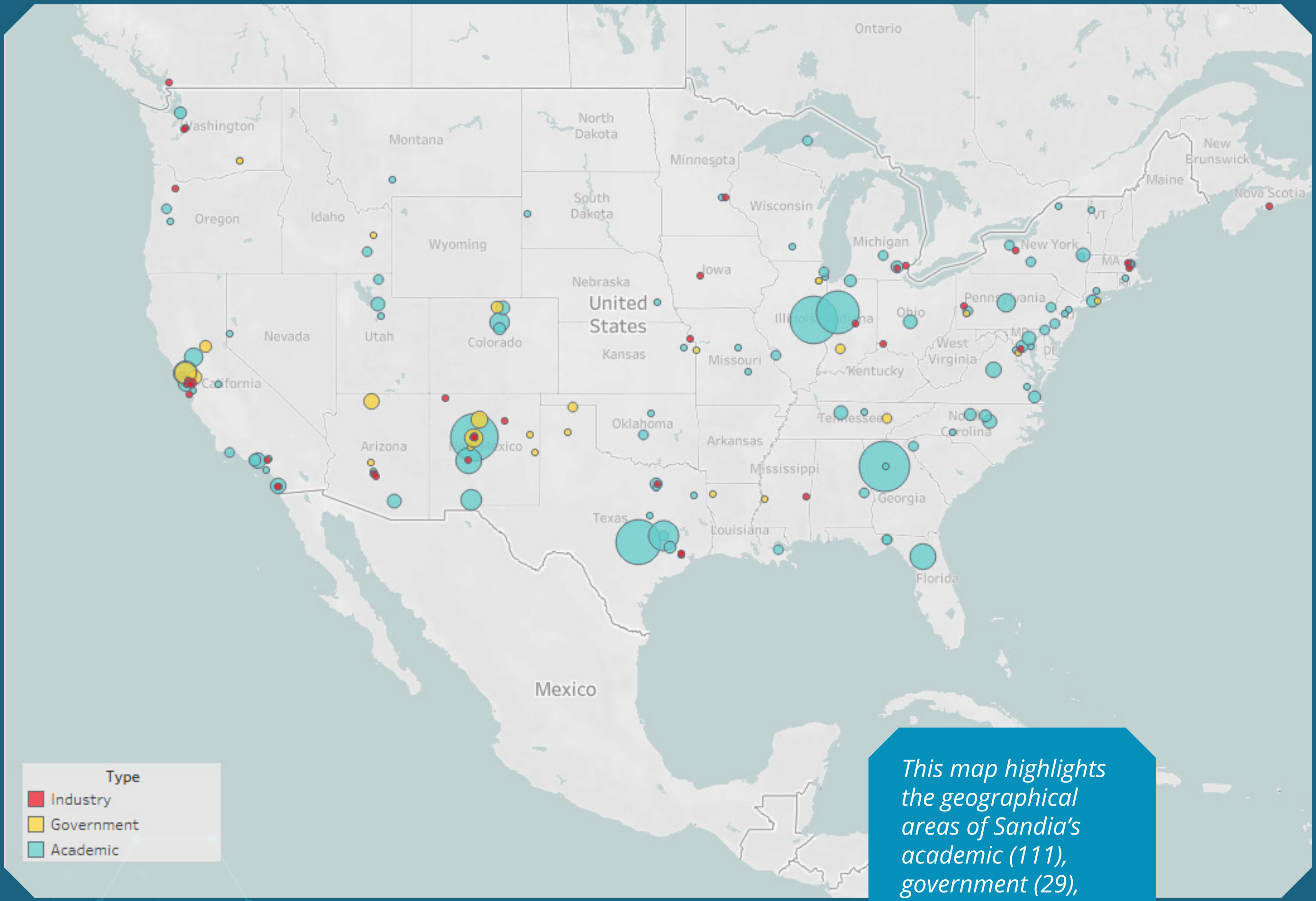
MITRE's ATT&CK framework in conjunction with cyber resiliency metrics and Bayesian Networks can be used to predict how an adversary accomplishes the unsafe control actions and the difficulty of an attack.

Sandia researchers Thushara Gunda, front, and Nicole Jackson examine solar panels at Sandia's Photovoltaic Systems Evaluation Laboratory as summer monsoon clouds roll by. Using machine learning and data from solar farms across the U.S., they uncovered the age of a solar farm, as well as the amount of cloud cover, have pronounced effects on farm performance during severe weather. (Photo by Randy Montoya)

Distributed energy resource honeypots and canaries. There are now over 2.5 million Distributed Energy Resource (DER) installations connected to the U.S. power system. These installations represent a major portion of American electricity critical infrastructure, so a cyberattack on these assets in aggregate would significantly affect grid operations. Virtualized Operational Technology (OT) equipment has been shown to provide practitioners with situational awareness and better understanding of adversary tactics, techniques, and procedures. Deploying synthetic DER devices as honeypots and canaries not only would open new avenues of operational defense and threat intelligence gathering, but also empower DER owners and operators with new cyber-defense mechanisms against the growing intensity and sophistication of cyberattacks on OT systems. Well-designed DER canary field deployments would deceive adversaries and provide early-warning notifications of adversary presence and malicious activities on OT networks. This Resilient Energy Systems LDRD team designed a high-fidelity, Python-based, cyber-physical DER honeypot/canary prototype that includes a SunSpec Modbus communication interface, which exposed data points for environmental, power system, and power electronics behaviors that mirrored physical DER equipment. To fully disguise and deploy authentic DER device technologies and to fool highly-sophisticated adversaries, further research is needed to increase realism in the communication systems, power conversion emulation, and unique environmental factors that dictate DER device behaviors. (PI: Jay Johnson)

Project Highlights - Workforce Development

Sandia's LDRD program enables principal investigators and research teams to collaborate with other national laboratories, academic institutions, and industry partners to revolutionize what is possible in science and engineering. This not only develops Sandia's workforce, but it also grows the nation's technical research capabilities overall, and even contributes to the economy. The highlights in this section are only a small subset of the impacts that have been made in 2021 through LDRD, but they give a glimpse of how significant the program is to the country and to the world.



This map highlights the geographical areas of Sandia's academic (111), government (29), and industry (46) LDRD collaborators during the 2021 fiscal year. The size of the circles corresponds directly to the number of collaborators of that particular type in a location.

International Awards

R&D 100 Awards

Sandia wins a record-setting seven 2021 R&D 100 Awards, four with LDRD roots.

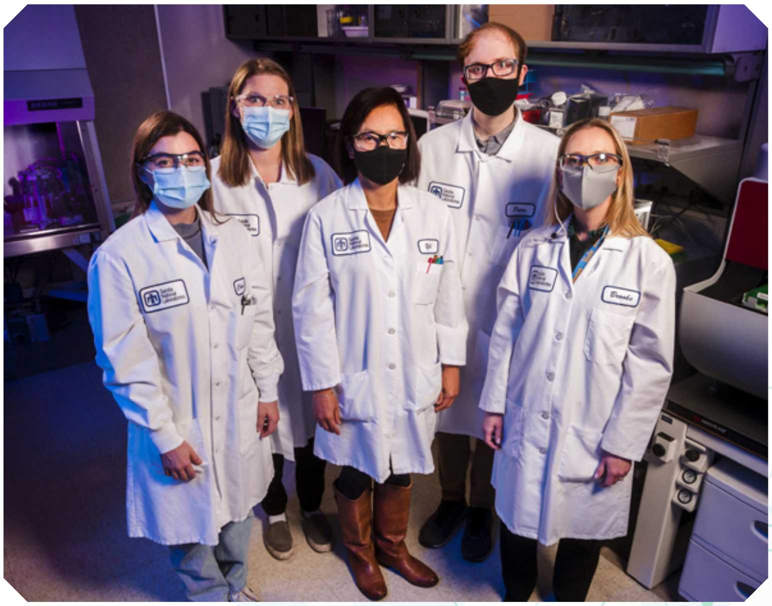
Sandia bested its own record in 2021 by winning seven R&D 100 Awards (one in conjunction with the National Renewable Energy Laboratory) and two specialty honors awards. For the nation, these awards indicate that the research and development done here, in support of the mission, is technologically significant and groundbreaking.

R&D 100 Award Winner

Extremely potent next-generation anti-COVID-19 neutralizing antibodies help create effective therapies.

Using a library of variable antibody fragments called nanobodies, Sandia researchers assembled extremely potent next-generation anti-COVID-19 neutralizing antibodies. The unique features of nanobodies offer easier manufacturability, increased versatility, smaller size, and the ability to bind to more than one target site to increase potency and resistance to viral mutants. Researchers have shown they can produce a nanobody-based countermeasure within 90 days, once a virus' genetic code has been identified. "Vaccines are very good at preventing infection, but they can take a long time to be developed and move through the regulatory process," principal investigator (PI) Brooke Harmon said. "We saw a critical need to create effective therapies that can be rapidly developed and deployed."

Sandia's research on nanobodies for emerging viruses also received acclamation at the 2021 National Lab Accelerator Pitch Event, where PI Brooke Harmon presented investors with business model ideas based on the innovations. View the award-winning presentation.



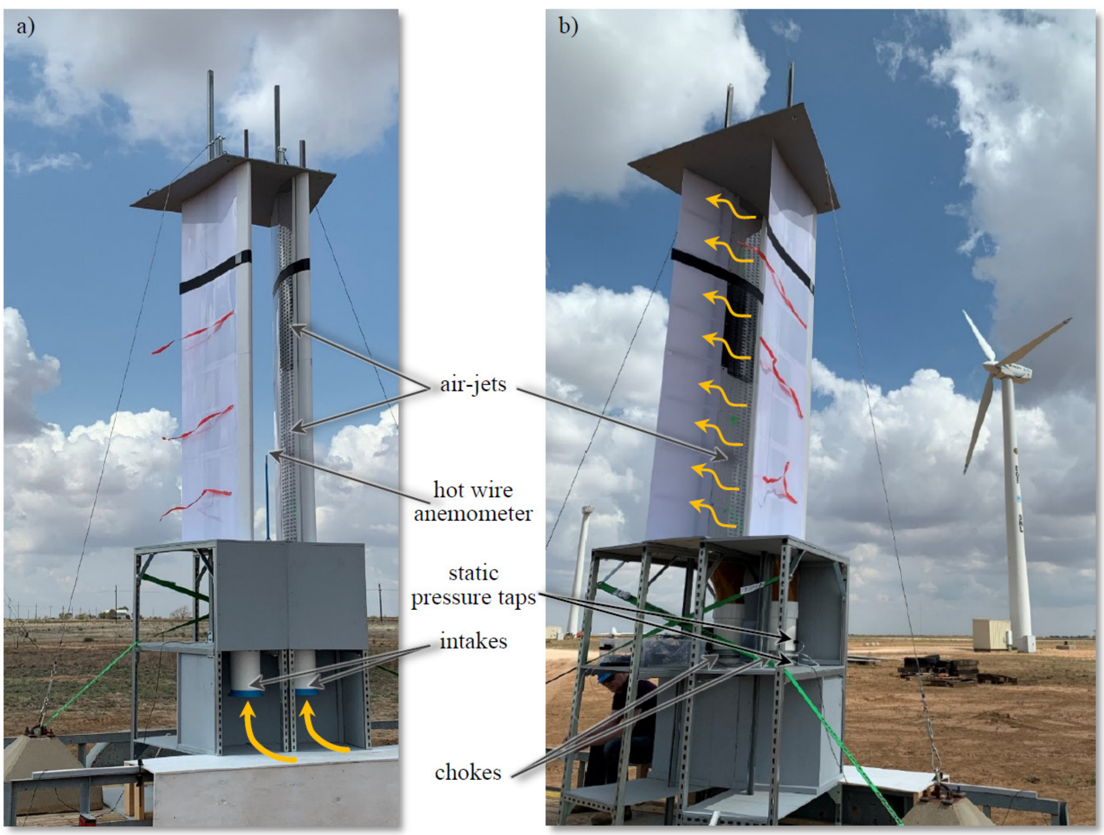
The research team filed for a patent on aspects of their work and are actively seeking commercial partners to help identify and engineer next-generation antibodies. (PI: Brooke Harmon) Watch the YouTube video.

The nanobodies research team from Sandia's Applied Biosciences and Engineering group developed a new process of screening for nanobodies that "neutralize" or disable the virus. This process represents a faster, more effective approach to developing nanobody therapies that prevent or treat viral infection. Pictured from left, Christine Thatcher, Jennifer Schwedler, Yooli Kim Light, Peter McIlroy, and Brooke Harmon.

R&D 100 Award Winner

AeroMINE opens up distributed wind power possibilities for rooftops and remote locations.

Distributed (point-of-use) wind energy has the potential to significantly increase world-wide green energy production and allow microgrids to supplement vulnerable electricity grids in many regions, but distributed point-of-use wind has remained an untapped market due to the weaknesses of distributed wind solutions. Enter AeroMINE (Motionless INtegrated Extraction). This stationary wind harvester can provide distributed electricity generation with no external moving parts. In 2020-2021, the LDRD project team, which included Texas Tech University and Westergaard Solutions Inc., built a pilot-scale (3 meters tall) AeroMINE at the Sandia Scaled Wind Farm Technology facility in Lubbock, Texas. Intern Elizabeth Krath, who has since joined Sandia as a postdoc to work on HydroMINE optimization, researched the optimal internal turbine design. Because AeroMINEs are incredibly resilient to environmental factors and require only minimal training to install, they can provide distributed wind-based power in underserved communities like coastal Alaska, the Arctic, and remote forward operating bases. Major project outcomes include the proof-of-concept at scale, the demonstration of negligible dependence to more than 30 degrees off-axis wind direction in low wind conditions, a 2021 R&D 100 Award, and a patent award (US 11,047,360 B1). (PI: Brent Houchens)
Watch the YouTube video.



Pilot-scale testing of a 3 meters (10 feet) tall AeroMINE at SWiFT shown from (a) in front and (b) behind.

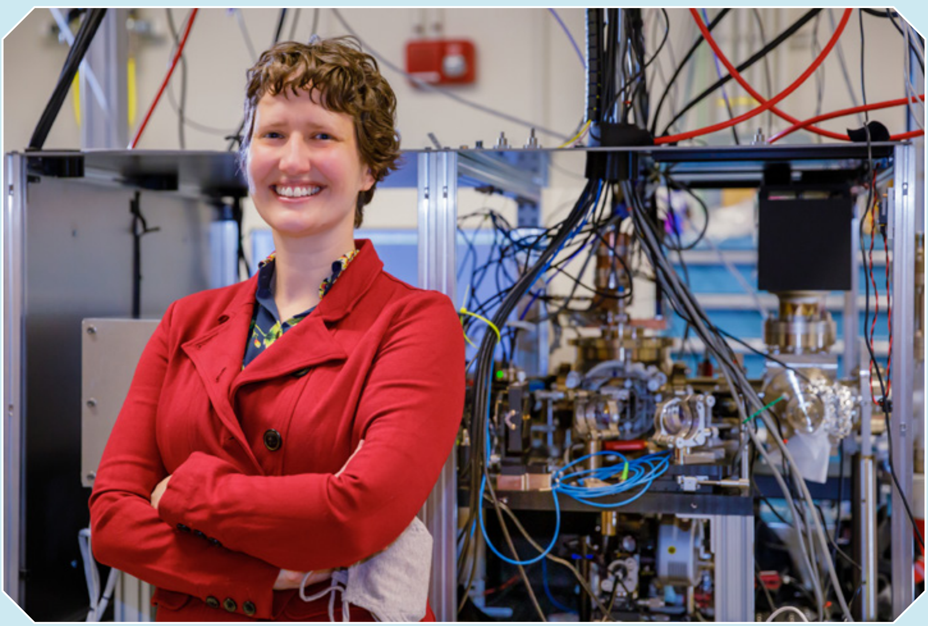
R&D 100 Award Winner

Quantum Scientific Computing Open User Testbed (QSCOUT) allows scientific community to study the quantum machine.

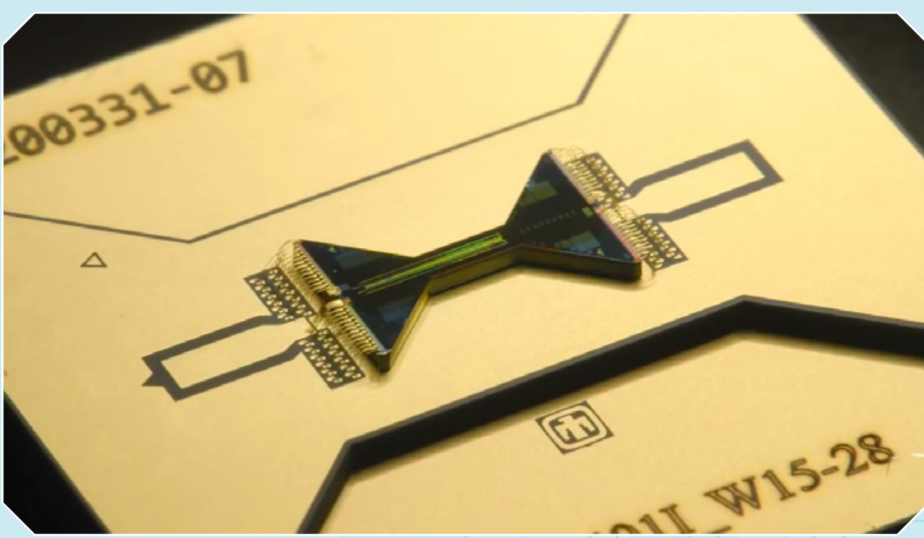
Quantum computing offers the allure of an exponential speed-up to the solution of important problems in an array of fields from basic science and medicine to national security. However, in order to realize the potential of quantum computing, research is needed not only on quantum devices and qubits but on quantum computers themselves. Now, for the first time, this has been made possible with QSCOUT.

The primary goal of the QSCOUT project is to build, maintain and provide access to a quantum processor based on trapped ion technology to the scientific community at large. QSCOUT has a rare design for a testbed—it uses what is called an ion trap. Trapped ions are held inside QSCOUT in a so-called "trap on a chip," a flat, bow tie-shaped device, about 2 cm (0.8 inches) long, overlaid on a semiconductor chip. This design means Sandia's testbed can run at warmer temperatures, plus trapped ions also yield clearer signals than circuits and hold on to information longer, enabling scientists to perform different types of experiments and compare the two platforms.

QSCOUT is a quantum computer for scientists, by scientists. (PI: Susan Clark) Watch the YouTube video.



Sandia physicist Susan Clark leads the team that built the Quantum Scientific Computing Open User Testbed. The ion-based quantum computer was made for outside researchers to use. (Photo by Bret Latter)



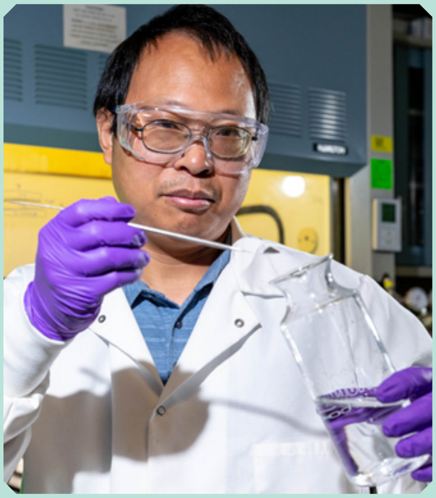
QSCOUT's ion trap uses an electromagnetic field to hold a chain of ytterbium-171 ions that function as qubits.

R&D 100 Award Winner

Slycat: Providing scalable ensemble analysis and visualization.
Traditional scientific visualization systems provide tools to explore and compare no more than a handful of simulation results at once. However, evaluating computational models through sensitivity analysis, uncertainty quantification, and parameter studies all require creating collections of runs, known as ensembles. Ensemble sizes can exceed 10,000 runs, each with hundreds of changing variables, plus multimedia outputs. So as the scale of ensemble data grows, ensemble-specific tools are needed to understand the results.

Slycat is a framework that addresses this capability gap by integrating data management, scalable analysis, abstract visual representations, and remote user interaction through a web-based interface. Slycat reduces data storage and movement costs by performing parallel analysis of the full data on the source cluster for the ensemble, then using the reduced-size analysis artifacts to model the ensemble on a Slycat server. Each Slycat model targets one or more specific result types, using multiple levels of abstraction to view the ensemble as a whole, results across variables, results between sets of runs, and components of individual runs. Slycat, inspired by an LDRD project led by PI Daniel Dunlavy in 2010, runs through a web-based interface designed for access-controlled collaboration between authenticated project members. Watch the YouTube video.

Members of the research team working on Slycat at Sandia. (Photo courtesy of Sandia)



R&D 100 Gold Special Recognition in Green Technology

Environmentally benign extraction of critical metals using supercritical CO2-based solvent.

Sandia researchers were recognized for a method that uses environmentally harmless citric acid in tandem with carbon dioxide to detoxify coal tailings by extracting critically needed rare elements and more harmful components at the same time. The extraction improves the environment instead of destroying it as conventional mining may do. (PI: Guangping Xu) Watch the YouTube video.

Sandia researcher Guangping Xu adds coal ash into a citric acid mixture. This solution will be fed into a reactor—operating at about 70 times atmospheric pressure—where supercritical carbon dioxide aids citric acid in extracting rare-earth metals. (Photo by Rebecca Lynne Gustaf)

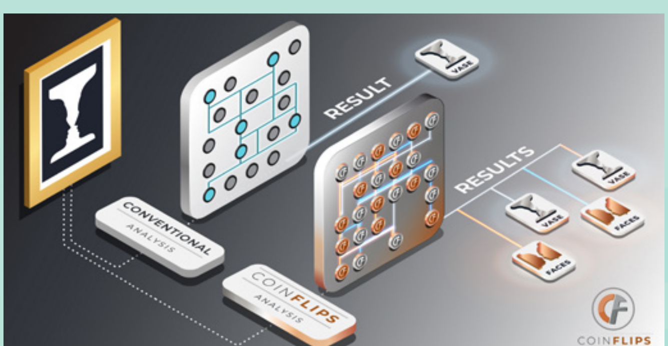
National/Federal Awards

2021 DOE Office of Science Award

Co-designed Improved Neural Foundations Leveraging Inherent Physics Stochasticity (COINFLIPS)

The COINFLIPS microelectronics co-design program, led by PI James Aimone, will receive $6 million over the next three years. The research, done in conjunction with Oak Ridge National Laboratory, New York University, the University of Texas at Austin, and Temple University in Philadelphia, will focus on designing a new kind of computer for solving complex probability problems. It is one of only 10 national laboratory-led projects selected for funding by DOE's Office of Science. "What we want to do in this project is to leverage randomness. Instead of fighting it, we want to use it." said Aimone, who has led many Sandia LDRD projects in the field.

Separately, Sandia is lending its expertise to two other projects selected for funding—one in nanotechnology and computer modeling led by Lawrence Berkeley National Laboratory, and another focused on improving the energy efficiency of information processing from sensors in autonomous vehicles, handheld devices and satellite led by Oak Ridge National Laboratory.



The 2021 COINFLIPS microelectronics co-design research program awarded for funding by DOE's Office of Science is a direct result of the successful workshop on AI-Enhanced Co-Design for Next-Generation Microelectronics that Sandia hosted April 2021.

Conventional computers can look at the optical illusion on the left and normally only see a vase or two faces. Sandia is laying the groundwork for a computer that, like our brains, can glance many times and see both. (Image by Laura Hatfield)

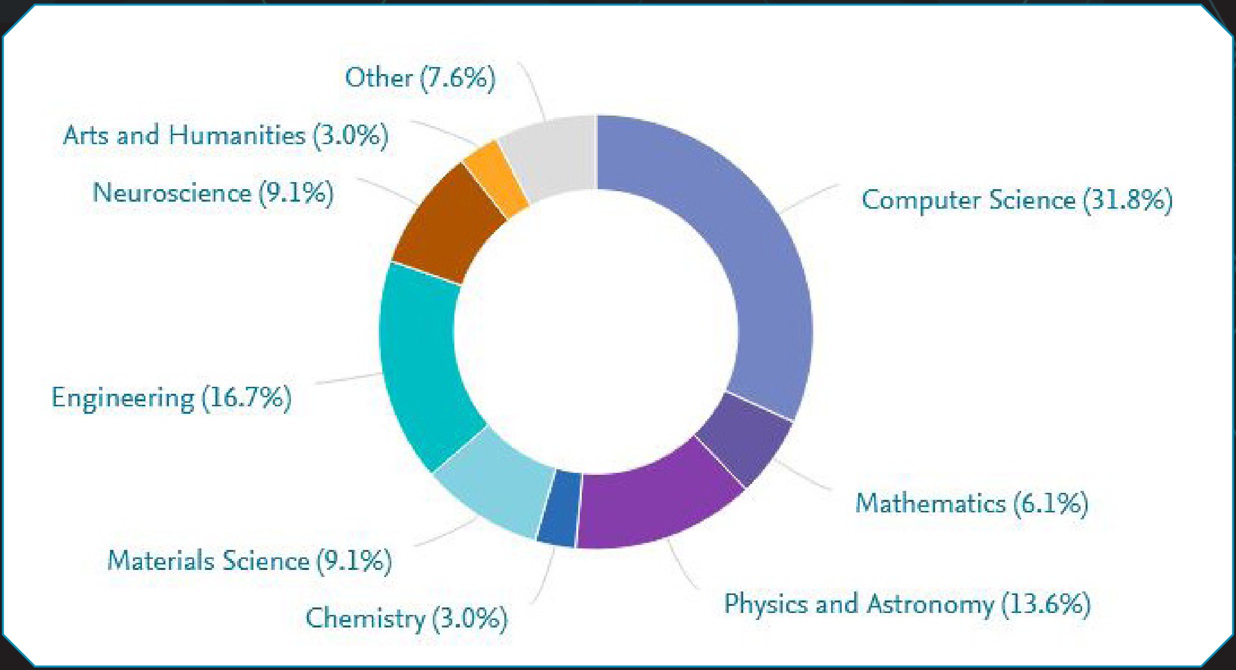
LDRD IMPACT STORY:

Hardware Acceleration of Adaptive Neural Algorithms (HAANA) Grand Challenge (2015-2017)

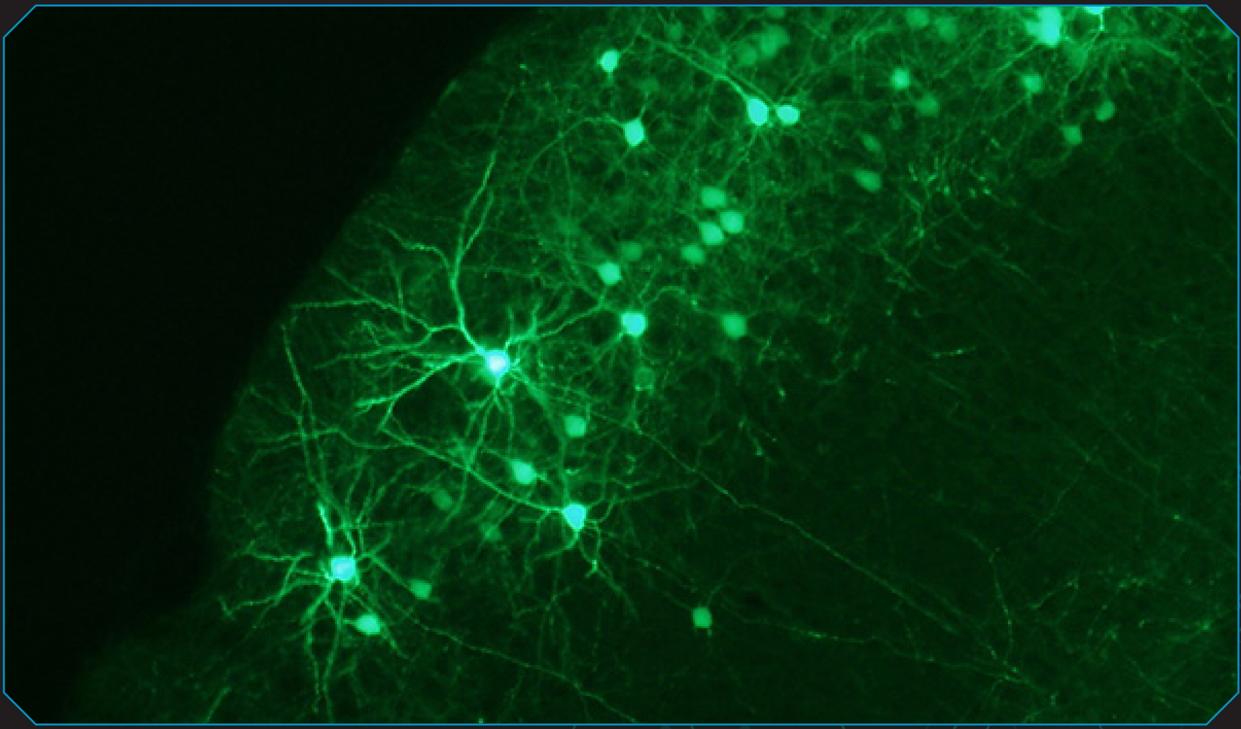
Situations are steeped in data. When computers are presented with a certain set of circumstances, microprocessors utilize programmed algorithms to synthesize the input and identify the best action to take in response. But as more variables are introduced, the data set grows exponentially, slowing down the system and response time. To solve the mounting problem created by big data, Sandia researchers, led by PI Conrad James, and academic partner, the University of Illinois Urbana-Champaign, conceptualized and developed a radical new approach. The new system integrated neural-inspired machine-learning algorithms with neural-inspired architecture cores, in conventional technology, allowing it to comb through large volumes of data and identify specific data patterns focused precisely on the activity of interest. The initial success of the endeavor, a Temporal Processing Unit, provided the nation with a mechanism for rapidly transforming raw cyber data into information for real-time, adaptive recognition and response, but the new technology also provided a neural network categorizer that spun off numerous other deliverables. Since 2015, the HAANA Grand Challenge has resulted in 19 worldwide patents, with 10 occurring in 2021 – one of those belonging to Sandia researchers, Matt Marinella and Sapan Agarwal (who originally hired in as a postdoctoral researcher to work on the HAANA Grand Challenge). Agarwal said of his experience, "When I joined Sandia, I was a primarily an expert in semiconductor devices. Through the HAANA GC, I was able to learn from neural algorithm and architecture experts and became an expert in multi-scale codesign of computing systems from material to algorithms. This [project] has provided me the opportunity to subsequently lead projects in the co-design of heterogenous radiation hardened systems, analog neural accelerators, solvers for linear systems and more."

The HAANA Grand Challenge has also resulted in more academic collaborations including a three-year LDRD project with the University of Texas at Austin, other workshops, and 39 publications directly associated with the effort.

> *"Through the HAANA GC, I was able to learn from neural algorithm and architecture experts and became an expert in multi-scale codesign of computing systems from material to algorithms."*



Twenty-four percent of publications from the HAANA Grand Challenge project ended up in the highest impact journals across numerous subject areas.

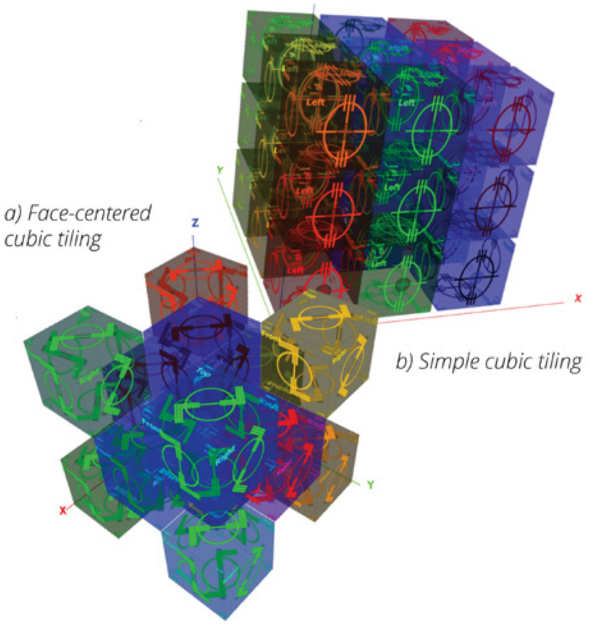


Sandia LDRD researchers are drawing inspiration from neurons in the brain, such as these green fluorescent protein-labeled neurons in a mouse neocortex, with the aim of developing neuro-inspired computing systems to reboot computing. (Photo by Frances Chance, courtesy Janelia Farm Research Campus)

2021 Federal Laboratory Consortium Mid-Continent Regional Awards

Sandia won three 2021 Federal Laboratory Consortium Mid-Continent Regional awards, two with roots in LDRD.

Excellence in Technology Transfer Award



MIRaGE, a futuristic design tool for metamaterials.
This research, rooted in a metamaterials science and technology Grand Challenge LDRD project, designs a metamaterial with comparable properties using scientific knowledge developed from molecular spectroscopy on how the symmetry of a natural molecule affects its optical behavior and properties. MIRaGE (PI: Ihab El-Kady) Watch the YouTube video.

Examples of 3D tiling options of metamaterial unit cells in MIRaGE.

Notable Technology Awards

Binary solvent diffusion for large nanoparticle supercrystals.
This project (rooted in LDRD) uses nanotechnology and chemistry to turn gold nanoparticles into supercrystals for optoelectronics, photovoltaics, and surface catalysis. (PI Hongyou Fan) Watch the YouTube video.

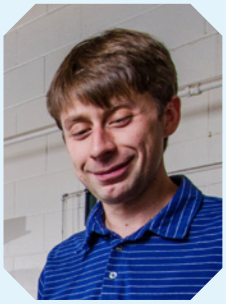
Prestigious Fellowships, Appointments and Memberships

Jim R. Stewart named Fellow of the U.S. Association for Computational Mechanics (USACM).

Jim R. Stewart was named USACM Fellow "for leadership and service to the USACM community, especially in the areas of uncertainty quantification and data-driven modeling." Stewart helps to guide the LDRD portfolio as an Advanced Science & Technology Mission Foundation IA team member.

Paul Kotula elected Fellow of the Microscopy Society of America (MSA).

Paul Kotula was elected MSA Fellow "for contributions to the field of statistical analysis of spectral data and dedicated long-term service to the Microscopy Society of America." Kotula served as a PI on an electronics and photonics LDRD project investigating correlated and comprehensive analytic techniques.



Justin Wagner named Associate Fellow of the American Institute of Aeronautics and Astronautics (AIAA).

Justin Wagner was named AIAA Associate Fellow for embodying the commitment, dedication, and ingenuity that are crucial for devising the best solutions to the complex questions raised in aerospace science. Wagner recently led an LDRD that developed a new capability to shock heat air and other gases to the extreme temperatures and pressures found in conventional explosive events.

Anne Grilled named Fellow of the American Institute of Chemical Engineers (AIChE).

Anne Grillet was named AIChE Fellow for advancing the understanding of battery performance, structure-function relationships in particle suspensions, and the manufacturing and aging of polymer gel systems. Her technical collaborations include leading numerous LDRD projects in Materials Science, Nuclear Deterrence, and Engineering Sciences research areas. An advocate for women in engineering and science, Grillet is also a leader of AIChE's Women in Chemical Engineering Committee.

Early Career Awards and Honors

Drew Kouri receives DOE Early Career Research Award.
Drew Kouri received the FY21 DOE Early Career Research Award for his Advanced Scientific Computing Research proposal on adaptive and fault-tolerant algorithms for data-driven optimization, design and learning. Since 2015, Drew served as PI for several LDRDs, including his current project focused on the fusion of simulation and experimental data.

FY21 Hruby and Truman Postdoctoral Fellowships

Jill Hruby Postdoctoral Fellowship

The LDRD-funded Jill Hruby Postdoctoral Fellowship was established in 2017 to encourage outstanding women with PhDs in technical fields to consider leadership in national security. Jill Hruby, the Under Secretary of Energy of the United States, was the first woman to lead a national security laboratory and served as Sandia's director from 2015 to 2017.

Elizabeth "Bette" Webster – FY21 Hruby Fellow
Bette Webster focused her PhD research at Stanford University on viral membrane platforms and host-pathogen interactions. Her work in fundamental studies is focused on gaining a better understanding of membrane entry mechanisms, which then can be used in technologies to address future viral threats. Bette has been widely published in journals such as *ACS Central Science, The Journal of Physical Chemistry C, Journal of the American Chemical Society*, and *Energy & Fuels*. Her fellowship research at Sandia's Biotechnology and Bioengineering department focuses on developing model membrane platforms to characterize enveloped virus entry and membrane-based delivery systems.

(Photo by Randy Wong)

Harry S. Truman Postdoctoral Fellowship

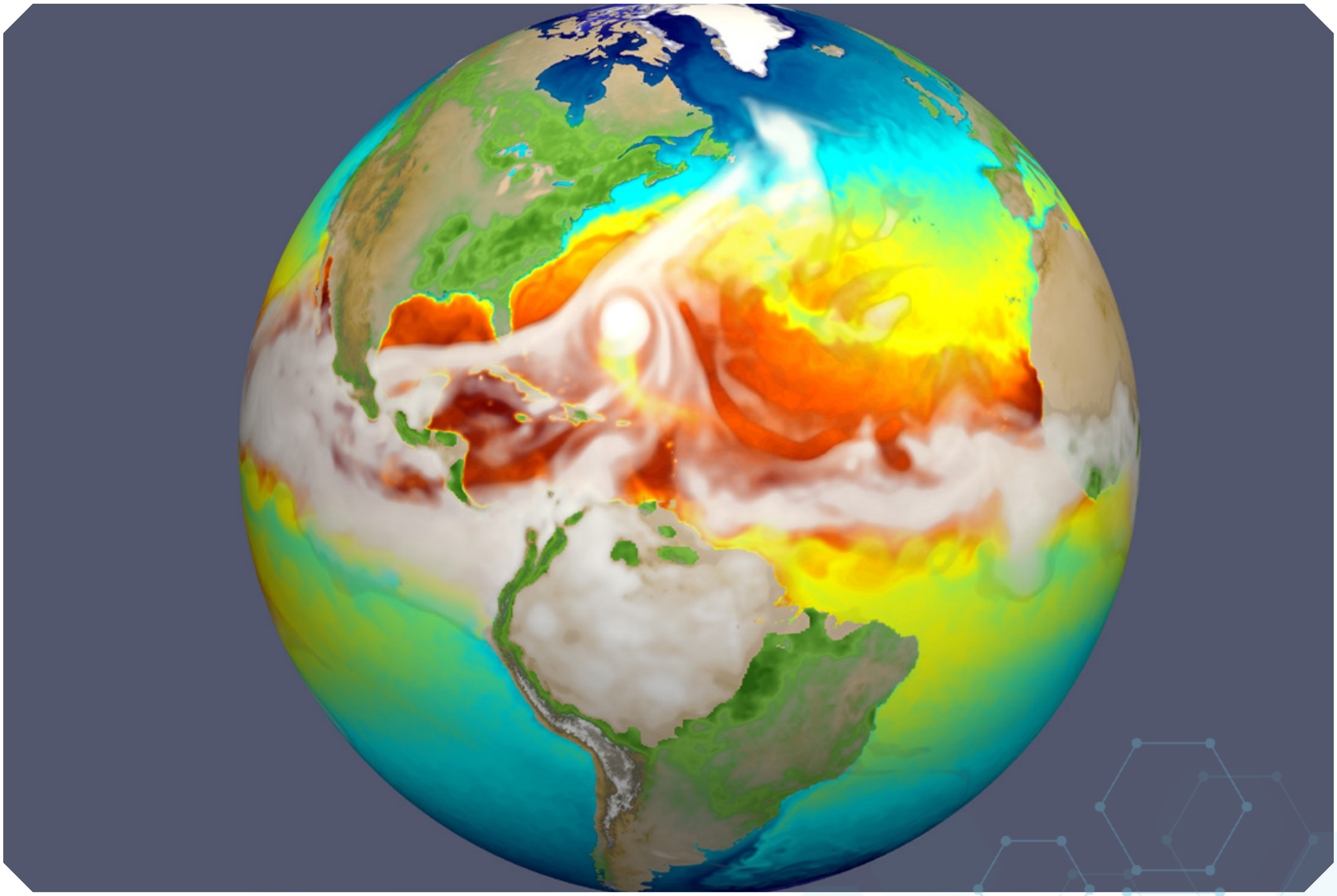
Sandia established the three-year fellowship, funded by LDRD, to attract the nationally recognized PhD scientists and engineers. Truman Fellows conduct independent groundbreaking research that supports Sandia's national security mission.

Nils Otterstrom – FY21 Truman Fellow
Nils Otterstrom received his PhD in Applied Physics at Yale, and his research focuses on harnessing inter-modal nonlinearities for flexible room temperature integrated quantum photonics. He has published in numerous journals including *Optica, Science Advances, APL Photonics, The Journal of Lightwave Technology*, and *Science Advances*. His most recent article, "Electrically Driven Acoustic-optics and Broadband Non-reciprocity in Silicon Photonics" was published in *Nature Photonics* in 2021.

(Photo by Randy Montoya)

Aaron Sharpe – FY21 Truman Fellow
Aaron Sharpe obtained his PhD in Applied Physics from Stanford with an expressed interest in condensed matter physics. His research into graphene superlattices has resulted in the discovery that graphene can become both a superconductor and a ferromagnet (a tunable platform). His work has been published in *Science, Nature, Physical Review Letters, Nature Communications*, and most recently in *Nano Letters* with an article focused on "Evidence of Orbital Ferromagnetism in Twisted Bilayer Graphene Aligned to Hexagonal Boron Nitride."

(Photo by Randy Wong)



Kelsey DiPietro, a Hruby Fellow who started at Sandia in FY20, is applying her computer model method to climate research, working with the Energy Department's supercomputer-powered Energy Exascale Earth System Model, or E3SM, which already has one of the finest resolutions ever achieved for simulating aspects of the planet's climate.

Professional Society and Conference Awards

Society of Women Engineers (SWE) Achievement Awards

Laura Biedermann, a Sandia physicist, received a 2021 SWE Spark Award for her mentoring work in co-founding the Principal Investigator Workshop in 2013 and co-creating Sandia's Peer Mentoring Steering Committee in 2016. Biedermann evaluates electrical conduction mechanisms in novel materials, investigates interactions between X-rays and materials, and conducts material aging and reliability studies, and she led projects across eight LDRD investment areas. Biedermann stated, "It is very important to not only have a strong technical depth in your field, but also to be exposed to the breadth of research and mission work at Sandia."

Photo by Lonnie Anderson

Annie Dallman, a Sandia mechanical engineer, received a 2021 SWE Distinguished New Engineer Award for her outstanding technical performance and contributions to several fields, and her leadership in SWE. She joined Sandia as a postdoctoral researcher in renewable energy and has applied her expertise in modeling and simulation, fluid dynamics and data analysis to other areas such as nuclear nonproliferation. Dallman, who has worked in a variety of research areas at Sandia, has acted as PI for several LDRD projects.

Photo by Lonnie Anderson

Black Engineer of the Year (BEYA): Most Promising Scientist — Professional Award

LaRico Treadwell is a chemist at the Advanced Materials Laboratory, who has led multiple LDRD projects at Sandia. His work covers the materials science spectrum, from basic materials discovery and characterization through applied materials reliability and device fabrication for a wide range of applications, including radiation, ultra-high-temperature systems, non-linear optics and thermo-electrics. His research advances science frontiers in chemistry, engineering, materials, and component reliability.

Black Engineer of the Year (BEYA): Modern Day Technology Leader Award

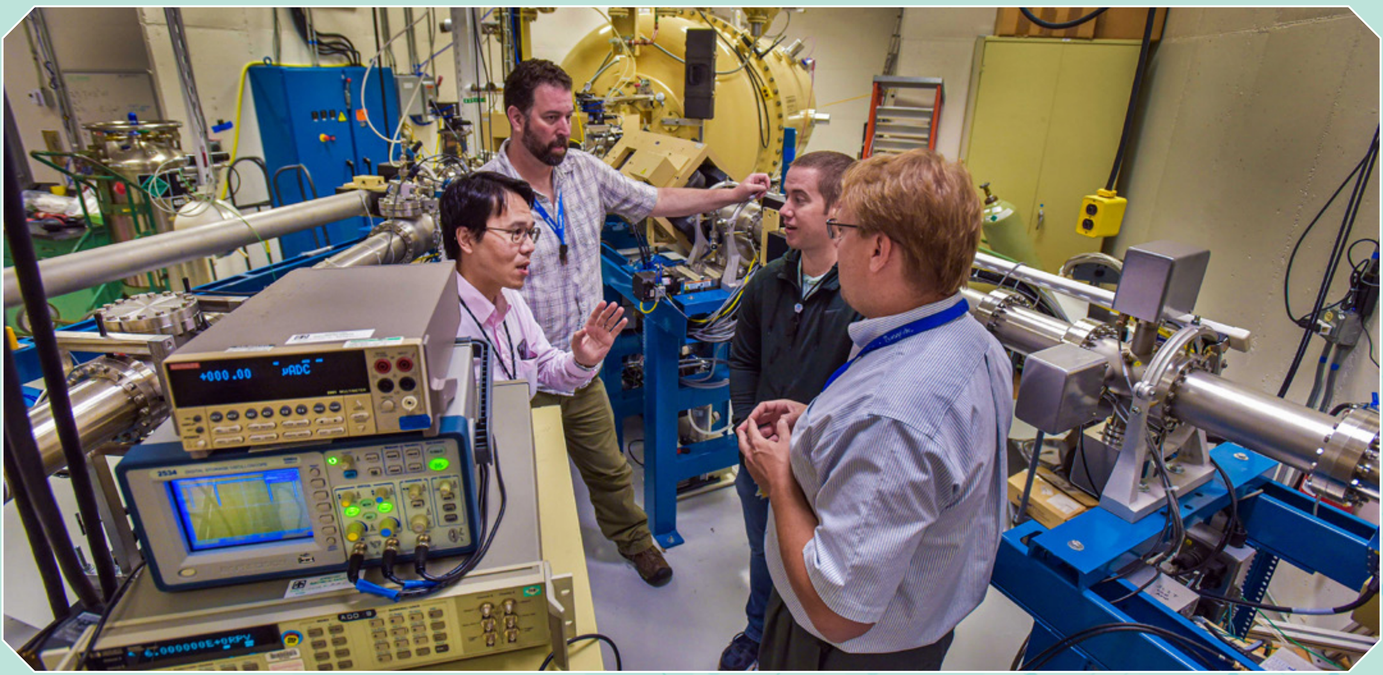
Uzoma Onunkwo, an electrical and computer engineer, leads efforts in cutting-edge research and development spanning high-speed data analytics, streaming machine learning, large-scale wireless network simulation and quantum information science. His work in multithreaded coding, data structure and algorithms, queue management and compiler optimization accelerated new analytics on high-speed streaming data while protecting government computer networks. He has achieved notable success as a PI in several LDRD areas.

Black Engineer of the Year (BEYA): Science Spectrum Trailblazer Award

Adam D. Williams, a systems engineer has made significant contributions incorporating systems-theoretic concepts, frameworks, and analysis techniques into Sandia's national-security mission areas. Williams, who led LDRD projects focused on global security, applied his technological aptitude to conduct high-consequence facility vulnerability assessments, design physical protection systems, analyze geopolitical implications of global energy development and support various global security engagement opportunities. He co-developed an analysis technique that is advancing cybersecurity for U.S. interests.

Society of Asian Scientists and Engineers Professional Achievement Award

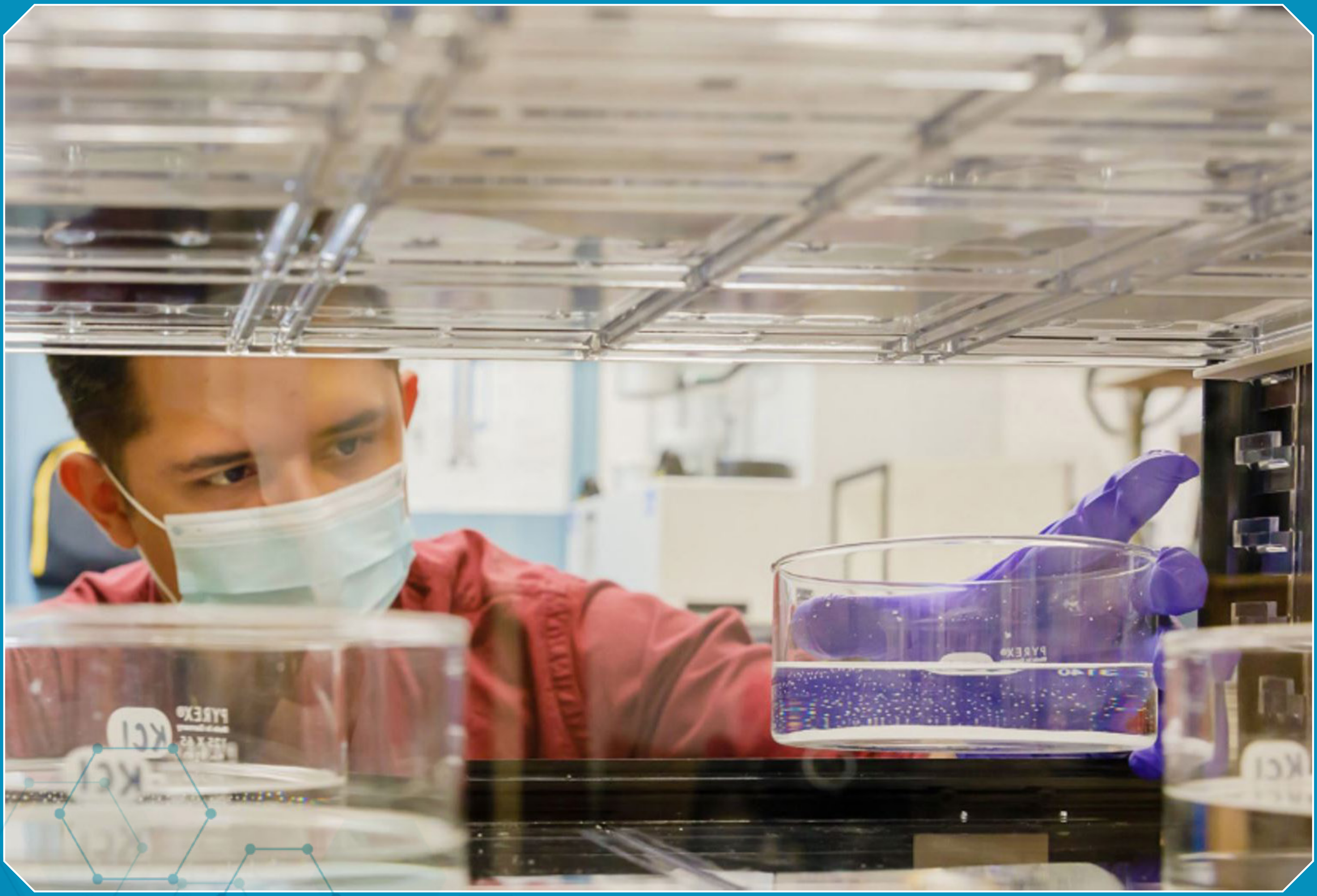
Yuan-Yu Jau, an atomic physicist, was nominated by Sandia Director James Peery for his extensive technical work and expertise. He has acted as PI for numerous LDRD projects across multiple investment areas, and his publishing record includes more than 40 high-impact, peer-reviewed papers primarily in *American Physical Society* journals, including *American Institute of Physics*, *Optical Society of America* and *Nature Portfolio*. He co-authored the foundational book "Optically Pumped Atoms," and his published work has been cited more than 2,000 times.



Sandia researchers, from left, Yuan-Yu Jau, George Burns, Justin Christensen and Ed Bielejec plan to test a future neutron generator for an electric-field imaging system at Sandia's Ion Beam Laboratory, pictured here. (Photo by Randy Montoya)

Hispanic Engineering National Achievement Award

Michael Omana, a mechanical engineer and aerosol and filtration scientist, was named a 2021 Most Promising Scientist, Masters. Omana spent the past year-plus serving as an aerosol and filtration science subject matter expert for numerous COVID-19 response efforts, including working with a team who developed a disposable respirator early in the pandemic made from materials not already used in the supply stream to sidestep the shortage of medical-grade personal protective equipment available to healthcare workers. Additional work in mask development yielded a reusable respirator that filters both inhaled and exhaled air with easily replaced N95 filter material stored inside two disc-shaped cases, protecting wearers and patients. Omana recently concluded a three-year LDRD using his expertise in aerosols.



Honors and Distinctions

Steve Slutz received the 2021 Distinguished Career Award from Fusion Power Associates in recognition of more than forty years of innovative as a theorist in Inertial Confinement Fusion (ICF) research. His LDRD work in pulsed power and high yield fusion is ground-breaking. His invention of the Magnetized Liner Inertial Fusion concept is now a leading approach to ICF.

Steve Beresh received the American Institute of Aeronautics and Astronautics (AIAA) Sustained Service Award for significant service and contributions to AIAA. Beresh has led LDRDs focused on hypersonic flows at Sandia.

Paul Clem, a materials physicist, received the 2020-2021 Distinguished Alumni Award from the University of Illinois Department of Materials Science & Engineering. His extensive LDRD work has crossed six research investment areas at Sandia and garnered a Federal Laboratory Consortium Award.

David Rademacher received the UNM Sigma Xi Chapter, "Noteworthy Technical Support Person Award" and Associate Membership in the Society. The award honors Rademacher's excellent record of helping staff mentor early career researchers in their projects, operating labs with exemplary safety practices, and providing vital technical support for realizing successful high impact scientific results. He assisted with an LDRD focused on tunable impedance spectroscopy sensors most recently.

Erica Redline was recognized as a 125th Anniversary Fellow for the College of Earth and Mineral Sciences at Penn State. Penn State selected a small group of dedicated alumni whose contributions to the fields of science and engineering have set them apart from their peers. She led LDRD projects in Materials Science and Nuclear Deterrence research areas at Sandia.

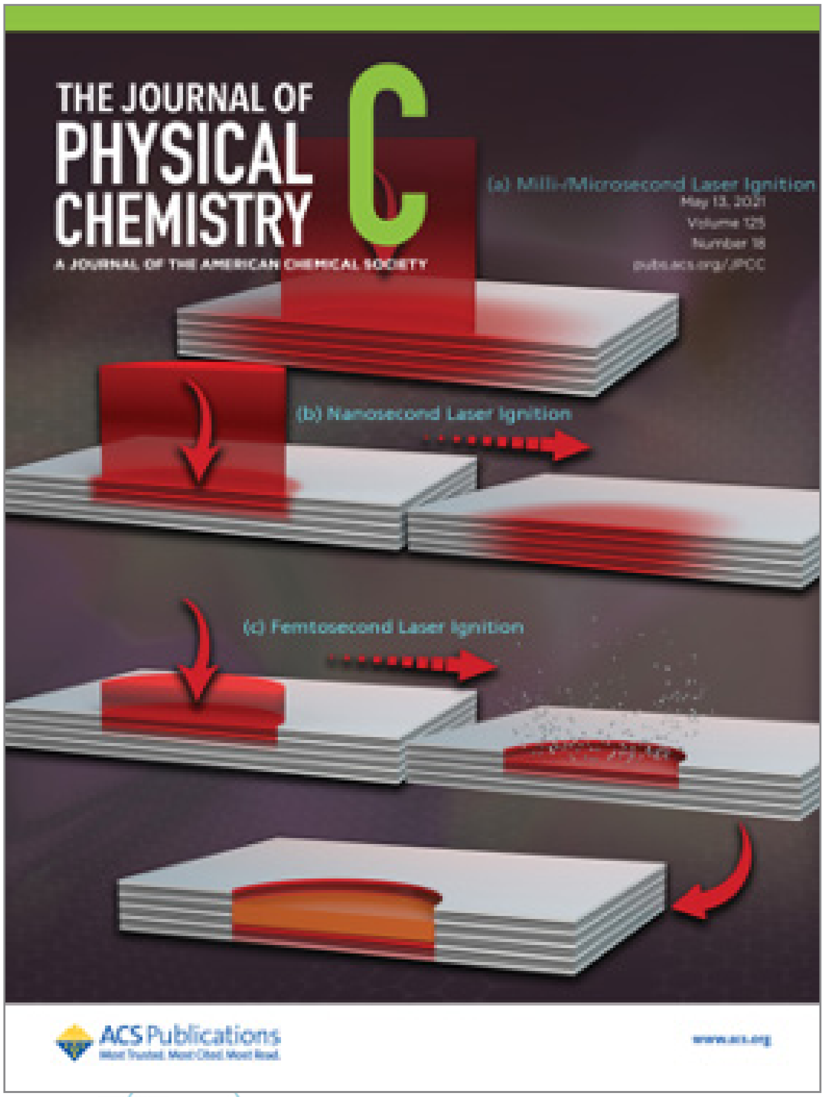
David Ching, a mechanical engineer and an early career staff member at Sandia, was recognized for significant contributions to hypersonics LDRD research.

Phillip L. Reu and Daniel P. Rohe co-authored a chapter on digital image correlation and photogrammetry in the recently published book, Handbook of Experimental Structural Dynamics. Reu has led LDRDs on materials reliability for Sandia.

Dolores Black, a PI for numerous LDRDs focused on radiation, electrical, and high energy density science, was invited to be the 2025 Nuclear and Space Radiation Effects Conference general chair.

Stephanie Hansen was elected to the National Ignition Facility User Executive Board. Hansen, an active LDRD PI, has led projects on improving predictive capabilities and the creation of a constitutive framework for multiphysics.

Michael L. McLain was elected vice-chair of the Hardened Electronics and Radiation Technology steering committee. McLain was a PI for several LDRD projects focused on radiation effects and high energy density science.



Nicholas Argibay, Michael Chandross, and Andrew Kustas were featured in *Industrial Heating*, where they describe their success in developing a new alloy with an extraordinary combination of mechanical properties. Each have been successful LDRD PIs in Materials Science and other Sandia research areas.

An article, "Variable Laser Ignition Pathways in Al/Pt Reactive Multilayers across 10 Decades of Pulse Duration," was published in *The Journal of Physical Chemistry C*. An illustration from this article, focused on the results from a Sandia LDRD project, was selected as the journal cover art.

ABSTRACT

This report provides an assessment of the value of the LDRD program to Sandia National Laboratories during fiscal year 2021.

2021 LDRD TEAM

Susan Seestrom, Basil Hassan, Wahid Hermina, Leigh Cunningham, Marie Arrowsmith, Ladonna Martin, Jenni Pandazis, Nicole Seay, and Amy Treece

Issued by Sandia National Laboratories, a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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