RESEARCH

LABORATORY DIRECTED
RESEARCH & DEVELOPMENT
FY20 ANNUAL REPORT

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

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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Laboratory Directed Research and Development FY20 Annual Report

From the Chief Research Officer

It often takes unprecedented times to achieve unprecedented success. During 2020, the national labs pivoted to meet the numerous challenges brought about by the COVID-19 pandemic. As CRO of Sandia National Laboratories, I'm privileged to see groundbreaking research every day, but it was my great honor in 2020 to see our staff meet critical needs with such exceptional speed and creativity. On March 15, one day after the national emergency announcement, Sandia finalized an integrated process to help direct research and development ideas to senior research leaders who could help vet their potential. Two days after the emergency announcement, I sent a memo to the 14,000+ individuals in our workforce asking them to submit revolutionary concepts that could potentially help our country. Within hours, proposals flooded the system. LDRD played a huge role during this time because innovation is at the very heart of the program.

Sandia's LDRD program fosters an environment conducive to innovation and mission success. When we read about new medical therapies, satellite systems, distributed energy technologies or radiation sensors, we rarely stop to consider their origin stories or the numerous components needed to pull off such advances. Discovery science is an essential ingredient in each recipe. It takes researchers and teams working on transformational science, technology, and engineering projects to fuel these innovations.

LDRD is inherently high risk and high reward. To achieve new techniques or create new applications, it takes knowledge, creativity, and a bit of fearlessness. The most successful innovators recognize that failure is part of the creative process. Projects that do not work as expected are not failures if they add knowledge and enable researchers to move on to ideas that may succeed; the only real failure is failing to try.

At Sandia, our principal investigators (PI) and LDRD teams see a bigger picture. The national labs are entrusted to deliver solutions for nuclear deterrence, national security, energy security, nonproliferation, and counterterrorism, among others. We are called on to combat climate change, guard the nation's data, protect our grid, advance energy storage, and combat terrorism in its many forms. Many of the new materials, forward-thinking prototypes and significant breakthroughs needed to fulfill these missions happen through LDRD.

Our nation's priorities are shaped by a changing global landscape; this is why we need to recruit and invest in inspired, innovative engineers and scientists. It's their leading-edge research and development ideas and our rigorous internal LDRD framework and strategic priorities that allow us to thoughtfully respond. During the 2020 fiscal year (FY), 672 idea proposals were submitted. Of those, 283 were invited to submit full proposals, and 172 new projects were funded. When added to ongoing projects and late-start projects, there were 447 active projects in FY20.

The FY20 LDRD Annual Report touches on many of the technological advances, awards, and patents achieved by Sandia's LDRD teams who rise up to meet today's emergencies while contributing to capabilities that will one day revolutionize the world.

Susan Seestrom

Chief Research Officer
Associate Laboratories Director
Advanced Science and Technology

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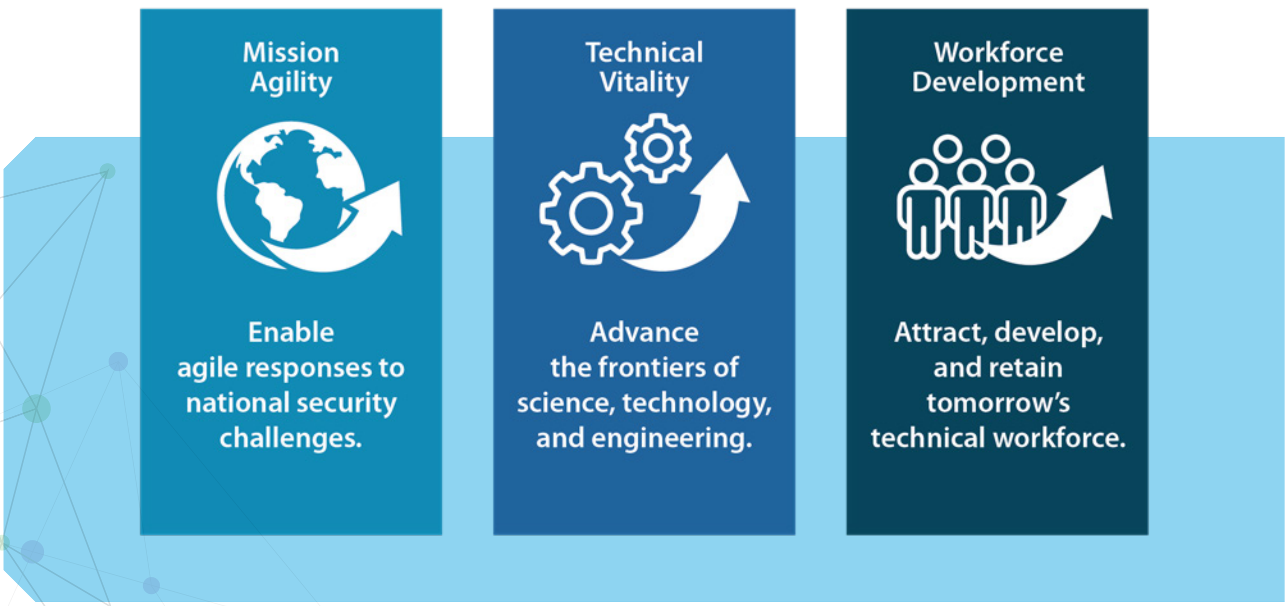
LDRD PROGRAM DESCRIPTION

Sandia is a federally funded research and development center (FFRDC) focused on 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 academia and industry.

Sandia's LDRD program maintains the scientific and technical vitality of the Labs and enhances the Labs' ability to address future national needs. The 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.

LDRD PROGRAM OBJECTIVES

Sandia's LDRD objectives guide the program overall and 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.

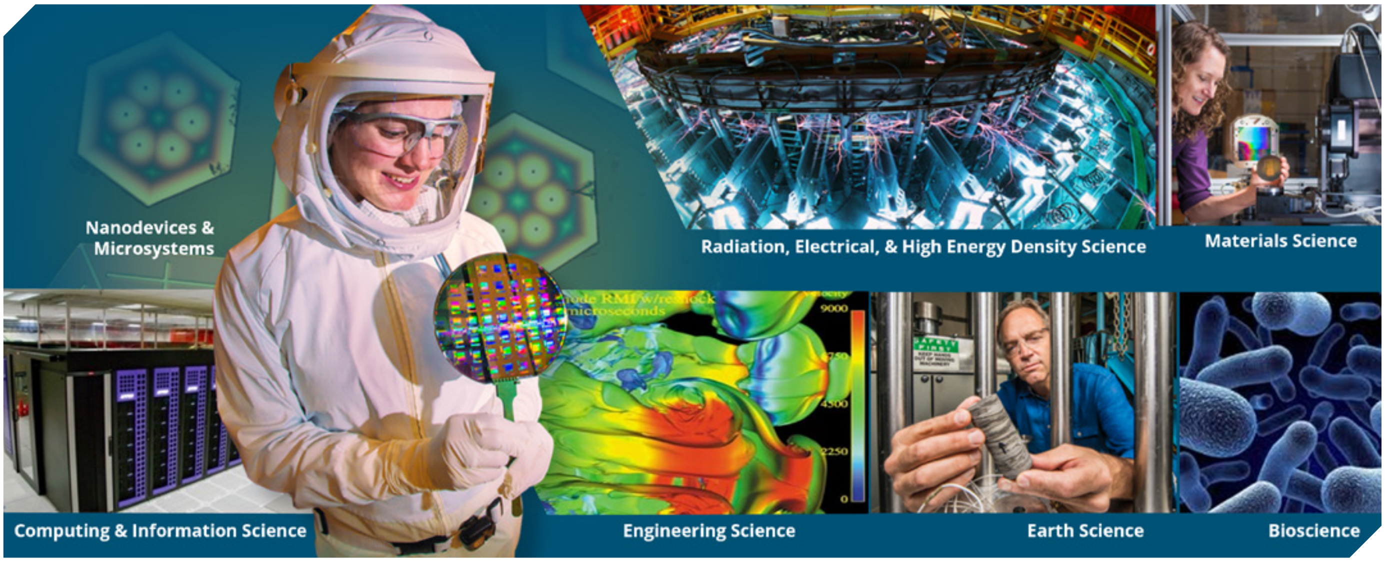


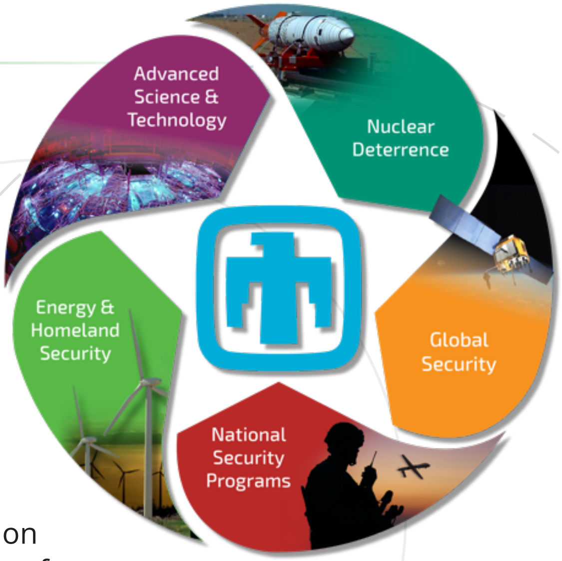
SANDIA'S LDRD PROGRAM STRUCTURE

Sandia's LDRD investments are structured around three Program Areas, which are further broken down into Investment Areas (IAs). Each IA is focused on discipline- or mission-based research priorities set by Sandia's leadership. The LDRD program structure and the allocation of funds to the associated IAs are designed to align LDRD investments with Sandia strategy and future national security mission needs.

LDRD INVESTMENT AREA ROLES

Research Foundations steward discipline-based science, technology, and engineering (ST&E) competencies that address the extensive national security challenges within Sandia's mission space. Each of the seven Research Foundations focuses on stewarding differentiating or unique capabilities.





Mission Foundations address national security mission challenges. LDRD Mission Foundations align with the five Sandia mission portfolios and conduct the applied research needed to develop capabilities and demonstrate solutions.

Strategic Initiatives promote strategic collaborations and CRO/Labs-directed initiatives. Strategic Initiatives include Grand Challenges projects (developing bold solutions to address major research challenges that require large multidisciplinary teams), Mission Campaign IAs (bridging ST&E to move intentionally from idea to mission impact), Exploratory Express (executing short-term projects of strategic importance), and New Ideas (pioneering fundamental R&D to discover game-changing breakthroughs). These initiatives also support strategic academic collaborations, and the Truman and Jill Hruby, and Foundation Postdoctoral Fellowships.

LDRD PROGRAM VALUE

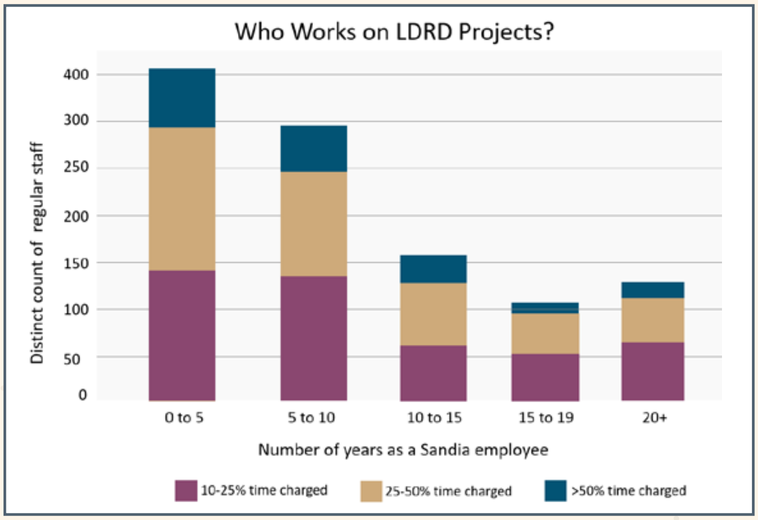
PERFORMANCE INDICATORS

While the FY 2020 LDRD program represented only about 5.4% of Sandia's total lab costs, the metrics shown below highlight how LDRD has a much larger relative impact on key performance indicators and metrics for the lab. The bar graph demonstrates the large percentage of early career staff, postdocs and students engaged in the LDRD program, validating the important role LDRD plays in attracting, developing, and retaining a world-class workforce to meet our most challenging national security needs.

FY 2020 LDRD Program Statistics

$188.9M	$354K	447	257
Total Program Cost (not including PM costs)	Median Project Size	Total LDRD Projects	New Projects in FY20

LDRD Participants



LDRD-Supported Postdocs	163	46% of Sandia total
LDRD-Supported Postdoc to Staff Conversions	25	53% of Sandia total
Refereed Publications	366	26% of Sandia total
Technical Advances	121	37% of Sandia total
Patents Issued	67	51% of Sandia total
Copyrights	40	24% of Sandia total
R&D 100 Awards	4	57% of Sandia total

...the large percentage of early career staff, postdocs and students engaged in the LDRD program...

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 will be updated annually. Data is expected to vary from year to year, so long-term running totals are also included and will be updated every five years.

Background

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

Alignment with LDRD Objectives

The collective selection of indicators (both numerical and qualitative) illustrate the long-term payoffs/success of LDRD, with respect to all three LDRD objectives (Technical Vitality, Mission Agility, Workforce Development). Since indicators crosscut objectives, a 1:1 mapping of indicators with objectives isn't possible.

Importance of Qualitative Data

The difficulty of developing numerical indicators for success in R&D programs is widely recognized. While the working group developed numerical success indicators for both Technical Vitality and Workforce Development, the team determined that "success or impact stories" best demonstrated the successes in Mission Agility, as well as some aspects of the other two LDRD objectives not well-captured by numerical metrics.

Tracing Impact Back to LDRD

When there are references to an accomplishment (invention, paper, capability, etc.) having "LDRD roots," it means one or more previous LDRD projects had a critical influence on the development. In the simplest scenario, if an idea for an invention arose during an LDRD project, and the team completed development during the period of LDRD investment, then the accomplishment would have LDRD roots. However, R&D doesn't typically advance on such a short timescale. Many times, current impacts are the result of technological gains achieved through LDRDs in prior years.

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

THE INDICATORS

Professional Fellows (American Physical Society)

One relevant indicator of advancement and leadership in a ST&E field is the election of individuals as fellows of professional societies. This indicator reflects success for both the researcher and the laboratory as a whole. American Physical Society (APS) Fellows were selected as the exemplar due to the important linkage of physicists with NNSA's core stockpile stewardship mission. Furthermore, APS Fellowships are awarded based on scientific merit and impact over an extended period of time. (In contrast, some professional societies may also award fellow status based on service to the society.)

Because of Sandia's unique role as a premier engineering and science laboratory, there are relatively fewer APS Fellows when compared to the NNSA physics laboratories. Of the three Fellows elected in the past three years, all of them had LDRD experience. Over the past ten years, over 80% of Sandia's APS Fellows had LDRD experience.

LDRD and American Physical Society Fellows at Sandia National Laboratories

	Single Years			Five Years		To Date*
	FY18	**FY19**	**FY20**	**FY11-15**	**FY16-20**	**FY11-20**
Total Awards	1	2	0	12	10	22
Awards with LDRD Roots	1	2	N/A	9	9	18
% with LDRD Roots	100%	100%	N/A	75%	90%	81%
Average Years from First LDRD Experience	22.0	12.0	N/A	14.7	13.0	14.8

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

APS Fellow Highlight

Senior staff emphasize the importance of LDRD in their early careers at Sandia. They also mention how LDRD seeds the cutting-edge R&D that helps motivate nominations and elections to prestigious societies, such as APS.

One example is that of Amalie Frischknecht, who was named an APS Fellow in 2012. Amalie is a Principal Member of Technical Staff at Sandia and a staff scientist at the Center for Integrated Nanotechnologies. She was nominated to APS for outstanding contributions to the theory of ionomers and nanocomposites, including the development and application of density functional theory to polymers.

Amalie Frischknecht, APS Fellow in 2012

"LDRD has been important, especially in my early career at Sandia. A large LDRD project ($2.8M total) that I obtained (as PI) in FY10 launched one of my major research areas and supported a great team including an excellent postdoc, who is now tenured faculty at The Ohio State University. The size of this project, which supported both computational and experimental work as well as multiple postdocs and students (through university collaborations), allowed us to make progress in this area and establish expertise. The research done under this LDRD project was an important part of my successful nomination as an APS Fellow. This large LDRD launched a line of research that has continued to the present through funding from the Center for Integrated Nanotechnologies (CINT). A paper supported by that FY10-FY12 LDRD and published in the Journal of the American Chemical Society is currently my most-cited paper, with 123 citations. While my continued success in research is due mostly to CINT, which supports long-term basic research, I have also remained engaged with LDRD, either as a PI, team member, or Truman Fellow mentor, continuously since I became a staff member in 2003 through the present."

A listing of Sandia employees with LDRD ties who were named to 2020 Prestigious Fellowships and Memberships is included in the Workforce Development section of this report.

Katie Jungjohann, PI at CINT, readies an experiment for the transmission electron microscope. (Photo by Randy Montoya)

R&D 100 Awards

Another relevant indicator of advancement and leadership in a ST&E field is R&D 100 Awards. 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 NNSA site often partner with sister organizations, such as the Intellectual Property Office and Public Affairs, to track whether R&D 100 winners (in the standard category or special awards) have "LDRD roots." Because of the long development time from idea (LDRD) to practical implementation (R&D 100 Award candidate) the staff who work on something that wins an R&D 100 Award may not be the same staff who worked on the original R&D. Each site's LDRD Program Offices engage in an extensive interview process to uncover how the LDRD work led to the celebrated invention.

Since 1976, Sandia has won 140 awards, illustrating the Labs' contributions in developing products and technologies with the potential to change industries and make the world a better place. Over the past three years, 60% of Sandia's R&D 100 winning contributions have been rooted in LDRD; over the past fifteen years, more than 70% have come from LDRD.

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*
	FY18	**FY19**	**FY20**	**FY11-15**	**FY16-20**	**FY06-20**
Total Awards	5	8	7	20	32	73
Awards with LDRD Roots	4	4	4	15	22	52
% with LDRD Roots	80%	50%	57%	75%	69%	71%
Average Years from First LDRD Investment	7	3.8	8	5	5.6	5

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

R&D 100 Award winner
Vincent Urias

R&D 100 HIGHLIGHT

Institute for the Design of Advanced Energy Systems (IDAES) Process Systems Engineering Computational Framework

One FY20 R&D 100 Award winner – the IDAES Integrated Framework – represents the efforts of a large collaboration led by DOE's National Energy Technology Laboratory and features scientists from seven institutions, including Sandia. The IDAES framework is a sophisticated set of modeling tools to that help users – including energy companies, technology developers, and researchers – rapidly design, analyze, and optimize new and potential technologies and processes to address demands for abundant and reliable energy.

The IDAES framework leverages another R&D 100 award-winning technology (2016) – Pyomo – an open-source software that features powerful optimization-based strategies to solve complex, real-world problems. Developed with several LDRD investments spanning from 2007 to 2013, Pyomo has also been used to design sensor networks to protect water distribution systems, schedule Department of Defense (DoD) satellite sensors, schedule production of nuclear weapon components, design cyber defense strategies, plan NNSA operations for nuclear weapon life extension programs, and control power grid operations. This latest R&D 100 Award highlights the continued payoffs of LDRD investments over time.

PYOMO

A full listing of FY20 R&D 100 Award winners associated with LDRD are included in the International Awards section of this report.

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. These staff members are named Senior Scientists/Engineers at Sandia, Fellows at Los Alamos National Laboratory (LANL), and Distinguished Members of the Technical Staff at Lawrence Livermore National Laboratory (LLNL). 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 award, in this case, for contribution to their laboratory's mission.

Each year at Sandia, a small number of staff are specially appointed to the rank of Senior Scientist/Engineer, an honor based on exceptional leadership and consistent outstanding contributions to national security missions. In FY20, nine out of the 16 staff promoted to Senior Scientist/Engineer were involved in the LDRD program as a PI or team member. Over the past decade, more than 60% of Sandia's Top 2% have LDRD roots.

In addition to the Senior Scientist/Engineer appointment, Sandia reserves a special recognition for an elite group of individuals – Sandia Fellows – who are recognized for careers of significant technical accomplishment for the Labs and for the nation. Only 15 individuals in Sandia's history have held this title. Seven of these Fellows are currently on staff, and all seven have been involved with LDRD in their careers. In a timely example, one Fellow, Gil Herrera, coordinated COVID-19 research efforts across Sandia's 14,000-strong workforce. Read more about how technology developed through LDRD investments helped with the pandemic response and how LDRD investments in rapid-response activities made a real-time difference.

LDRD and Top 2% Technical Staff at Sandia National Laboratories

	Single Years			Five Years		To Date*
	FY18	FY19	FY20	FY11-15	FY16-20	FY11-20
Total Awards	9	11	16	22	46	68
Awards with LDRD Roots	3	9	13	9	34	43
% with LDRD Roots	33%	81%	81%	40%	73%	63%
Average Years from First LDRD Experience	15.0	19.9	19.8	13.7	18.2	16.5

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

"Top 2%" – staff are specially appointed to the rank of Senior Scientist/Engineer, an honor based on exceptional leadership and consistent outstanding contributions to national security missions.

SHORT-TERM METRICS

Intellectual Property

Patents

Number of U.S. and foreign patents issued in a given FY.
LDRD-supported patents: Patents issued that would not exist if not for initial work funded by LDRD.

	FY16	FY17	FY18	FY19	FY20
Sandia Patents	139	157	148	159	131
LDRD-Supported	75	86	76	76	67
% Due to LDRD	54%	55%	51%	48%	51%

Copyrights

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

	FY16	FY17	FY18	FY19	FY20
Sandia Copyrights	145	101	107	104	163
LDRD-Supported	31	25	17	25	40
% Due to LDRD	21%	24%	15%	24%	24%

Invention Disclosures

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

	FY16	FY17	FY18	FY19	FY20
Sandia Disclosures	310	296	260	252	320
LDRD-Supported	135	125	112	102	121
% Due to LDRD	44%	42%	43%	40%	37%

Peer-reviewed Publications

Number of peer-reviewed publications, as a function of publication year.
LDRD-supported publications: Publications that would not exist if not for initial work funded by LDRD.

	FY16	FY17	FY18	FY19	FY20*
Sandia Publications	1064	1251	1170	1399	N/A
LDRD-Supported	291	293	363	366	N/A
% Due to LDRD	27%	23%	31%	26%	N/A

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

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.

	FY16	FY17	FY18	FY19	FY20
Graduate Students	75	71	82	106	127
Undergraduate Students	94	98	104	115	100

Postdoctoral Researcher Support

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

	FY16	FY17	FY18	FY19	FY20
Sandia Postdocs	291	316	302	388	350
LDRD-Supported >10%	124	132	133	148	163
% Due to LDRD	43%	42%	44%	38%	46%

Postdoctoral Researcher Conversions

Number of conversions from postdoctoral researcher to a member of the staff.
LDRD-supported conversions: Conversion of postdoctoral researchers who charged at least 10% time to LDRD in the fiscal year preceding the conversion.

	FY16	FY17	FY18	FY19	FY20
Sandia Conversions	43	47	53	68	47
LDRD-Supported >10%	24	22	25	34	25
% Due to LDRD	56%	47%	47%	50%	53%

"In the midst of this COVID-19 pandemic, Sandia is uniquely positioned to positively impact our nation as we possesses numerous technical areas of excellence staffed by some of the most innovative scientists, researchers and engineers in the world. You, and all who work here, can make a difference during this time." – Sandia COVID-19 Wiki post

Michael Omana and a team of Sandia researchers tested materials for Albuquerque companies looking to manufacture N95-like respirators that could be used in local medical facilities. The project originated from the urgent need for personal protective equipment when the COVID-19 outbreak began. (Photo by Bret Latter)

LDRD IMPACT STORY: COVID-19 pandemic.

Eight weeks. Seven research areas. Thirty-four LDRD projects.

MISSION MOTIVATION: Immediately assist the nation with pandemic crisis.

LDRD CHALLENGE: Leverage Sandia expertise and capabilities to provide technical solutions to key COVID-19 challenges.

March 13. The U.S. declared a national health emergency.

March 15. A Sandia COVID-19 internal site launched to incubate ideas and encourage team building.

March 16. Susan Seestrom, CRO, sent an email to the entire workforce soliciting ideas that could enable Sandia to respond quickly to the needs of the nation.

March 16-25. Senior leadership from all LDRD areas participated in an accelerated peer review and approval process to maintain quality while executing same-day reviews for the hundreds of innovative ideas flowing in from across Sandia Labs.

March 26 – May 12. Sandia set up a special “Rapid Response” LDRD program and allocated $1.7M of internal LDRD funding to leverage the Labs’ extensive and relevant capabilities in modeling and simulation, machine learning, biodefense, and materials science for research efforts in manufacturing of medical equipment and critical consumables, epidemiological modeling-based tools for decision support, development of improved therapeutic candidates, next-generation testing platforms, and understanding viral transport and fate in the environment. Approximately $4M more supported longer-term LDRD research in COVID-19-related challenges. The limited project duration ensured the results would make an impact, and by partnering with local hospitals, medical industry, and other national laboratories, Sandia assured viability, adoption, and deployment.

MISSION IMPACT: To summarize just a few LDRD COVID-19 impacts:

- To help local hospitals with ventilator shortages, Sandia converted respiratory machines into machines that can be used as ventilators to help treat patients with severe cases of COVID-19.
- A Sandia Materials Science LDRD team evaluated 2,000,000 design combinations for face coverings and shields and provided methods to make quick to market face coverings and face shields using commonly available materials.
- A Bioscience LDRD team started creating a deployable antiviral countermeasure using CRISPR-based technology. This project is continuing through funding provided by the DoD's Defense Advanced Research Projects Agency. The technology developed will be able to respond to many different viruses, including coronavirus.
- Sandia LDRD researchers assessed the viability of using gamma radiation for sterilizing used personal protective equipment (PPE) to address the national shortage of PPE. The project is continuing through DOE Office of Science and supports gamma sterilization of Coca Cola preforms for use in COVID-19 test kits.

In cases where Sandia's COVID-19 work tightly aligns with current LDRD investment areas and strategic priorities, the research will continue.

Exceptional service in the national interest.

COVID-19 LDRD PROJECTS

BIOSCIENCE

- COVID-19 infection prevention through natural product molecules (PI: Cody Corbin)
- Rapid assessment for COVID-19 (PI: Susan Caskey)
- Testing a novel peptide drug to treat COVID-19 (PI: Raga Krishnakumar)
- Betacoronavirus sequence server (PI: Kelly Williams)
- Handheld biosensor for COVID-19 screening (PI: Darren Branch)
- Development of novel medical countermeasures against COVID-19 (PI: Brooke Harmon)
- Pre-symptomatic COVID-19 screening (PI: Ronen Polsky)
- Computational modeling to adapt neutralizing antibody (PI: Mike Kent)
- COVID-19 prognostics based on RNA profiles of patient specimens (PI: Steve Branda)
- Efficacy and delivery of Novel Facile Accelerated Specific Therapeutics agents for coronaviruses (PI: Colleen Courtney)

COMPUTING & INFORMATION SCIENCES

- Rapid response data science (PI: Travis Bauer)
- Modeling for epidemiology (PI: Patrick Finley)
- Dynamic modeling value of rapid screening (PI: Robert Frederic Jeffers)
- Forecasting COVID-19 (PI: Cosmin Safta)
- Detect misinformation campaigns (PI: Monear Makvandi)
- Robust estimation of transmission parameters for COVID-19 policy planning (PI: Carl Laird)
- Quantified pandemics decision making with Partially Observed Markov Decision Processes (PI: Alex Outkin)
- Contact network modeling to inform return-to-work decisions (PI: Walt Beyeler)

EARTH SCIENCE

- Big-data-driven geo-spatiotemporal correlation between precursor pollen and influenza: Implication to the novel coronavirus outbreak (PI: Yifeng Wang)

ENGINEERING SCIENCE

- Bioparticle transmission (PI: Stefan Domino)
- Computational fluid dynamics modeling safe separation distances (PI: Cliff Ho)
- Science-based understanding of PPE degradation after sterilization for reuse (PI: Anne Grillet)
- Direct Simulation Monte Carlo method for COVID-19 prediction (PI: Jose Pacheco)
- Aerosol transport through masks (PI: Martin Nemer)

MATERIALS SCIENCE

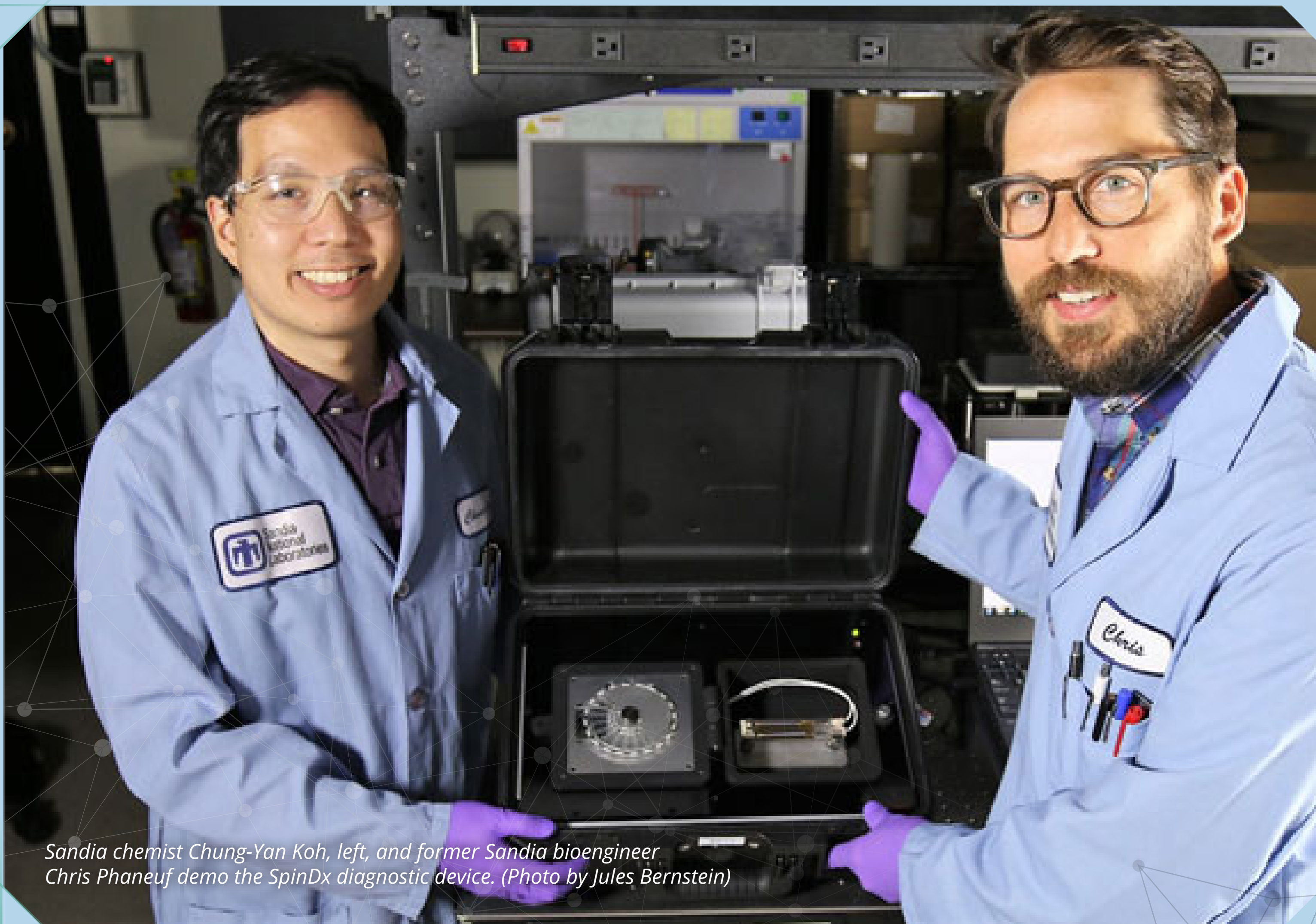
- PPE pipeline (PI: Grant Rossman)
- Supercritical CO_2 for PPE (PI: Jeff Koplow)
- Spray-on active layer (PI: Mat Celina)
- Boronic acid-functionalized polymer (PI: Brad Jones)
- Carboxylic acids as sanitizers (PI: Patrick D. Burton)
- Self-cleaning coatings (PI: Cody Corbin)
- CPAP ventilators for COVID-19 by modification of CPAP equipment (PI: Ryan Haggerty)
- Addressing corrosion concerns with the DF-200 decontamination chemistry for use on military infrastructure (PI: Michael Melia)

NANODEVICES & MICROSYSTEMS

- Catalytic materials for SAR-COV-2 (PI: Robin Jacobs-Gedrim)

RADIATION EFFECTS & HIGH ENERGY DENSITY SCIENCE

- Gamma Irradiation Facility sterilization (PI: Paul Thelen)



Sandia chemist Chung-Yan Koh, left, and former Sandia bioengineer Chris Phaneuf demo the SpinDx diagnostic device. (Photo by Jules Bernstein)

LDRD IMPACT STORY: Medical diagnostic capability developed through LDRD investments enables rapid response to the coronavirus pandemic

MISSION MOTIVATION: Rapidly identify trace levels of chemical and biological agents to contain and mitigate outbreaks and attacks.

LDRD CHALLENGE: Develop technology for the detection of threats in environmental and clinical settings that are rapid, portable, automated, and highly accurate.

MISSION IMPACT: Sandia's deployable diagnostic and detection systems have been used in numerous national security and medical applications ranging from toxin diagnostics to environmental monitoring to biodosimetry. One such technology, SpinDX, was utilized to provide rapid diagnosis of SARS-CoV-2 early in the coronavirus pandemic.

Sandia has a long history of developing novel detection systems. LDRD investments in "lab-on-chip" technology have allowed researchers to create portable diagnostic devices enabling the rapid detection of chemical and biological agents. Beginning in the mid-1990s, the development of a handheld chemical analysis system called µChemLab helped spur the growth of Sandia's now enduring capability in biological science and technology. Additional investments from LDRD, government, and technology partnerships over the next two decades led to improvements in detection capabilities for national security and medical applications.

One LDRD-enabled technology – SpinDX – came out of a need to rapidly identify trace levels of biotoxins to combat terrorism. After initial LDRD investments in 2009, SpinDX continued to receive funding from multiple sponsors, including the U.S. Armed Forces Radiobiology Research Institute, National Institutes of Health, and National Institutes of Allergy and Infectious Diseases, to address critical issues in biodefense and healthcare. Numerous companies have licensed SpinDX as a platform for point-of-care diagnostics testing, water pathogen testing, and other applications.

Investments in SpinDX continue to pay dividends through the issuance of seven patents and eight commercial licenses, the development of new partnerships, and the expansion of novel applications beyond what was first envisioned beginning with the original LDRD in 2010. Notably, in 2020, Sandia began using SpinDX for rapid detection of viral antigens and SARS-CoV-2 antibodies during the coronavirus pandemic. As a result, SpinDX was able to offer healthcare professionals a powerful way to diagnose SARS-CoV-2 at all stages of the disease.

How does SpinDX work?

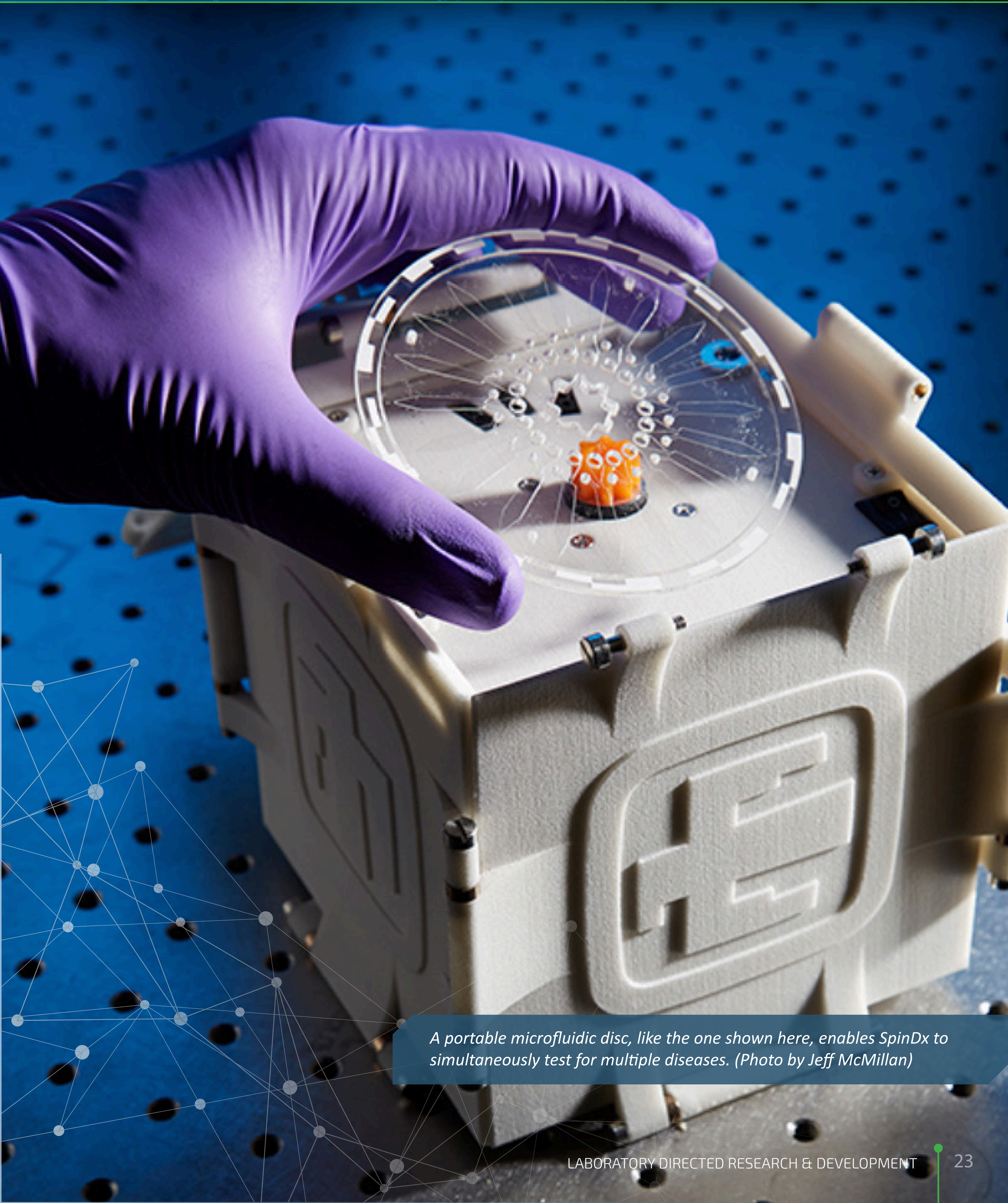
SpinDX is a portable, medical diagnostic platform that uses a disposable, centrifugal disc with microfluidic flow paths to manipulate a biological sample. This allows multiple tests to be carried out on a single sample with no preparation required. The device operates by distributing drops of raw, unprocessed samples into different channels that function as dozens of tiny test tubes. When the disc spins, the samples interact with test reagents inside the channels. If there is a chemical interaction between the sample and the reagent, the tip of the channel will produce a fluorescent glow indicating an infectious agent is present. The data is then transferred to a software interface that displays the test results.

Conventional viral testing requires both heating and cooling of a biological sample multiple times to multiply any viral DNA or RNA (an important biological macromolecule that functions to convert the genetic information of DNA into proteins) to detectable levels. An early version of SpinDX used conventional viral testing to perform protein tests that searched for pathogen-specific proteins and antibodies. To make viral testing more efficient, Sandia developed an assay and detection scheme that allows the sample to be heated only once. The newest version of SpinDX does this by using a tiny infrared heat emitter that hovers at the top of the device, targeting a part of the spinning disc to heat the sample. Using this method, SpinDX can conduct nucleic acid tests that identify causative pathogens (viruses and bacteria) as well as pathogen-specific proteins.

Read more about SpinDX here.

Watch the YouTube video.

"Notably, in 2020, Sandia began using SpinDX for rapid detection of viral antigens and SARS-CoV-2 antibodies during the coronavirus pandemic. As a result, SpinDX was able to offer healthcare professionals a powerful way to diagnose SARS-CoV-2 at all stages of the disease."



A portable microfluidic disc, like the one shown here, enables SpinDx to simultaneously test for multiple diseases. (Photo by Jeff McMillan)

LDRD IMPACT STORY: *Multi-mission radio frequency architecture*

MISSION MOTIVATION: DOE national security applications benefit from radar capabilities that enable smarter sense, analyze, and respond cycles.

LDRD CHALLENGE: Enable advanced real-time multi-mission sensors that can send/receive/process arbitrary signals with large instantaneous bandwidth using multiple channels.

In 2017, a Sandia LDRD team, led by PI Jacques Loui, sought to develop a multi-mission digital radar architecture to simplify and modularize a radar's radio frequency frontend by replacing application-specific analog detection methodology with flexible and programmable digital signal processing. After a year of work, they successfully obtained real-time digital-detection radar impulse response from a prototype and demonstrated multi-channel synchronization.

With such positive results, the Sandia Multi-Mission Radio Frequency Architecture (MMRFA) LDRD team continued the effort into 2019 and demonstrated an ultra-wide-band multimission modular digital radar architecture that overcame limitations of single-application analog radar designs by leveraging commercial-off-the-shelf (COTS) hardware, existing/new firmware/software intellectual properties, and available radio frequency (RF) apertures. They demonstrated several Sandia firsts in real-time ultra-wideband sensing, including multi-channel

A high-resolution Digital Synthetic Aperture Radar image from the successful initial flight test in 2019.

clock synchronization, advanced arbitrary waveform generation, frequency domain channelization, and single-stage-heterodyne conversion using advanced COTS and custom RF modules.

The High-Performance Digital Radar (HPDR) significantly advanced the state-of-the-art for Sandia radar system architectures by replacing static analog waveform generation and detection with agile digital waveform synthesis and signal processing. The project culminated with a successful flight test that demonstrated integration of the HPDR with an operational radar and creation of high-resolution synthetic aperture radar imagery.

In 2020, the MMRFA team demonstrated the first ever instance of real-time, parallel and fast Fourier transform-matched filtering of large instantaneous bandwidth signals. Pulse compression, important for imaging applications, requires real-time digital matched filtering when using agile waveforms. To overcome motion compensation challenges, the team implemented real-time pulse extension with efficient interpolative post processing that improved bandwidth utilization without performance (resolution and throughput) degradation. They also configured and tested simultaneous dual-channel receive operation that improved range performance while doubling data throughput. This set an important precedent that facilitates the configuration and setup for simultaneous multi-channel digital signal processing of agile waveforms in the future.

MISSION IMPACT: Thanks to the dedication of the MMRFA team and continued LDRD funding, major NNSA, Army, Air Force, and Navy programs are now utilizing aspects of these revolutionary Sandia radar system architectures.

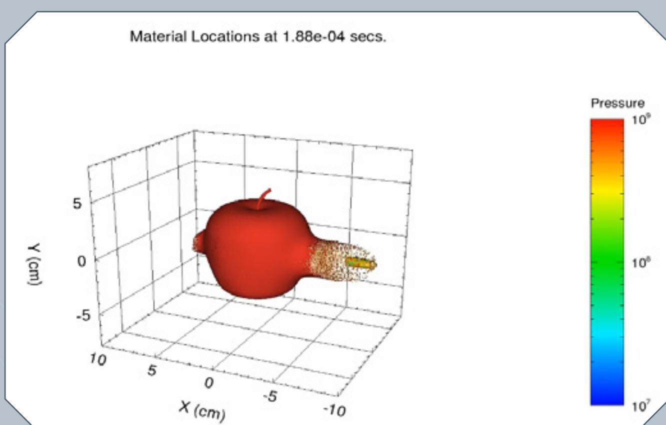
Overcoming COVID-19 pandemic challenges through virtual means, teams from Sandia and the U.S. Air Force, under the guidance of NNSA, performed a critical B61-12 flight test. (Photo by Dale Green)

Watch the YouTube Video.

LDRD IMPACT STORY: CTH software code use in scalable shock physics

MISSION MOTIVATION: Obtain greater understanding of material strength, fracture, porosity, and explosive detonation so the data can aid in national security and defense, health, and space applications.

LDRD CHALLENGE: Use Sandia expertise to create software that solves multi-dimensional problems characterized by large deformations and strong shocks within various material configurations.



CTH calculation of a .50 caliber round against a fruit

Sandia's CTH journey started more than 30 years ago with its predecessor codes, CHARTD and CSQ, which were developed in the 1970s for one-dimensional problems and expanded to simulate problems in two- and three-dimensions in the 1980s. CTH software was then created to expand Sandia's production shock physics code suite to 3D. The code, written in FORTRAN 90 and C, was modified to run on massively parallel computers in 1992-1993 and enhanced with parallel adaptive mesh refinement.

In the last 20 years, many Sandia LDRD projects have contributed to the development and application of CTH, which can successfully analyze a variety of materials for high-speed impact, penetration, perforation, and explosive detonation. Applications are numerous and include astrophysics, safety assessments, accident investigations, blast design, threat assessments, fracking predictions, and medical research. Two Sandia LDRD projects focused specifically on wound injury mechanics and traumatic brain injuries.

Sandia researchers developed specialized computer modeling and simulation methods (CTH software) to better understand how blasts on a battlefield can lead to traumatic brain injury and injuries to vital organs, such as the heart and lungs. (Photo by Randy Montoya)

MISSION IMPACT: CTH is one of the most highly used computational structural mechanics codes on DoD high-performance computing platforms, as well as the number one code at Sandia in terms of computing hours. CTH has been used to mimic the entry process of the Chelyabinsk asteroid in Russia, simulate the penetration (a first-of-its-kind simulation), breakup and fireball of Comet Shoemaker-Levy 9 hitting Jupiter, and aid in the accident investigations of the Space Shuttle Columbia disaster and the USS Iowa naval training accident. The CTH code is currently being used to design and improve high-velocity and high-temperature national security applications that ultimately provide security to the country.

This 3D simulation of the Chelyabinsk meteor explosion by Mark Boslough was rendered by Brad Carvey using the CTH code on Sandia's Red Sky supercomputer. Andrea Carvey composited the wireframe tail.

LDRD Program Accomplishments

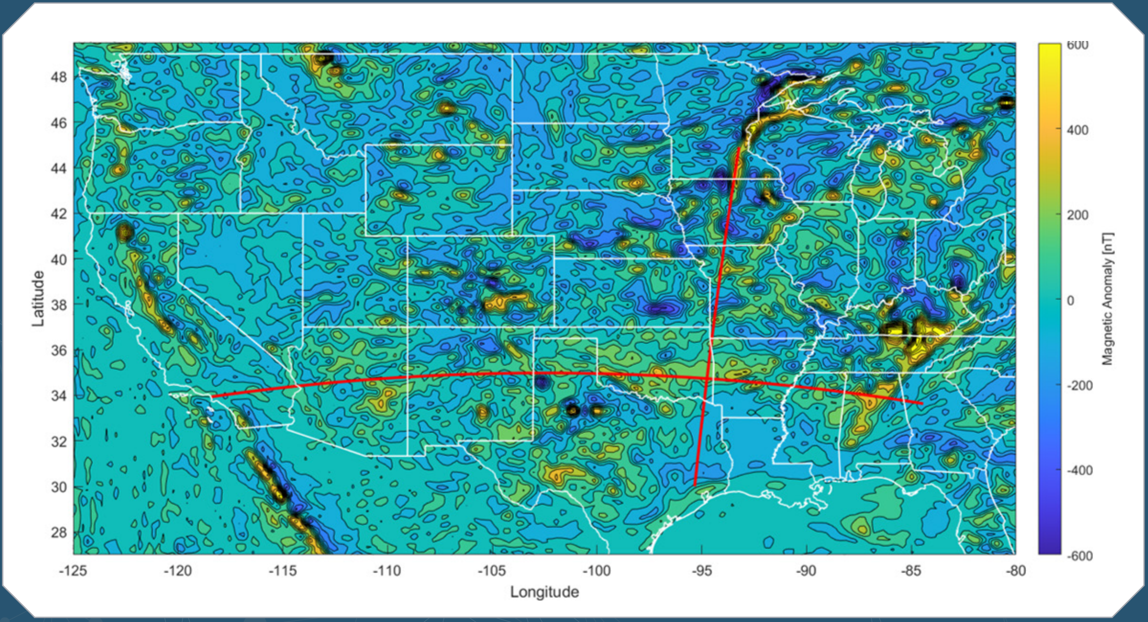
This section highlights some LDRD program accomplishments, organized around the three themes of mission agility, technical vitality, and workforce development. These highlights are from projects that ended in FY20 or are continuing into FY21 but have already realized some significant research accomplishment.

Project Highlights – Mission Agility

Enabling agile responses to national security missions

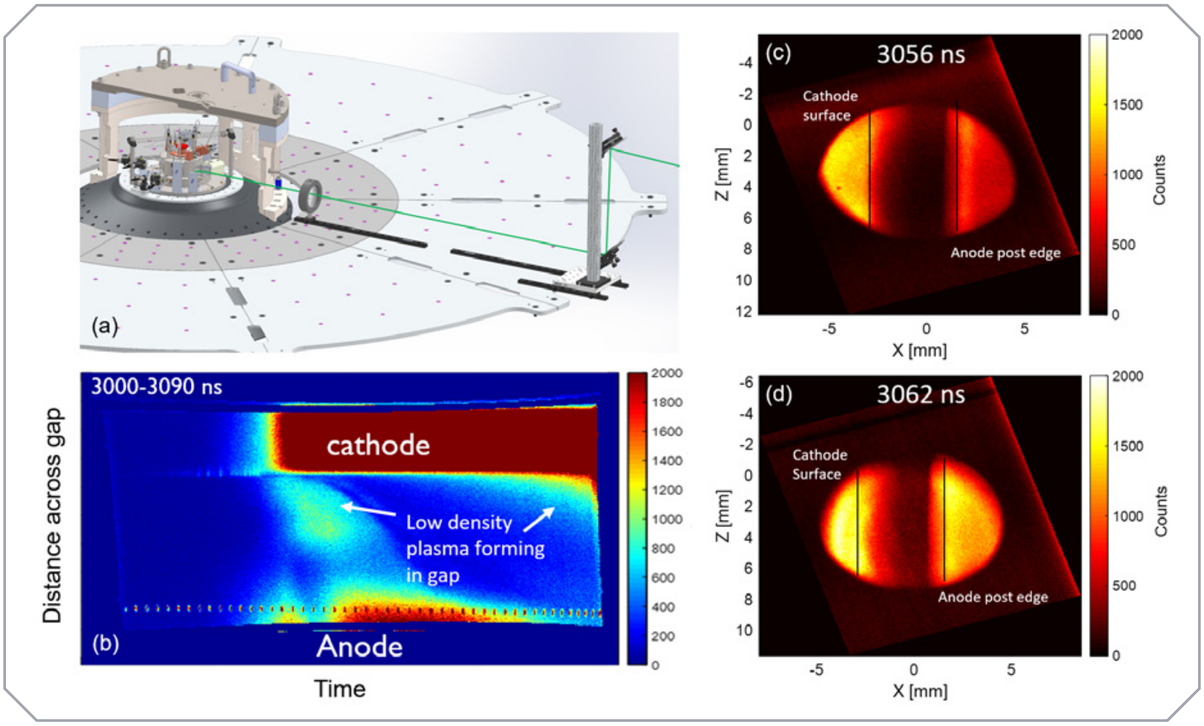
It takes innovative ST&E to create and enhance the capabilities needed to ensure the U.S. is ready to respond nimbly to national security mission needs. LDRD is a critical resource at the heart of what it takes to lead into the future.

Magnetometer-aided navigation for hypersonic strike vehicles. GPS-denied navigation is a top concern for national security and finding a suitable alternative that is effective over featureless terrain and ocean is a priority. The accuracy of weapon systems such as hypersonic missiles is limited by their positioning capability. Sandia's Autonomy for Hypersonics (A4H) Mission Campaign research on magnetic navigation (MagNav) leveraged the Earth's magnetic field to determine vehicle position via high-fidelity magnetic field models, sensor fusion, and nonlinear, non-Bayesian filtering techniques. This effort resulted in the development of a realistic MagNav simulation capability – providing quantitative estimates for magnetic navigation performance over land and water, including altitude dependence. MagNav is a promising alternative navigation solution, especially when combined with other inertial measurement unit-aiding sensors. The research team is currently investigating machine learning techniques to reduce platform magnetic interference and investigating opportunities to further validate this technology. (PI: Neil Claussen)



Shown is a magnetic field anomaly as a function of position at fixed altitude of 4km height above ellipsoid. The red lines indicate two model trajectories for evaluating magnetic navigation algorithms. The south-north trajectory connects Houston and Minneapolis while the east-west trajectory joins Atlanta and Los Angeles. Along these two trajectories, the region of lowest magnetic character occurs on the coastal plain just north of Houston.

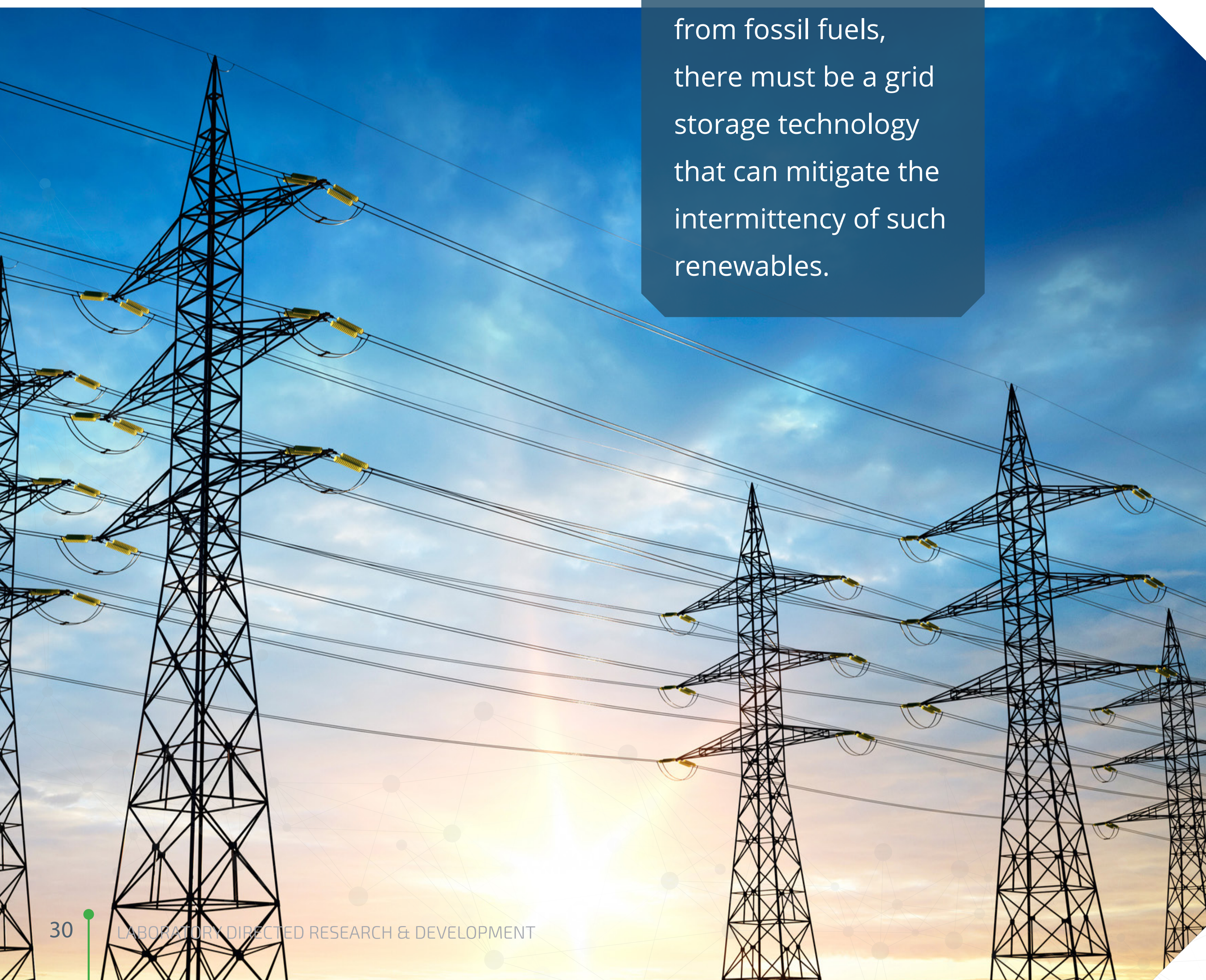
Developing self-emission optical imagers in pursuit of advanced diagnostics. This project is developing a visible imaging diagnostic to observe: (1) fast phenomena such as self-emission from inertial confinement fusion targets and powerflow surfaces, and (2) slow phenomena such as post-shot debris and pre-shot target motion induced from the long-pulse coils that magnetize the Magnetized Liner Inertial Fusion concept. This is a standalone diagnostic utilizing the Z Line VISAR (Velocity Interferometer System for Any Reflector) optical system, but its completion is an essential step toward more advanced diagnostics such as laser imaging. Improved measurements of the initiation and evolution of magnetically-driven targets will contribute to improved understanding, validation of, and performance of targets on the Z machine, which could be utilized in numerous security applications and high energy density physics. (PI: David Yager-Elorriaga)



(a) The optical imager diagnostic consists of an in-chamber periscope and lens that couples to the Z Line VISAR infrastructure to create and relay an image to two 1D streak cameras and eight gated cameras. Streaked data in (b) and 2D image data in (c) and (d) show the evolution of low-density plasmas in the anode-cathode gap.

Cost-competitive, scalable and safe grid storage: Sandia's radical ion flow battery technology. To transition away from fossil fuels, there must be a grid storage technology that can mitigate the intermittency of such renewables. But such a battery must be dirt cheap, derived from Earth-abundant materials, have a 30-year service lifetime, and be massively scalable in size. To address the intermittency problem of photovoltaic solar and wind power, the team investigated the feasibility of the electrochemical half-reaction, low-cost, battery-based grid storage. The Radical Ion Flow Battery (RIFB) is uniquely suited to the most challenging grid storage application, addressing known pitfalls including: (1) use of prohibitively expensive materials, (2) lack of scalability due to limited material abundance, (3) sluggish electrochemistry at one or both electrodes, (4) unwanted side reactions leading to capacity fade and/or internal corrosion, and (5) comingling of highly reactive chemical reagents (making fire suppression extremely difficult in the event of an accident). The unique battery chemistry uses only earth abundant materials (NaCl, N_2, O_2, and steel), avoids electrochemical kinetic and transport penalties, prevents capacity fade via simplified battery chemistry, achieves the functionality of a flow battery without pumps, and exploits the anomalously low activation energy barrier for radical-ion electron transfer half reactions. Results of the LDRD effort confirm that the $NO_2 + e^- \rightleftarrows NO_2^-$ redox couple can be carried out effectively on nonexotic electrode materials (e.g. stainless steel) despite the challenge of a triple-phase boundary for the nitrogen dioxide reduction. This study also allowed the team to work out how RIFB can be implemented in a planarized, series-connected form factor that meets stringent requirements for battery efficiency, manufacturability, and materials compatibility. (PI: Jeffrey Koplow)

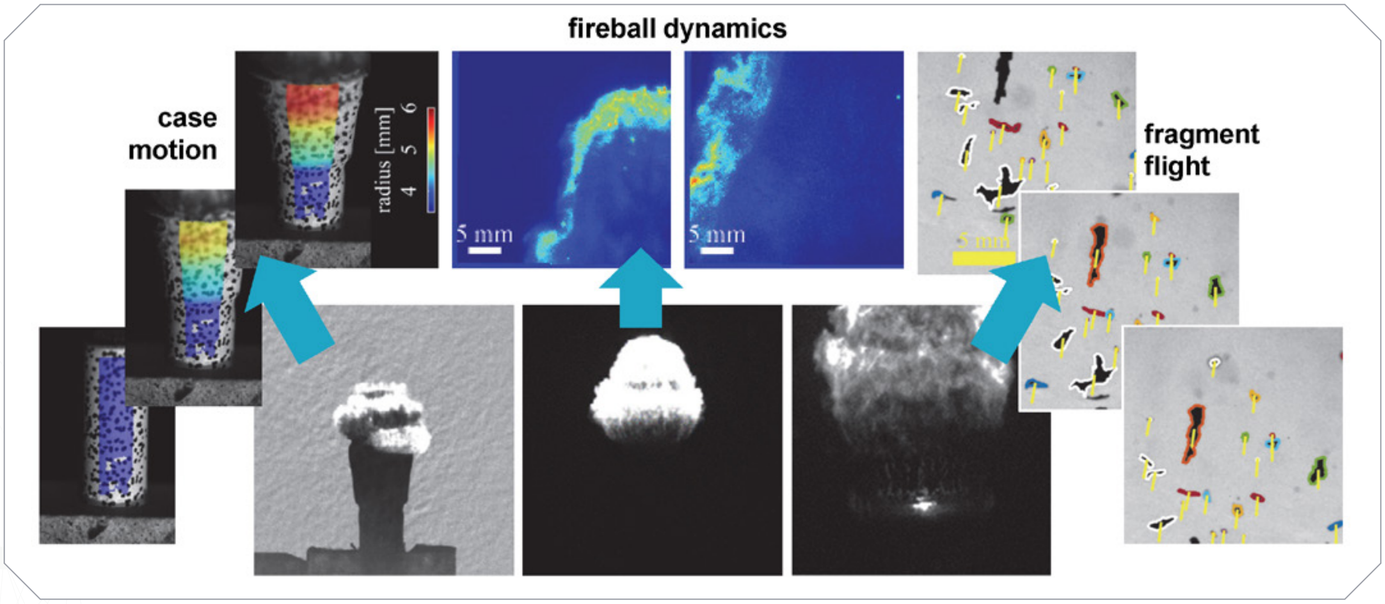
> To transition away from fossil fuels, there must be a grid storage technology that can mitigate the intermittency of such renewables.



A predictive model for Arctic coastal erosion. Current tools for quantifying permafrost erosion are unable to explain the episodic, storm-driven erosion events; however, the treatment of transient erosion events can be enabled by mechanistically coupling oceanographic predictions with a terrestrial model to capture the thermo-mechanical dynamics of erosion. The Arctic Coastal Erosion (ACE) model consists of oceanographic and atmospheric boundary conditions that force a coastal terrestrial permafrost environment in Albany. This modeling approach enables failure from any allowable deformation. Extensive experimental work underpins the ACE model development, including field campaigns to measure in-situ ocean and erosion processes, strength properties derived from thermally-driven geomechanical experiments, and extensive physical composition and geochemical analyses. This work, done in collaboration with the University of Texas at Austin, offers the most comprehensive and physically grounded treatment of Arctic coastal erosion available in literature. The ACE model and experimental results can inform scientific understanding of coastal erosion processes, contribute to estimates of geochemical and sediment land-to-ocean fluxes, and facilitate infrastructure susceptibility assessments. (PI: Diana Bull)

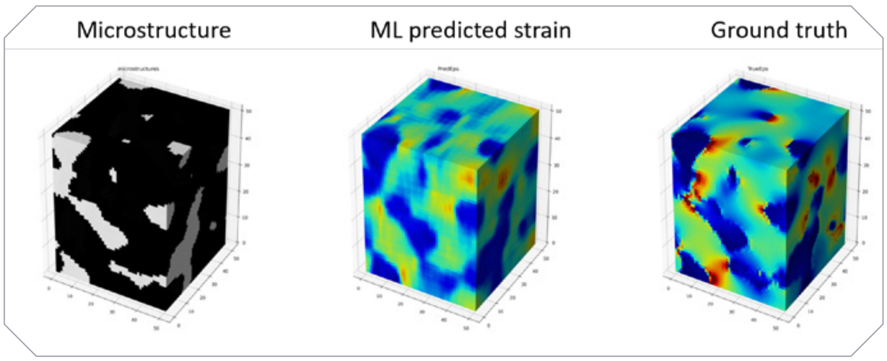
A Sandia researcher holds up a core sample of thermokarst-cave ice with vertical frost cracks; this indicates thawing degree days occurred in this Arctic area.

Explosive challenge: Revolutionizing spatial and temporal blast characterization. Numerous defense and national security challenges require accurate prediction of the hazardous fragments and fireballs produced by large explosive devices. Prior to this work, the pace of model development was hindered by the limited data measurable during full-scale, outdoor testing. To accelerate these efforts, an LDRD team demonstrated benchtop-scale explosive devices, which replicate the fragment and fireball dynamics while greatly reducing per-shot costs. This enabled the first successful demonstration of many advanced laser and imaging diagnostics within post-detonation environments. Insights revealed by the new high-fidelity experimental data led to several subsequent model improvements. These successes inspired a follow-on Grand Challenge LDRD that brings together over 30 Sandia staff with faculty from four preeminent U.S. universities. Grand Challenge efforts will attempt to closely couple the multiscale experimental philosophy developed at Sandia, with advanced modeling and simulation to revolutionize R&D pathways for the prediction of post-detonation environments. (PI: Daniel Robert Guildenbecher)



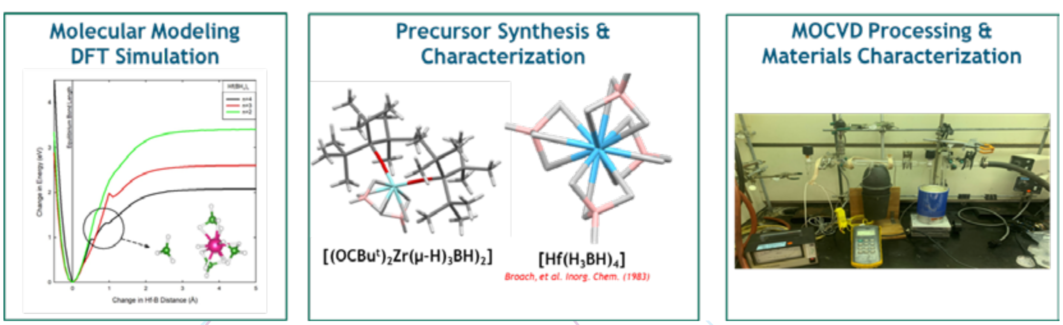
Accelerating rapid-turnaround benchtop-scale explosive testing through development of laser and imaging diagnostics for post-detonation environments.

Physics-informed deep learning for fast and accurate multiscale simulations in computational solid mechanics. Sandia developed a deep learning framework to accurately predict the localized elastic microstructural responses at the microscale. This framework could replace crystal plasticity finite element models. In addition, the team developed an unsupervised deep learning framework for learning latent representations of microstructures, thereby reducing the dimensionality of the microstructure representations. Using these approaches may allow the solution of direct numerical simulation problems for macroscale objects at a small fraction of the computational cost of traditional simulations. Therefore, the methods developed in this research can be used to lower the computational cost of high-fidelity simulation in computational materials science, and to assess and improve the materials reliability in extreme and critical conditions. (PI: Anh Tran)



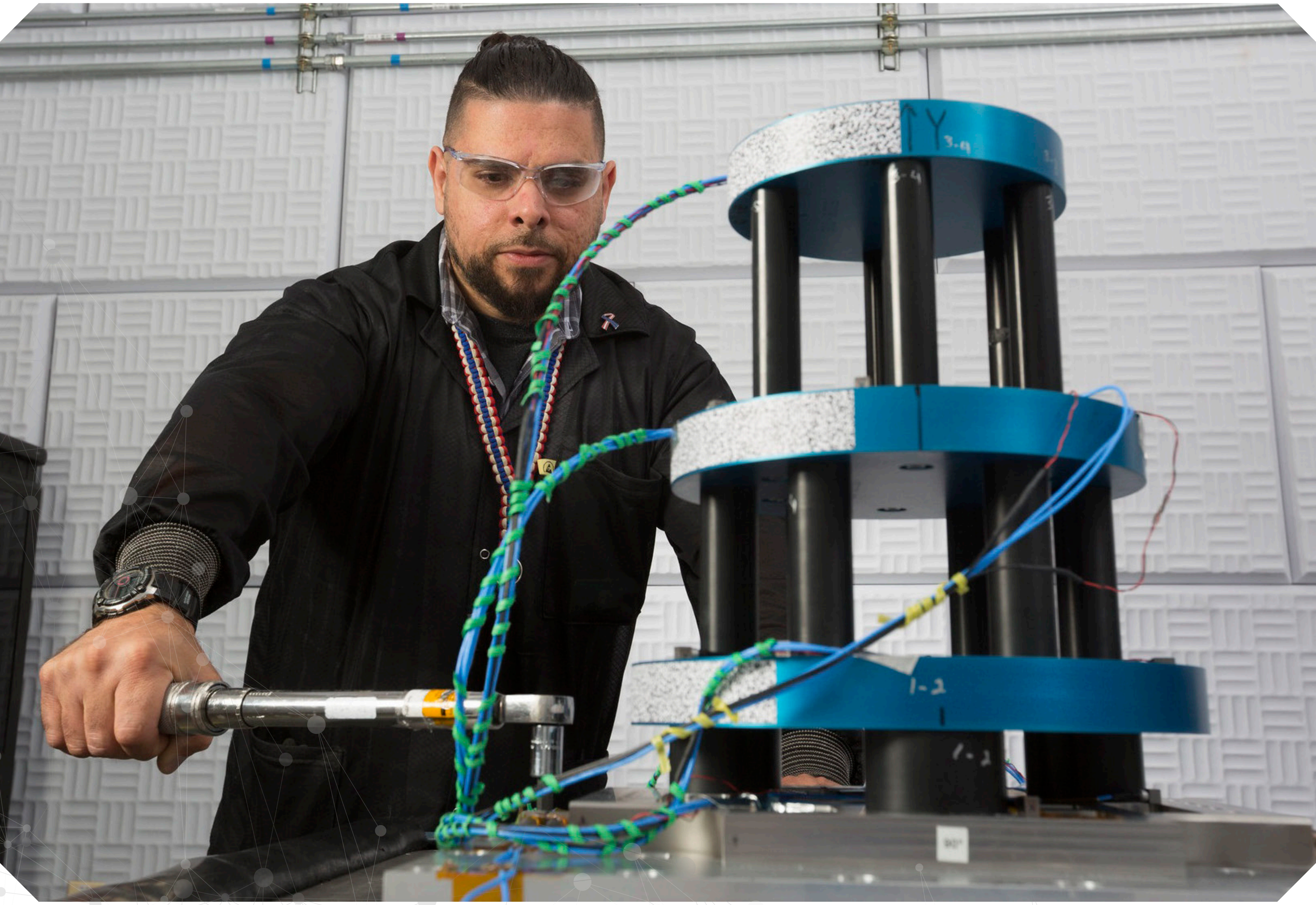
The machine learning framework can accurately predict strain with only a fraction of the computation burden of traditional methods.

Hafnium-boron-based precursors for vapor deposition of ultra-high temperature materials. High-temperature protection applications require refractory hafnium diboride ceramic coatings. This project employed density functional theory calculations to identify candidate hafnium-based precursors for chemical vapor deposition processing, synthesized the new precursors, and experimentally demonstrated the deposition of hafnium using the new precursors. Demonstrating the preparation of hafnium diboride precursors helps advance U.S. initiatives in the manufacture of thermal management and protection capabilities. (PI: Bernadette Hernandez-Sanchez)



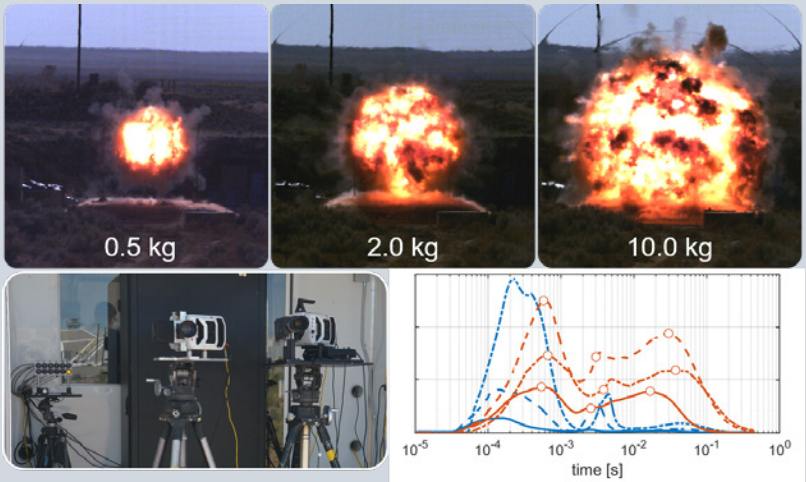
(Left) Simulation of $[Hf(BH_4)_2L_2]$ precursors for metal-organic chemical vapor deposition (MOCVD) applications; (Middle) Precursors explored and synthesized, and (Right) MOVCD setup used to produce films.

Efficient real-time cognition at the point of sensing. Sensors operating on the principles of "compressive sensing" (CS) can accurately represent a signal with dramatically fewer data points than traditional sensors. However, translating this data into a form humans can interpret requires a computationally-intensive reconstruction algorithm. Traditionally, machine learning algorithms have been applied to CS systems after the reconstruction step. Sandia researchers asked the question, "If a machine is performing the analysis, why put the data in a format a human can understand?" They successfully demonstrated that machine learning techniques can be employed on CS data in their native domain without the reconstruction. This reduces power and computational requirements and enhances algorithm performance and speed. This new sensing paradigm will enable faster, more efficient automated systems for a wide variety of national security missions. (PI: Eric Shields)



Data collected from sensors aboard HOT SHOT sounding rockets is allowing researchers to improve computer- and ground-based simulations of flight vibrations. Ralph Lied-Lopez helped to study the amount of vibration that mechanical objects endure in flight, including the so-called "wedding cake" hardware, a mock rocket component. (Photo by Norman Johnson)

Advanced manufacturing brings threat representative explosive systems to new scales. Researchers at Sandia pushed explosive designs to unprecedented small scales by employing advanced manufacturing and novel scaling approaches while preserving mission relevance. Explosive source term data is critical for development of remote sensing methods and phenomenological study of the available data. Historically, high-fidelity experiments have been prohibitively expensive. By exploring limits of geometric scaling, costs have been reduced by over an order of magnitude per test with an increased responsiveness. Further, the reduced size enables colocation of advanced diagnostics and testing in a controlled laboratory chamber rather than in the field. The testbed is being adopted as an enabling capability for further in-depth phenomenological studies. (PI: Ryan Marinis)

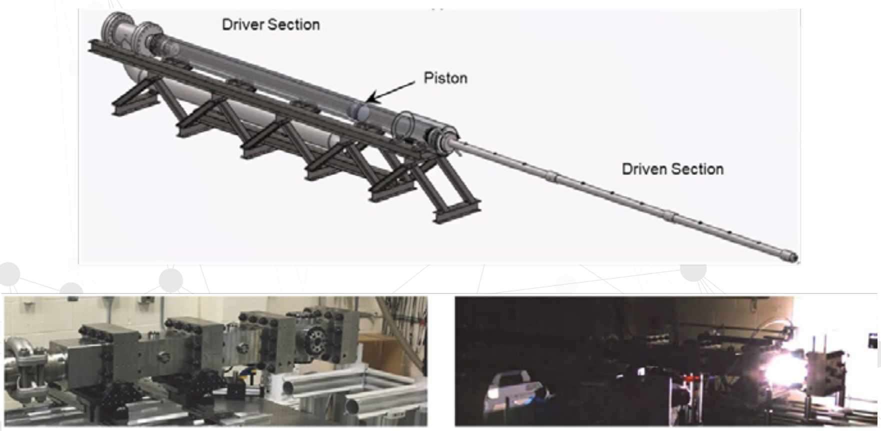


Three scales of threat-relevant explosive source term fireballs (top row) produced by novel manufacturing techniques produced signals remotely collected (bottom left). Collected data is spectrally narrow and spatially integrated, showing relevant phenomena produced across scales (bottom right).

PI Theodore Grabowski led a significant LDRD project in FY20 that utilized the Hermes III accelerator, the world's largest gamma radiation simulator. In this image, one of Sandia's technicians arms a series of triggering lasers for a test.

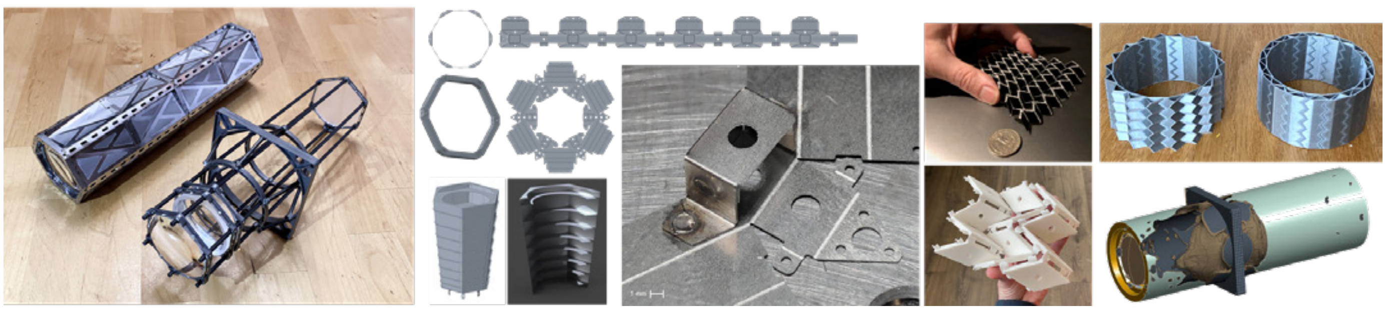
Rebecca Nylen first interned at Sandia in 2018 as a civil engineering doctoral candidate from Georgia Tech. She's now a full time staff member on Sandia's Computational Shock Physics team.

Extreme conditions in the Sandia high-temperature shock tube enable the remote sensing mission. Sandia researchers developed a new capability to shock heat air and other gases to the extreme temperatures and pressures found in conventional explosive events. The method uses a "free-piston" shock tube to generate intense air luminosity, which is then sensed by high-speed emission spectrometers. The LDRD team also developed a novel, highly accurate optical diagnostic to concurrently measure the gas temperature using a pulse-burst laser and Raman spectroscopy. This, in combination with the spectral emission data, enables validation of opacity tables used in NNSA codes to model fireball optical signatures. Collectively, this technology is expected to provide a scientific underpinning to support multiple national security applications. (PI: Justin Wagner)



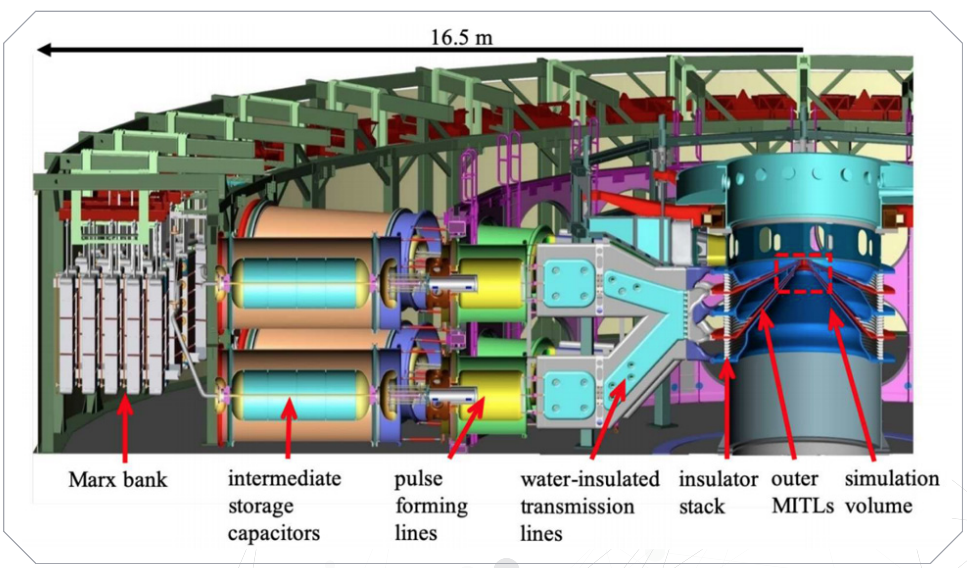
Illustrative schematic of the free-piston shock tube (top), optical test section (bottom left), and photo of shock-heated air emission obtained during a 7000 K shot (bottom right).

Extremely lightweight optical structures for rapid deployment. Sandia researchers used origami-style folding of photo-etched and micro-welded sheet metal along with 3D-printed metal, to create ultra-lightweight structures for spaceborne optical systems. While traditional light-weighting starts with a heavy block of material that is then cut away to make thin walls and ribs, this research effort starts with much thinner material and folds it to create the stiff structures required by the design. Photo-etching creates the shapes and fold lines for easy assembly. The new method realized structure weight savings of >90% and 20% diameter reduction compared to traditional space system optical design methods, with designs that are both less expensive and more quickly realized than standard machined assemblies. This technology can enable compact, affordable, and rapidly produced systems for cubesats/smallsats with scalable advantages for larger space payloads. (PI: Edward Winrow)



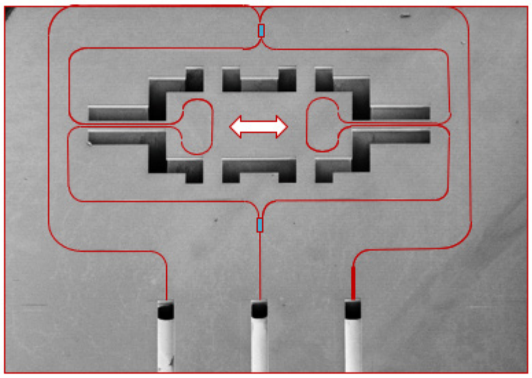
(Left to right) Folded and hybrid 3D-printed ultralight optical structures (folded and unfolded lens sub-cell components), solar shade design (fold and weld detail), flexible structures based on miura-ori fold patterns, miura-ori reinforced cylinder, and topology optimization model.

Developing a validated multiscale plasma engineering design tool. The Plasma Science & Engineering Grand Challenge LDRD developed advanced multiscale computational plasma physics models and demonstrated integration between modeling and surface physics theory and supporting experimentation. This led to 30-40X speed and reduced 150-day power flow design calculations to several days. With the speed up, Z machine programs have increased shot resources for power flow studies by 2.5X. This enabled a revolutionary plasma engineering capability impacting pulsed power accelerators, select nuclear weapon components, radiation effects qualification, reentry vehicle plasma sheaths, high-power electromagnetic diodes, and high energy density science. Efforts on development and application are continuing. (Leads: George Laity, Allen Robinson, Michael Cuneo)



The Plasma Science & Engineering Grand Challenge demonstrated and verified rapid full-physics Z power flow simulation through development of complementary CHIGACO and EMPIRE code technologies. (Above) A cross section of the Z generator that notes the portion simulated by the Grand Challenge as "simulation volume."

Miniature accelerometers with sub-microsecond timescales for characterization of structural dynamics. Looking to greatly improve ground-based or *in-situ* testing of weapon components or other systems, Sandia researchers developed highly miniaturized, solid-state accelerometers that can measure significantly higher vibration frequencies and displacements far more accurately than current technologies, by using nano-optomechanical systems. This technology results in devices that are almost 6X smaller than typical accelerometers and use laser interferometry to test over the full range of operation. The new vibrometers were tested in a hypersonic wind tunnel as well as a shock tube, yielding promising results, with plans to test at higher frequencies in pulsed power facilities. (PI: Katya Casper)

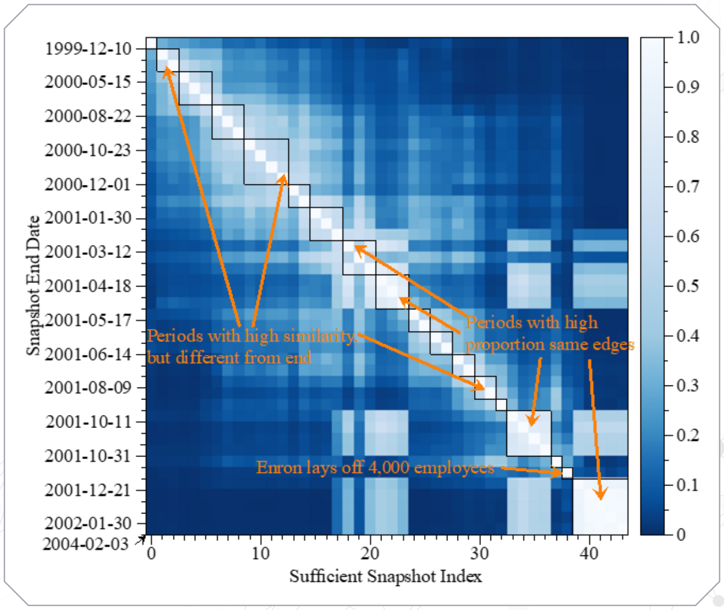


The uniaxial high-frequency accelerometer provided 100X higher response in shock tube testing in comparison to a traditional sensor.

With its hypersonic wind tunnel and advanced laser diagnostic technology, Sandia is in an excellent position to help U.S. defense agencies understand the physics associated with aircraft flying five times the speed of sound. "The physics are enormously difficult at hypersonic speed," said Sandia aerospace engineer Steven Beresh. (Photo by Randy Montoya)

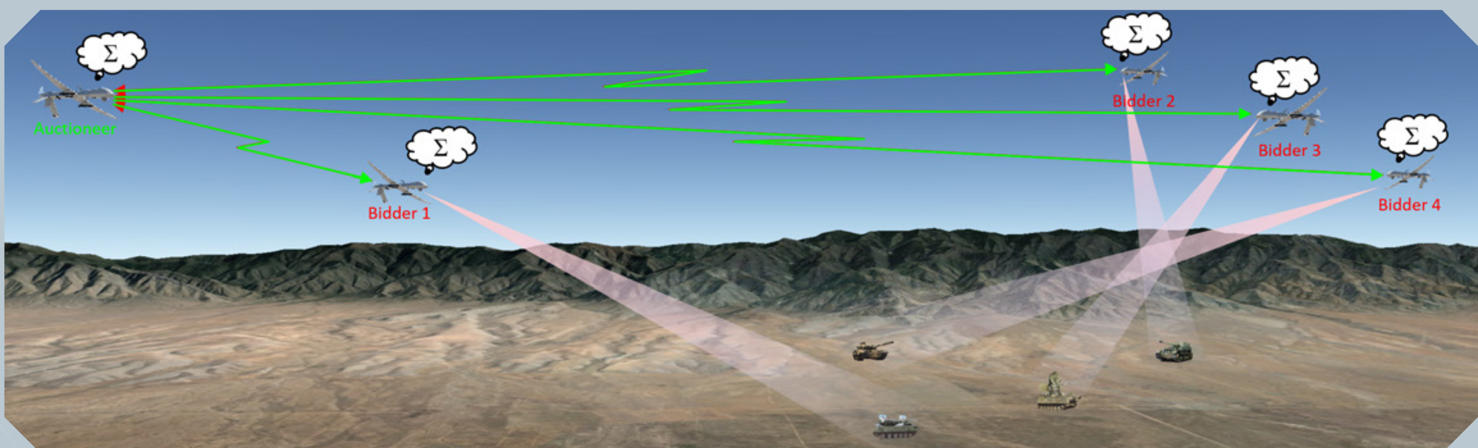
Aerial cross-polarized nuclear quadrupole and magnetic resonance allows for explosive detection at a safe distance. New technology now allows for the safe and remote detection of nitrogen-containing explosive materials possibly buried in landmines or hidden in contraband in airport luggage or in/on passengers. During this LDRD, the PI conducted additional experiments, doping a polymer with quadrupolar nuclei. He showed that a stress in the polymer stresses the dopant particles, shifting the nuclear quadrupole resonance frequency. The techniques used to detect small amounts of explosive material quickly and safely will significantly enhance our nation's ability to prevent casualties in warzones and improve security in the transportation sector. (PI: Eric Sorte)

Automated analysis finds stable graph data. As communication is evaluated, relationships can be seen to change over time (people join/leave or new relationships form). Graphs formed from all communication events in a limited time period provide "snapshots" of the relationships. As change events are detected, a new graph snapshot should be generated from the communication events. Since graph snapshots are often used by downstream analysis tools to facilitate important national security decisions, it is critical to ensure that they properly represent the underlying communication stream. A new technique developed at Sandia can now efficiently identify these fundamental changes in real-time. It was tested against synthetic, known-answer datasets (providing significant improvements over previous techniques) and against a variety of real-world datasets (highlighting previously unreported features). The technique is expected to be foundational to future graph analyses. (PI: Jeremy Wendt)



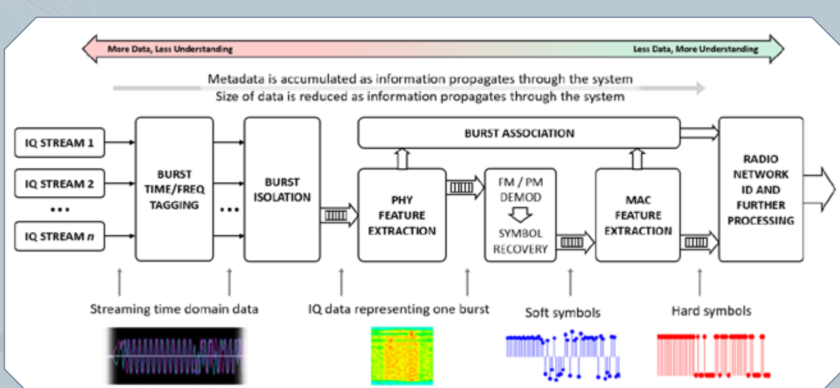
Sandia's technique automatically splits years of the Enron Email Dataset into 44 distinct static graphs of varying duration based on underlying shifts in communication patterns. A second step highlights periods of high similarity (lighter, white colors). This visualization shows that some of those high-similarity periods repeat across many months, interrupted by periods of low similarity.

Autonomous sensor tasking and scheduling across multiple platforms. This LDRD project investigated the use of multiple distributed sensors to enable autonomous execution of collaborative, multiplatform intelligence, surveillance, and reconnaissance (ISR) missions. The innovative auction framework involved the use of low-bandwidth communication and rigorous optimization of mission utility measures to provide a flexible, robust capability for autonomous multiplatform ISR in dynamic environments. Developed techniques were recently incorporated into Air Force and Navy efforts to autonomously detect and track mobile threats using distributed collections of mobile sensors, and also to support simultaneous execution of multiple ISR missions with distributed, federated collections of platforms and sensors. The work through this LDRD, done collaboratively with Purdue University, has yielded new technologies enabling development of emerging autonomous systems that provide important new warfighter capabilities. (PI: John Richards)



Autonomous collaborative intelligence, surveillance, and reconnaissance mission execution through auction framework and rigorous optimization of sensing utility.

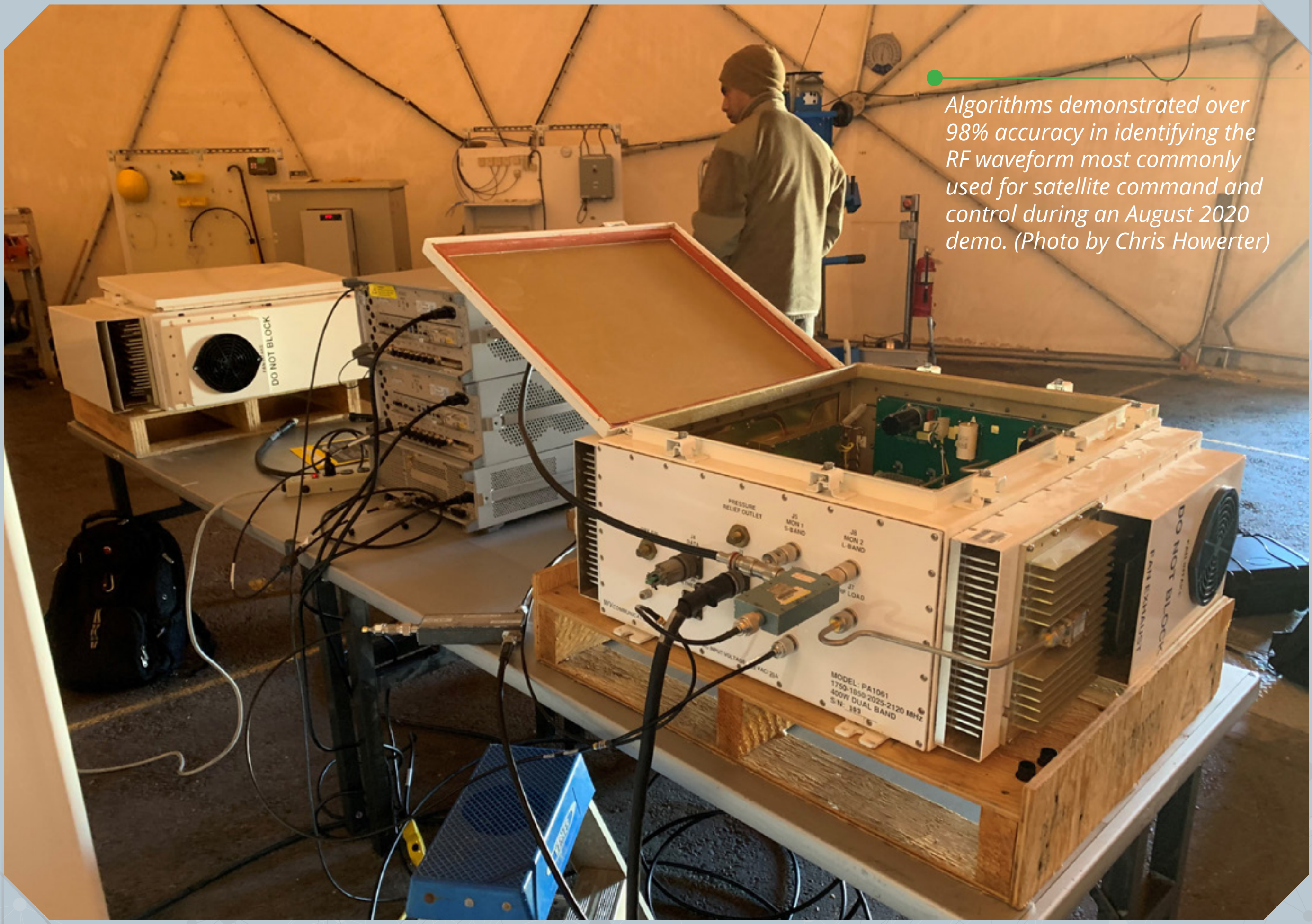
New Counter-Unmanned Aerial System radio frequency techniques bring agility in protection applications. Sandia developed new semi-autonomous methods for rapid prototyping of software-defined radio frequency counter-unmanned aerial system technology. The technique brings agility beyond current static library-based effects and reduces the amount of skilled operator input required for development of defeat capabilities. This is a significant advancement in the Counter-Unmanned Systems RF effect domain and enhances posture for these capabilities to be leveraged for critical asset/ force protection applications. (PI: Jacob Alan Gilbert)



Metadata-aided RF system detector for bandwidth-constrained cooperative sensing and RF situational awareness.

Developing an EMP-resilient electric grid for national security. The Resilient Energy Systems Grand Challenge project is pioneering a comprehensive approach to defend the grid against electromagnetic pulses. The primary task focused on identifying potential component and system vulnerabilities and providing quantitative hardness-level requirements through modeling and testing facilities unique to Sandia. A material and device innovation subtask is investigating EMP surge arrestors and "smart" transformer oil additives. A further grid-scale assessment sub-task will develop scalable approaches to grid-scale probabilistic outages models. (PI: Ross Guttromson)

Radio frequency feature extraction using wireless protocol informatics, pattern matching, and natural language processing. Identifying radio frequency (RF) emitters and assessing the sophistication of a potential cyber-attack through RF means on U.S. space assets requires the development of RF fingerprinting techniques and algorithms. To identify how sophisticated the attacker may be, it is essential to identify the level of protocol-compliant knowledge the attacker is employing such as jamming characteristics and/or waveform utilization, which may also provide information on the potential target(s). The research on this Science and Technology Advancing Resilience for Contested Space Mission Campaign LDRD project includes pattern matching and machine learning techniques to help identify waveform and protocol information. During a demonstration in August 2020, the algorithms demonstrated over 98% accuracy in identifying the waveform most commonly used for satellite command and control. (PI: Chris Howerter)

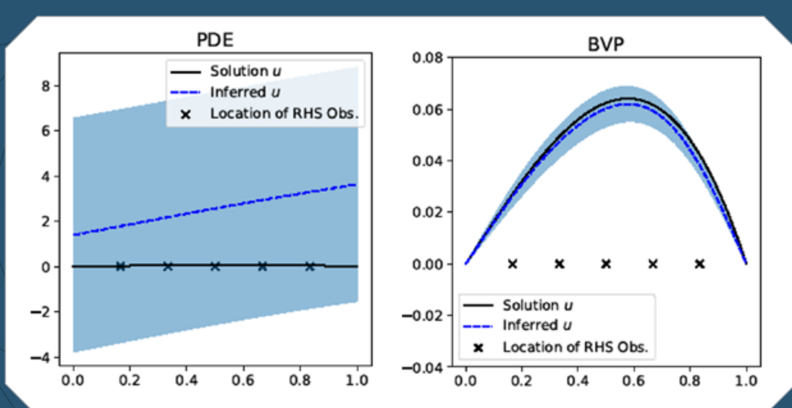


Algorithms demonstrated over 98% accuracy in identifying the RF waveform most commonly used for satellite command and control during an August 2020 demo. (Photo by Chris Howerter)

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 advance our scientific understanding, enable national security, and result in technology transfer to industry that is commercialized under licensing agreements and brought to market for the U.S. public good.

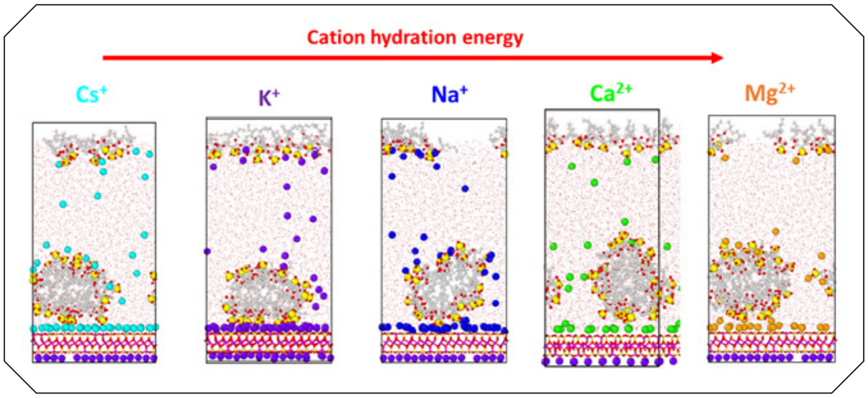
Incorporating physical constraints into Gaussian process surrogate models. Surrogate models are widely used as emulators for expensive physics simulations, but previously no open source or commercial class of machine learning (ML) models, called Gaussian processes (GP), treat constraints. The incorporation of physical constraints and domain knowledge into ML algorithms is a significant challenge when it comes to the application of ML algorithms to scientific and engineering problems. Sandia researchers are investigating Gaussian processes and examined bound constraints, monotonicity constraints, linear operator constraints that represent physical laws as partial differential equations, and intrinsic boundary condition constraints. The resulting approaches are expected to serve as a foundation for physics-constrained Gaussian process applications. (PI: Laura Painton Swiler)



Effect of enforcing a boundary condition when developing Gaussian process surrogates to model the solution of a one-dimensional problem: $-\frac{\partial^2 u}{\partial x^2} = f(x) \quad x \in (0,1),\ u(0) = 0, u(1) = 0$

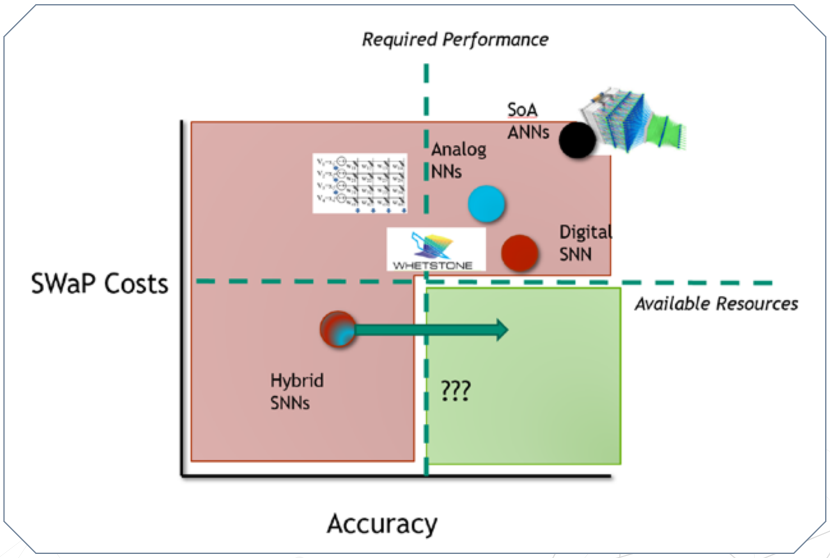
Five scattered observations of f are provided at the points labeled with X. The left panel shows a formulation that incorporates the differential equation information into the GP, but the inference fails with only information about f and not u. The right panel shows the GP with incorporation of the boundary value problem and the improved prediction.

Complex fluid partitioning revealed in surface and pore environments. Understanding the interaction of complex fluids in surface and pore environments is critical for technical advancements in energy-water applications such as resource recovery and water purification. This project combined experimental measurements and molecular modeling to investigate fundamental properties of these fluid interactions with mineral surfaces to provide a more complete picture of surfactant interactions. This research focused on an anionic surfactant and a well-characterized mineral phase representative of oil- and gas-producing shale deposits with the results demonstrating that the presence of surfactant significantly affects the mineral-fluid interfacial structure. Molecular modeling results also reveal details of the surfactant structure at the interface, and how this structure varies with surfactant coverage and fluid composition. This project will enable a broader Sandia capability to solve technical challenges critical to the country's energy-water future. (PI: Jeffery Greathouse)



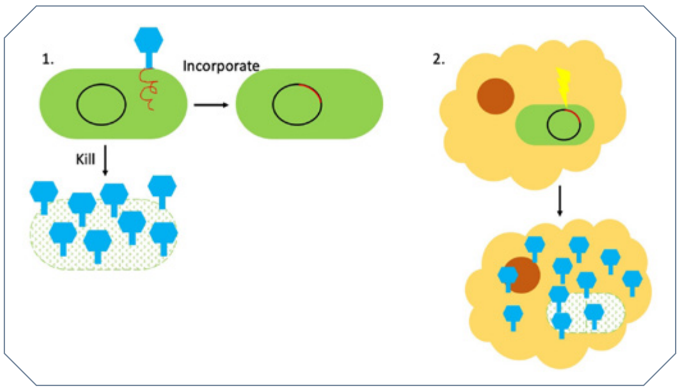
Snapshots from molecular dynamics simulations showing the effect of cation on surfactant micelle structure at a negatively charged mineral surface.

A flexible, highly scalable, configurable neuromorphic architecture. Neuromorphic architectures are proving to be very attractive options for computing since they have, in the past decade, provided potential 100X-1000X efficiency gains over conventional Von Neumann architectures. Both neuromorphic analog and digital technologies provide low-power and configurable acceleration of challenging artificial intelligence (AI) algorithms. This project explored placing deep artificial neural networks onto a hybrid analog-digital neuromorphic architecture that amplifies the advantages of both high-density analog memory and spike-based digital communication while mitigating their limitations. This approach provides a possible avenue for maximizing the benefits of these emerging complementary approaches to neuromorphic computing. It can further U.S. leadership in advanced computing technology by forging a path to widespread applicability of brain-inspired computing from embedded domains to large-scale simulation tasks. (PI: James Bradley Aimone)



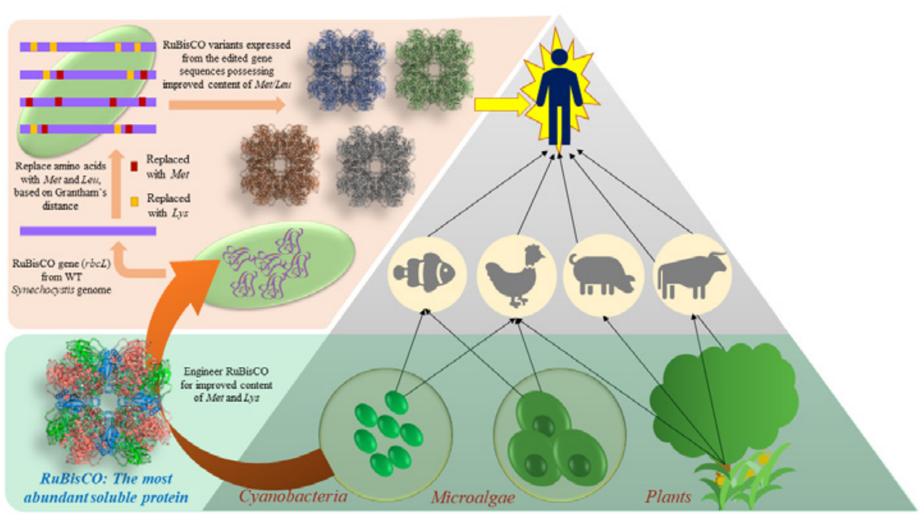
This project focused on techniques allowing hybrid analog-spiking artificial neural networks to get into the "sweet spot" of low computational costs with high performance.

Inducing self-destruction of bacterial pathogens. Bacteria have evolved defenses against the viruses that would otherwise prove lethal to them by incorporating the viral DNA into their own genomes. Some of these bacteria cause human infections and are becoming more resistant to antibacterial therapeutics such as antibiotics. In preliminary research, Sandia scientists demonstrated it is possible to cause the bacteria to self-destruct when they have infected human cells by triggering the expression of this latent viral DNA harbored in the bacterial genome. This work draws on existing computational approaches to identify viral DNA within bacterial genomes and has developed a computational pipeline to identify potential genomic targets. It also builds on and expands Sandia's experimental molecular biology capabilities. Ultimately, this work could lead to new techniques to counter intracellular and antibiotic-resistant bacterial infections. (PI: Catherine Margaret Mageeney)



When bacterial viruses infect bacteria, they have a choice to kill the bacteria or incorporate the viral genome into the bacterial genome. (2) Many pathogens contain at least one of these viruses. When the bacteria infect human cells, the incorporated virus can be activated, causing self-destruction of the bacterial pathogen.

Engineering the most abundant soluble protein on earth to support food security. Global demand for high-quality, digestible protein as a food source is expected to substantially outpace population growth over the coming decades, necessitating gains in feed-to-food conversion efficiency for sustainable food security. Toward these ends, identifying and producing new protein feedstocks that supplement existing agriculture will be of major importance and have significant impacts that intersect with energy and water infrastructure. Ribulose bisphosphate carboxylase/oxygenase (RuBisCO) is the most abundant soluble protein on Earth, produced by photosynthetic organisms such as plants, algae, and cyanobacteria, but is not optimal as a food source because it lacks sufficient amounts of methionine and lysine, which are its first nutritionally limiting amino acids. Sandia's research team genetically engineered a cyanobacterium to significantly increase the amount of these two amino acids in the RuBisCO it produces. This opens the door to use the modified RuBisCO as feed in agricultural and maricultural applications. Sandia is developing commercial partnerships to exploit this advance. (PI: Ryan Davis)



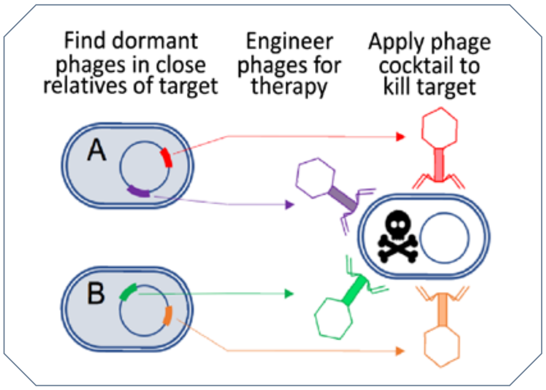
Schematic for bioengineering of RuBisCO, the most abundant soluble protein, for use as a complete, low-carbon protein source from biomass.

Permafrost resilience bioindicators to improve climate model fidelity. Increasing temperatures in the Arctic are thawing permafrost soils that previously remained frozen. The increased microbiome activity in these soils has been shown to release trapped carbon as potent greenhouse gases, such as methane, but with large degrees of uncertainty. To better understand the role of permafrost biology, this project developed approaches to improve genomic and metabolomic analyses of the permafrost microbiome by enriching metabolically active, dormant, and dead microbes through fractionation and sorting of microbial populations. Researchers developed techniques for high-throughput microbial enrichment, repurposed an existing targeted assembly and annotation pipeline to identify a potential bioindicator of methane production in permafrost ecosystems, and applied these approaches to permafrost core samples. These analyses will provide data to improve the biological fidelity of permafrost impact on climate models. (PI: Chuck Smallwood)

Enhanced genomic and metabolomic analyses on permafrost cores, such as the one shown here, will provide biologically relevant input to climate models.

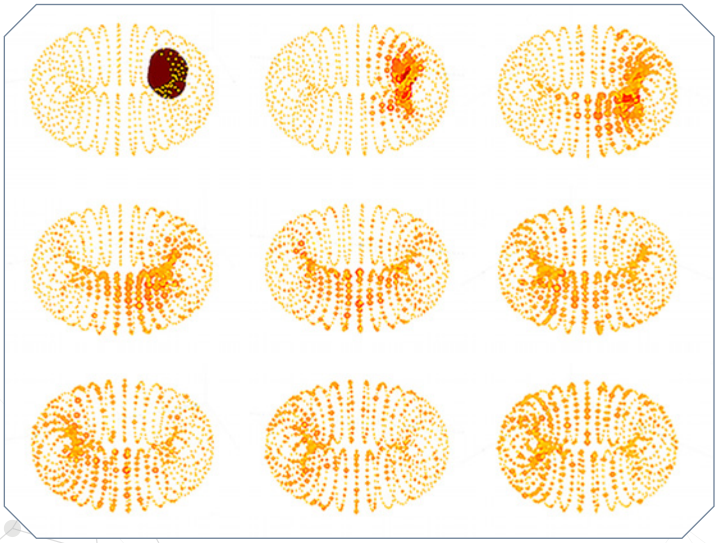
Engineering cells for personalized antimicrobial therapy. Increasing use of antibacterial and antiviral drugs has led to microbial infections that are resistant to these types of therapies, requiring new approaches. One promising broad-spectrum approach is to enhance the human immune system itself to better deal with pathogens on its own. The Sandia and UC Davis research teams have demonstrated that by applying the gene engineering technique CRISPR to mesenchymal stromal cells (MSC), one type of human stem cell, the specific antimicrobial properties in these cells are enhanced. They also proved that modifying MSC surface protein expression can control their behavior. To characterize the properties in these engineered MSC populations, they established and utilized a novel combination of high-throughput population and single-cell nucleic acid sequencing, mass-spectrometry-based protein expression surveys, and high-throughput imaging capabilities. Although animal and human studies are necessary next steps, the work provides a roadmap for engineering of MSCs for immunomodulation applications. Ultimately, these results can lead to expanded antimicrobial therapies and increase the resilience of our healthcare system to future pandemics. (PI: Raga Krishnakumar)

Diversified therapeutic phage cocktails from close relatives of the target bacterium. Bacteriophages are viruses that evolved to attack and kill specific bacteria, making them promising candidates for treating bacterial infections. This approach, known as phage therapy, is more urgent now that bacteria are developing resistance to antibiotics. Software tools developed in this project by Sandia, the University of Florida, and New Mexico Tech collaborators, helped discover new bacteriophages for pathogenic bacteria by searching the genomes of these bacteria for viral genetic sequences that the bacteria have incorporated into their own. This is a significant improvement in our ability to identify bacteriophages, which used to require searching through environmental samples collected in the field. Upon identification, viruses are reconstructed in the laboratory from their genetic blueprints and modified to enhance their lethality to the target bacteria. Choosing bacteriophages from close relatives of the target makes them more effective. Testing against infections in model systems has demonstrated the potential of this approach. With further testing, these results promise quick development of countermeasures that specifically target any bacteria emerging as national security biothreats. (PI: Kelly Williams)



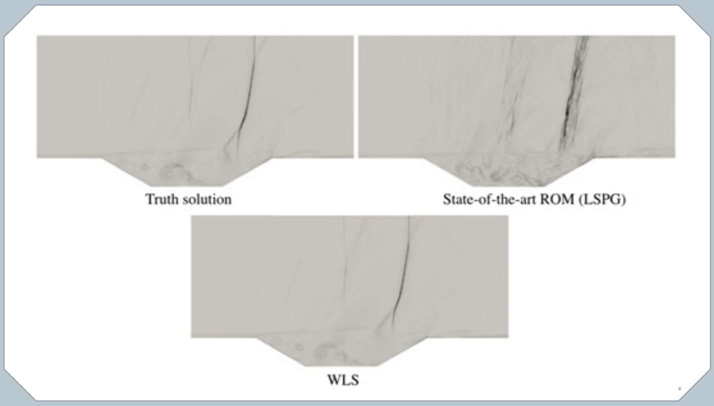
Method for countering any bacterial pathogen using bacteriophages discovered in their genomes.

Energy-efficient implementation of partial differential equations by stochastic and deterministic neuromorphic algorithms. Neuromorphic computing is a new approach to achieving low-power computing solutions by leveraging inspiration from the brain. Since it is critical to stockpile stewardship to facilitate low-power neuromorphic architectures, the team researched computational foundations for solving partial differential equations (PDE). They developed neural algorithm approaches for Monte Carlo-dependent mission relevant PDEs that can be mapped to emerging brain-inspired computer architectures and demonstrated a random walk algorithm with an overall energy consumption (speed/power) that is 20X to 100X better than conventional computing. This is the first formal demonstration of a neuromorphic advantage on a numerical computing application. (PI: James Bradley Aimone)

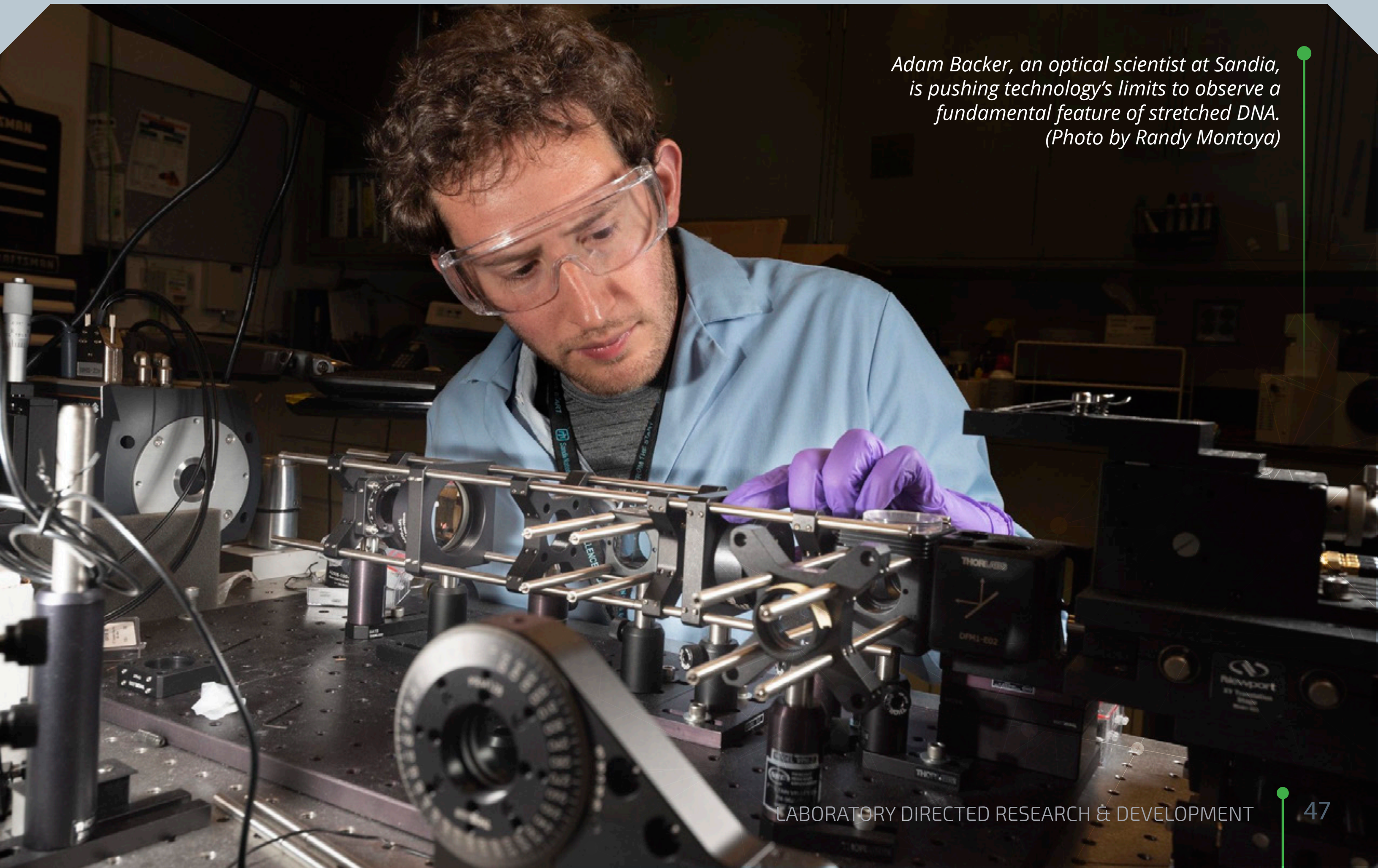


While estimating a solution to a 2D diffusion equation, this figure represents the simulation of 1,000 random walkers moving in parallel over a torus-shaped mesh that represents the networked connections on the Intel Loihi system. The entire random walk process is performed exclusively on the neuromorphic platform.

Integrating state-of-the-art machine learning technologies with multiscale modeling frameworks. Projection-based reduced-order models (ROMs) provide a promising approach for enabling accurate, low-cost simulations of dynamical systems for applications such as engineering design and uncertainty quantification. Unfortunately, state-of-the-art ROM approaches can become inaccurate when applied to systems characterized by nonlinear, nonsymmetric, and multiscale dynamics. In this research, Sandia developed a novel ROM methodology — termed windowed least-squares (WLS) — to address these shortcomings. WLS leverages ideas from space-time model reduction and residual minimization to develop a ROM approach capable of providing accurate and efficient reduced-order models of complex dynamical systems. The methodology was additionally integrated into an open-source reduced-order modeling code developed at Sandia, termed Pressio, and the approach demonstrated on benchmark supersonic and geophysical fluid dynamics problems. The research article, "Windowed least-squares model reduction for dynamical systems," published in the *Journal of Computational Physics*, provides more details. (PI: Eric J. Parish)

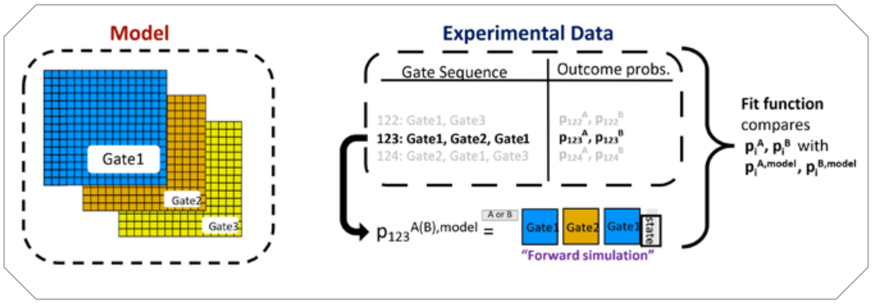


Numerical schlieren of supersonic cavity flow reduced-order model simulations. The new WLS method is closer to the truth solution than other state-of-the-art methods such as least-squares Petrov-Galerkin.



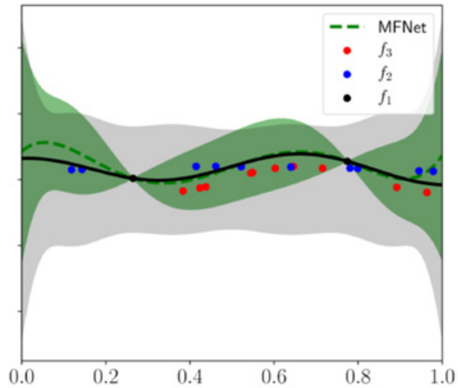
Adam Backer, an optical scientist at Sandia, is pushing technology's limits to observe a fundamental feature of stretched DNA. (Photo by Randy Montoya)

Efficient tomography of many qubit quantum processors is a state-of-the-art advance. The development and evaluation of efficient characterization of many-qubit quantum processors are key to enabling quantum computing hardware. This project focused on the development of multi-qubit tomography protocols that allow for increasing the size (number of qubits) and quality (and hence utility) of quantum processors. The ability to perform useful tomography on 10+ qubits represents a significant advance in the state-of-the-art, which was only two qubits prior to this LDRD. The work will benefit national security missions through its potential to achieve and accelerate applications of quantum computing including cryptography, simulation, and computing beyond Moore's Law. (PI: Erik Nielsen)



Pictorial view of approach: PyGSTi provides efficient forward simulations of quantum circuits, including classes of cloud noise, that enables comparison to experimental data from emerging quantum processors.

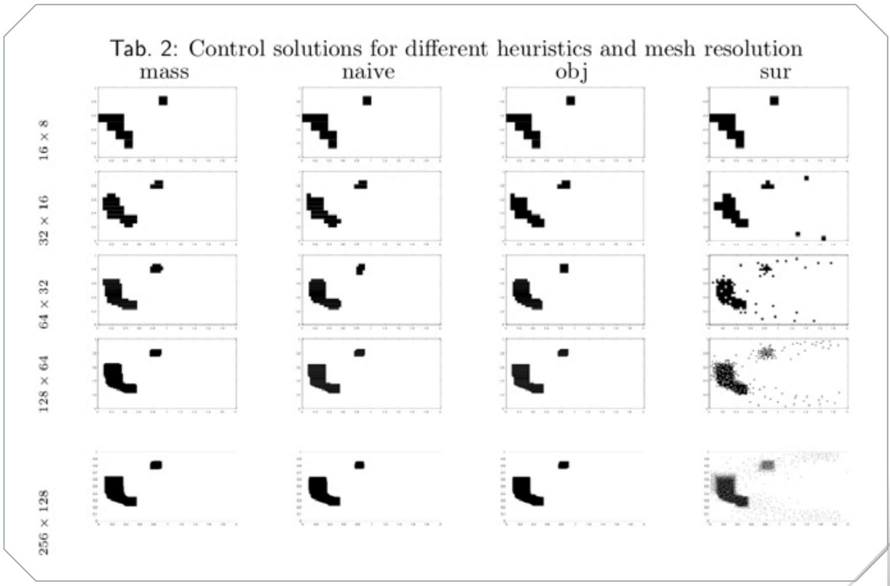
Learning hidden structure in multifidelity information sources for efficient uncertainty quantification. An automated learning framework was developed for efficient analysis and prediction of complex systems that uses multiple sources of data of varying trustworthiness and cost. The Sandia team's approach maximized confidence in predictions by employing approximation strategies that fuse heterogeneous experimental and numerical simulation data in a way that maximizes information gain subject to resource limitations. Predictions are endowed with probabilistic estimates of error, which can be used to create trusted analytics and inform the future design of experiments. (PI: John Davis Jakeman)



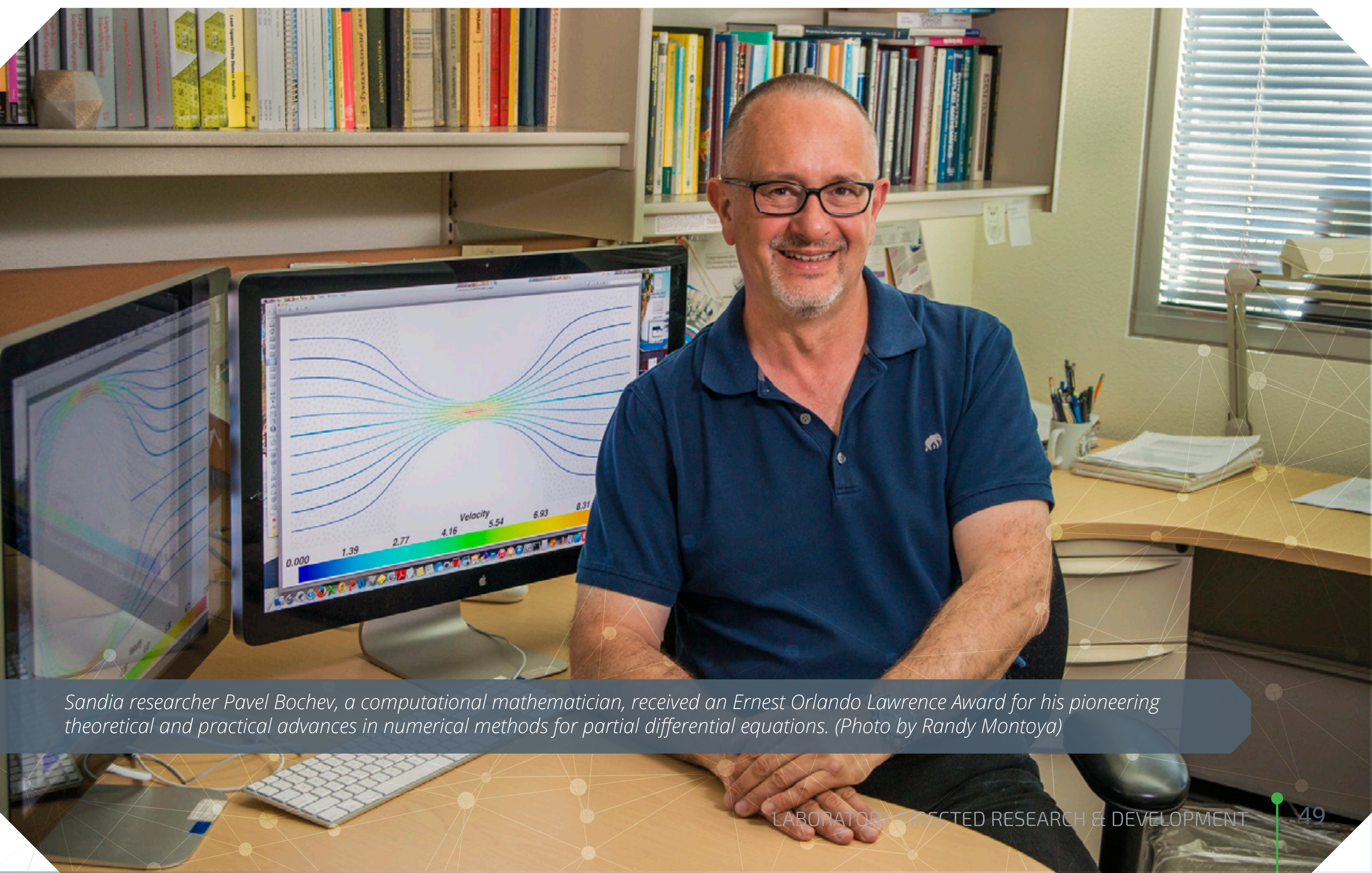
Multifidelity (MF) approximation built using both 1D and 2D low-fidelity and lower-fidelity information sources. The green dashed line is the MF approximation of the high-fidelity function (black line) using two high-fidelity evaluations (black dots) and 10 evaluations of each low-fidelity information source (red and blue dots). The gray region is the original uncertainty, and the green region is the new uncertainty.

Solving specific mixed-integer partial differential equation constrained optimization problems. Sandia and collaborator Georgia Tech created the first highly parallel code for solving mixed-integer PDE-constrained optimization (MIPDECO). Partial differential equations, or PDEs, describe the behavior of objects under constraints such as physics and chemistry. PDE-constrained optimization involves making choices of parameters to solve an inverse, control or design problem involving a physical system. When some of the variables in PDE-constrained optimization must take discrete values, the problem becomes MIPDECO. For example, discrete choices might involve a fixed set of controls on an additive manufacturing machine, selecting materials or making yes/no decisions. The code, called ROL-PEBBL, is C++ and MPI-based. It combines a code to efficiently search over integer choices (PEBBL = Parallel Enumeration Branch-and-Bound Library) and a code for efficient nonlinear optimization, including PDE-constrained optimization (ROL = Rapid Optimization

Library). Creating a general-purpose MIPDECO solver is perhaps a decade away, but this is the first parallel code that can solve specific MIPDECO problems with customized branch-and-bound methods. MIPDECO technology could impact many national security applications such as energy harvesting for weapon systems. (PI: Cynthia Phillips)

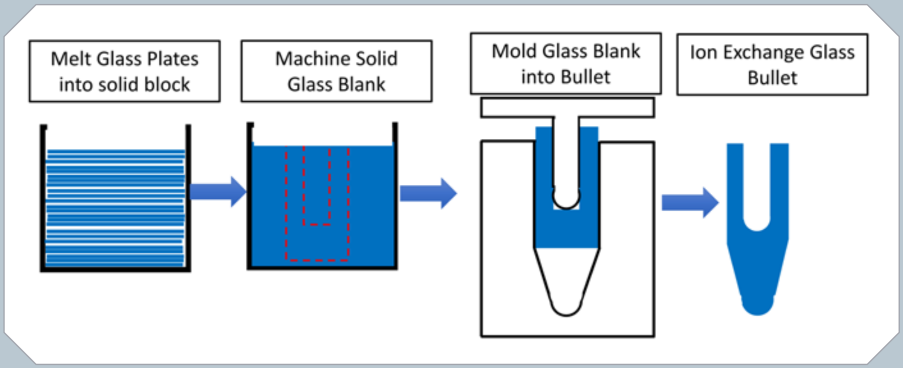


Given sparse measurements of pollution moving by advection and diffusion, the team attempted to approximately locate the pollution source (source inversion) when the sources are restricted to a grid. The input is pollution concentration from the example on the right at sparse random points (.006 samples per grid point) with added noise. ROL-PEBBL gives the solution on the left, with the best optimization guarantee for any general solver that gives both a solution and a quality guarantee.)



Sandia researcher Pavel Bochev, a computational mathematician, received an Ernest Orlando Lawrence Award for his pioneering theoretical and practical advances in numerical methods for partial differential equations. (Photo by Randy Montoya)

Unmanned aerial systems neutralization using disintegrating bullets. Unmanned Aerial Systems (UAS) pose a national security threat. Current counter-UAS technology has limited effectiveness against interdiction of a UAS attack. Disintegrating munitions offers an opportunity to utilize kinetic means to interdict UASs without causing down-range collateral damage. A bullet-shaped glass was developed from Corning 0317 glass and ion-exchanged to create a stressed glass bullet. The glass bullet fragmented into many pieces when a crack was intentionally created with a diamond punch. The glass bullet was successfully fired from a .50 caliber smooth bore muzzle-loading musket with a muzzle velocity of 784.97 ft/sec. A model was developed to predict the stresses produced in the glass bullet during the ion-exchange process, and diffusion-mechanics and viscoelastic constitutive solutions were implemented into a finite element code. Data from this project and resulting disintegrating munitions could prove beneficial to numerous agencies. (PI: Kevin Strong)



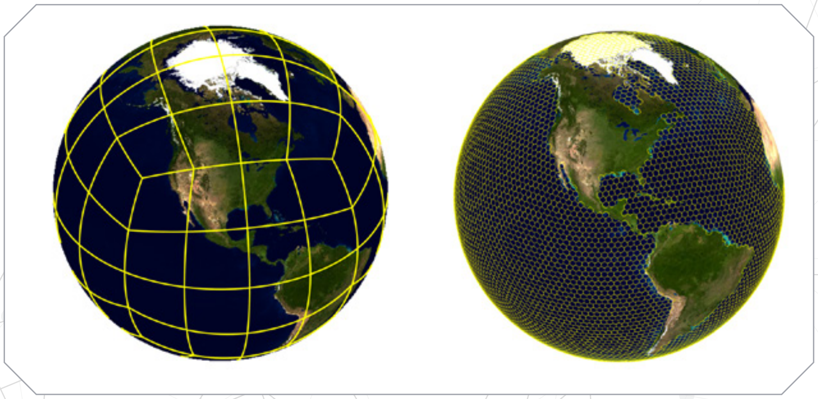
The process of developing a stressed glass bullet.

A glass bullet as it is successfully fired from a .50 caliber smooth bore muzzle-loading musket.

Automated threat modeling for cyber security analytics and emulation. Current state-of-the-art in automated adversary emulation relies on endpoint or network actuation. This Sandia project, done collaboratively with Georgia Tech and Purdue University, created new design tools enabling designers to efficiently generate detailed models of benign and malicious human actors at scale. The resulting Emulytics platform enables automated human actor traffic generation by taking advanced persistent threat actions as inputs and generating automated threat responses. The threat modeling capability includes application-layer artifacts, allowing for selection and design time experimentation. The traffic generation capability captures, encodes, and leverages user activities to develop highly faithful user models. This allows for encoding of benign and malicious traffic and provides a mechanism to derive uniquely identifiable models from a base dataset. Actors were derived from well-described profiles of typical human behaviors and assembled into a library of highly mutable and composable benign and malicious artifacts. This novel Emulytics platform allows for experimenting with human and non-human threats. (PI: Vince Urias)

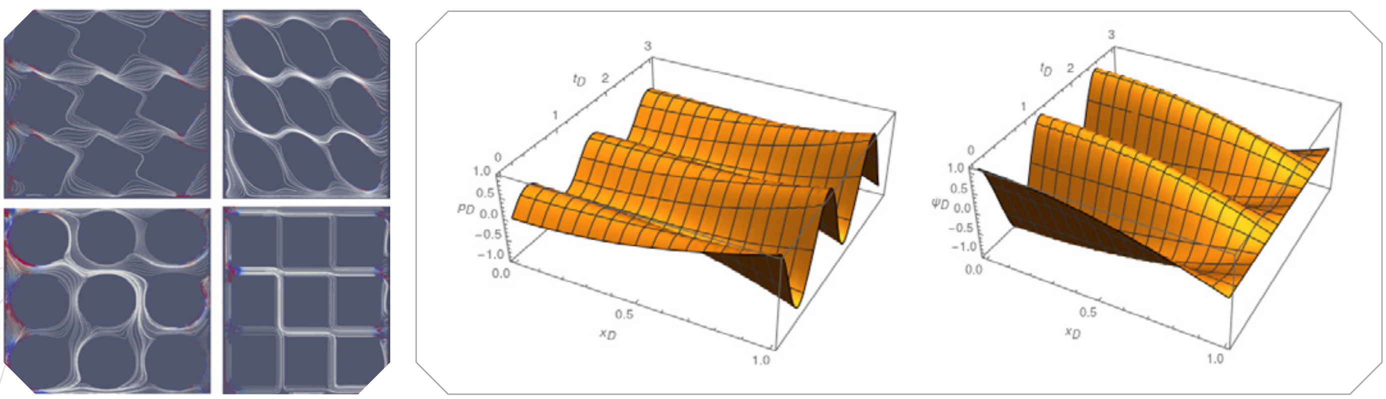
Investigating the Arctic tipping points triggering global change. Tipping events, or small magnitude changes with state-altering effects, are anticipated in the Arctic with the potential to disrupt the global Earth system. By leveraging Sandia's unique data analytics and climate modeling resources, this team developed a framework of computational methods with uncertainty quantification to enable Arctic-focused tipping event prediction. As a first step in quantifying uncertainties in simulated Arctic climate response, Sandia researchers performed a global sensitivity analysis (GSA) on more than 100 perturbed simulation ensembles of one hundred years on 12 Arctic quantities of interest using a fully coupled ultralow-resolution configuration of the Energy Exascale Earth System Model (E3SM). The parameter variations showed significant impact on the Arctic climate state with the largest impact coming from atmospheric parameters related to cloud parameterizations. In addition, significant interactions between parameters from the atmosphere, sea ice, and ocean components of E3SM were found. To the team's knowledge, this is the first GSA involving the fully coupled E3SM. The results can be used to inform model tuning work as well as more targeted studies at higher resolution.

Sandia researchers also trained machine learning models (MLMs) on observational and simulation data from five historical ensembles generated by the E3SM to elucidate the most influential factors in predicting September average Arctic sea ice extent and investigate differences between observed and simulation data. MLMs can help illuminate differences in sea ice response between observational data and simulations in order to guide improvements in sea ice prediction. PhD candidate and year-round intern Jake Nichol, who collaborated with the LDRD team, won the award for best student presentation at the June 2020 *European Seminar on Computing* (ESCO) workshop for his presentation on this work. (PI: Kara Peterson) Watch the YouTube video.



Ultra-low atmosphere grid (left) and ultralow ocean grid (right).

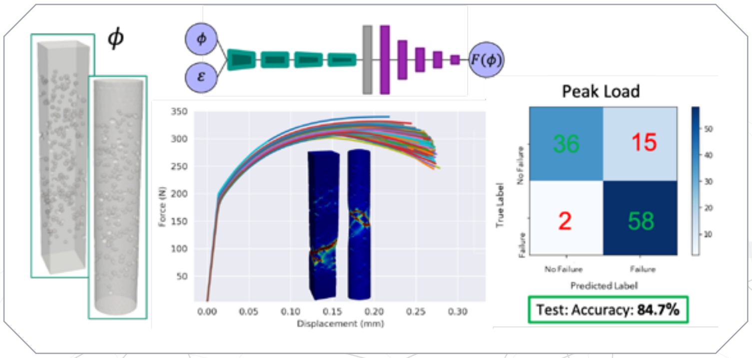
Characterization and sampling of ultralow permeability geomaterials using electrokinetics. Ultralow permeability geomaterials are critical to missions including advanced energy, infrastructure, and nuclear waste disposal. In this project, Sandia, the University of Illinois Urbana-Champaign and Cal Poly San Luis Obispo investigated hydrogeophysical coupling between water movement and electric current flow in tight rocks and developed new transient electrokinetic laboratory methods to sample and characterize properties of fractured ultralow permeability geomaterials (e.g., granite or cement). Characterization of low-permeability rocks – with micron-scale pores – is important for applications like radioactive waste disposal, borehole sealing, water resource management, and CO_2 sequestration. Pressure-driven fluid flow through a porous medium drags along ions, creating a streaming potential. Similarly, applied AC or DC electric current will move ions in the same porous medium, which drags along water, creating an electroosmotic pressure. The team used combined oscillatory tests of these reciprocal effects to estimate steady-state permeability (a parameter of interest in tight rocks) without a traditional Darcy flow test. Sandia PI Kris Kuhlman said, “Leveraging an Academic Alliance partnership, we combined Sandia’s expertise in geomaterials and earth science applications with Illinois’ capabilities to simulate nano- and micro-fluidics, incorporating laboratory, theoretical, and numerical approaches to tackle the electrokinetics problem. The project resulted in journal publications on general approaches to solving coupled multiphysics problems and new insights into the relationship between streaming potential and electroosmosis for a range of pore and path complexities in idealized 2D porous media.” These methods have fundamentally contributed to physical understanding of transient electrical phenomena in rocks, revolutionized Sandia’s ability to understand and control them, and broadly advanced the state of the art. (PI: Kris Kuhlman) Watch the YouTube video.



(Left) Pore-scale flow simulations by the University of Illinois illustrating streamlines around grains of variable shape and orientation. Electroosmosis is stronger in a more tortuous medium, while streaming potential is stronger in a less tortuous medium. (Right) Predicted pressure (p_D) and electrical (ψ_D) response in space (x_D) and time (t_D) for a harmonic streaming potential test, based on simple analytical solutions using the new uncoupling approach.

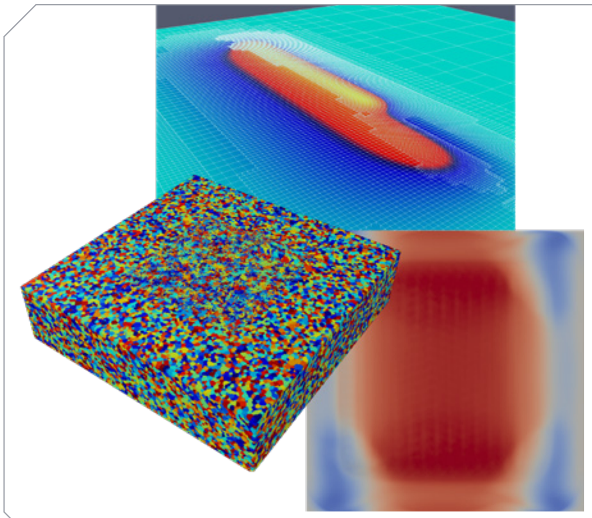
The Sandia Fracture Challenge morphed from a materials scientists and engineers' competition into a collaborative community of researchers refining their techniques for engineering reliable structures made from a variety of materials. (Photo by Randy Montoya)

A new paradigm for failure prediction using 4D materials science and deep learning. Accurate and efficient performance prediction in weapon components is crucial to maintaining a safe and secure nuclear deterrent. Even with rich characterization of the existing microstructure and defect population, simulating the behavior of these parts remains challenging and computationally intensive. This LDRD utilized a 3D convolutional neural network (CNN) to predict mechanical performance based on experimentally measured initial pore structures in additively manufactured tensile samples. High-fidelity simulation results using the Sierra/Solid Mechanics code suite served as training data for the CNN, which classified several metrics of part performance five orders of magnitude faster than traditional finite element analysis. The trained network also remained predictive when the sample geometry and loading condition were varied from what was used in training data. This work is now being extended in a new LDRD to predict failure in conventionally processed metal components using cutting-edge experimental characterization and multiscale modeling. (PI: Kyle Johnson)



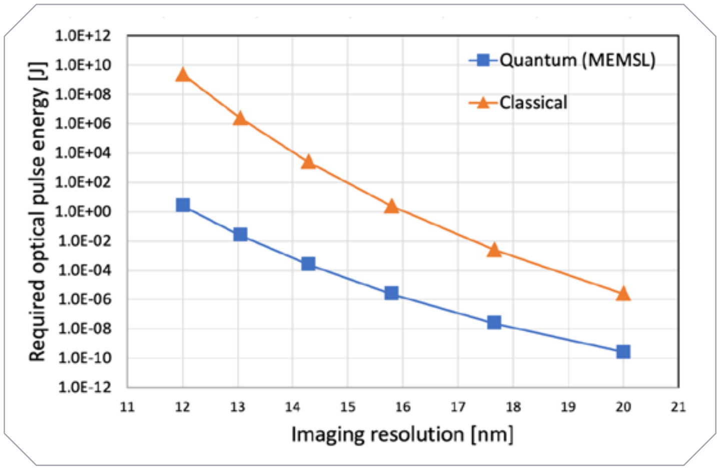
(Left) Sample meshes of porous additively manufactured square and cylindrical tensile specimens were generated based on computed tomography measurements. The simulated force-displacement histories of 1,000 microstructure samples (lower middle) were used to train a deep-learning algorithm (upper middle) to classify samples based on peak load predictions with 85% accuracy. The confusion matrix (right) shows predicted labels and true labels for a reserved test set of tensile samples.

Multiscale approach to fast ModSim for laser processing of metals benefit future nuclear deterrence environments. New modeling capabilities, developed to predict laser-processed metal part performance from manufacturing process parameters, resulted in a thermal modeling technique able to run 72X faster than previous methods. Rapid predictive models of advanced manufacturing processes are critical tools needed to achieve a flexible and responsive nuclear deterrent. The models resulting from this project continue to be developed by Sandia and will result in a full suite of rapid, predictive laser-metal process models that will facilitate a more agile advanced manufacturing design and qualification process for system components needed by the nuclear deterrence mission. (PI: Dan Moser)



Simulated temperature, microstructure, and residual stress distributions for a laser-processed metal part.

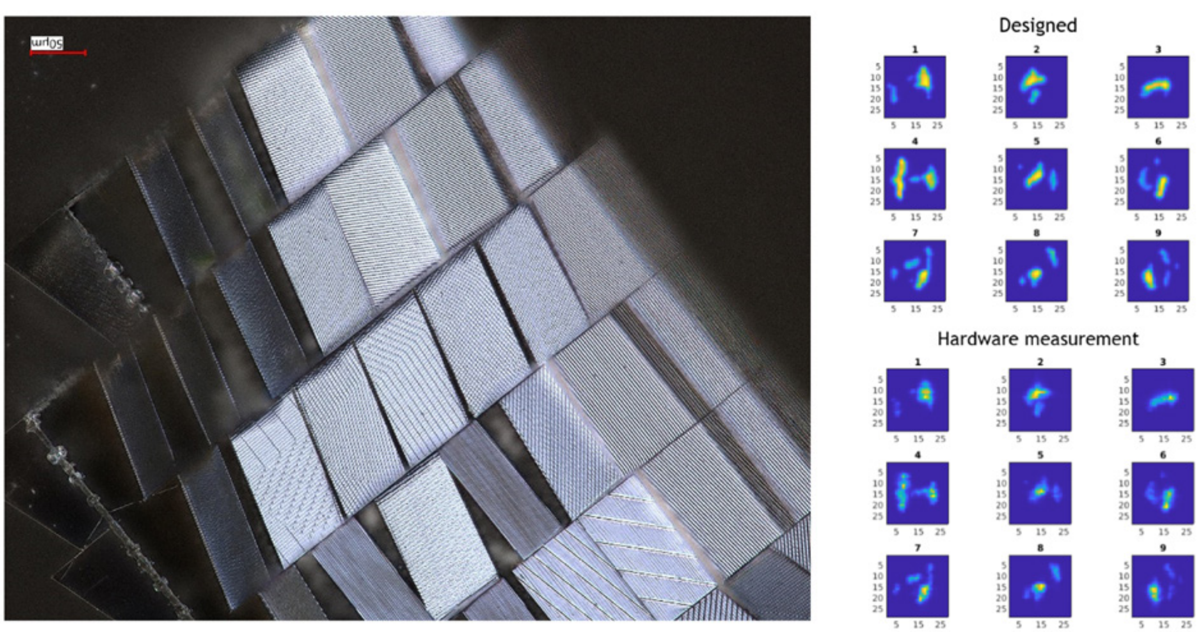
Quantum-enabled bioimaging using a multipartite-entangled light source. This project studied the feasibility of a quantum-enabled super-resolution bioimaging technique to monitor various bio-activities of the nanoscale (~25 nm). Observing the detailed biological mechanisms at the nanoscale will dramatically increase the understanding of sub-cellular biology — the mechanisms for cellular response to disease. During the course of this work, the team discovered a working quantum imaging configuration using multimode entangled squeezed light and showed that quantum imaging noise can be lower than classical imaging noise. These successes promise to usher in nanoscale in-situ bioimaging, impacting basic science to reduce global biological security threats and guarding against the bio-technological surprise. (PI: Daniel Soh)



Quantum imaging can achieve equivalent signal-to-noise performance with orders of magnitude lower optical energy.

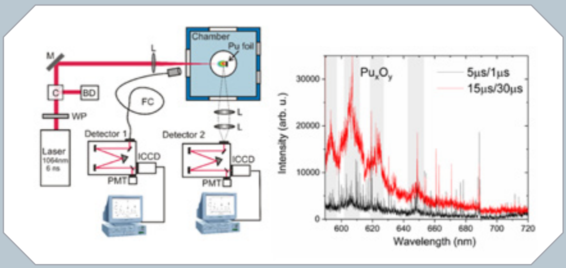
High-throughput discovery of tools for brain protection. Protection of the brain from chemical, biological, and radiological threats is dependent on successful non-invasive delivery of medical countermeasures across the blood-brain barrier. Existing delivery methods of cargo to the brain lead to inefficient or non-specific penetration of the blood-brain-barrier, so the team focused on using functional and selective screening of brain-penetrating nanobodies under physiological conditions to identify novel noninvasive routes of delivery to the brain. Through this project, the team generated a large >10^{10} library of nanobodies already being utilized in multiple Sandia studies, including COVID-19 research. Several of these nanobodies were identified as promising blood-brain-barrier shuttles and are being further investigated. If successfully developed, these blood-brain-barrier shuttles will assist in national security threat mitigation. (PI: Maxwell Stefan)

Ultra-efficient sensing system through holistic design. Many metrics used to evaluate high-quality optical devices are focused on imaging, and therefore biased by what observers perceive to be “good” images. Many optical devices, however, are now being used as part of a larger system to perform machine learning and are therefore less constrained by traditional imaging performance. This project developed computational imaging techniques that design the optical component while simultaneously developing the machine learning algorithms. By leveraging the photonics, optical science, and machine learning capabilities at Sandia, the team developed generalizable techniques to create nearly arbitrary linear optical systems. These systems can directly measure significantly compressed data while still retaining the ability to classify scenes via a machine learning element. Creating task-specific optical devices can enable lower size, weight, and power-consuming sensors ultimately capable of performing a machine learning task. This technology could influence the growing domain of ubiquitous sensing and suggests that computational imaging can play a practical role in national security relevant problems. (PI: Gabriel Carlisle Birch)



(Left) Microscope image of a multiphoton lithography-generated refractive computational optical element, designed via a machine learning optimization process. (Top right) The predicted output for the computational sensing device from simulations. (Bottom right) The measured output of the computational sensing device.

Optical spectroscopy of plutonium project provides critical data for remote-sensing proliferation detection and nuclear detonation applications. There is a critical need to measure optical emission characteristics of plutonium (Pu) and its isotopes in high-temperature plasmas, such as those encountered in a detonation fireball or laser ablation plume. Previously, less than 20 unpublished transition probabilities (Einstein A coefficients) were measured using low-temperature lamps. The research team used laser-induced breakdown spectroscopy (LIBS) as a tool for creating high-density plasma and determining spectro-temporal signatures of Pu at high temperatures (3,000-8,000K), including the first published optical emission spectrum attributed to Pu oxides. The results are documented in the Atomic Plutonium Atlas, a comprehensive digital reference on the optical spectrum with thousands of energy levels and transition probabilities of atomic Pu. Through this work, critical data was provided on the identification and characterization of Pu in small samples for proliferation detection and in nuclear detonation remote-sensing applications. (PI: Sudeep Mitra)



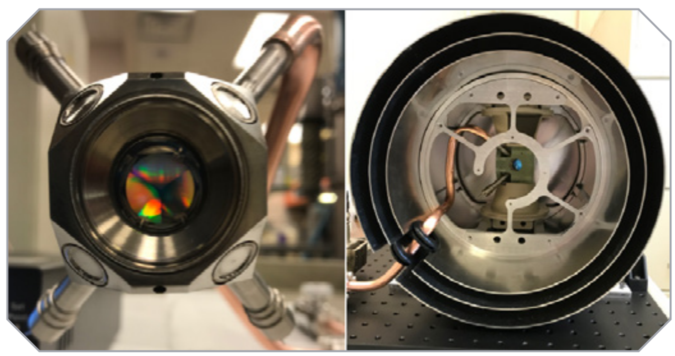
First-published spectrum of Pu oxide emission using LIBS.

Integrated challenge defends the grid against high-altitude EMPs. Sandia's EMP Grid Grand Challenge LDRD, which completed in September 2020, pioneered a comprehensive approach to defending the grid against high-altitude EMP (HEMP). The research team determined risk to the grid if a HEMP event were to occur, developed the ability to predict EMP-coupled insults to grid equipment, and conducted pulse tests up to 500kV. The probabilistic failure rates of equipment were identified and models established to understand grid cascading and how to dynamically recover. In addition, a polymer for transformer thermal management was created. Follow-on development and application work will continue in this emerging area of national security. (PI: Grant Biedermann)

Developing the world's first low-SWaP inertial sensor based on atom-interferometer technology. Atom interferometers could provide a GPS-denied solution for applications using a Size Weight and Power (SWaP) slightly larger than HG9900 but less expensive than traditional strategic grade sensors. Traditional strategic-grade inertial sensing can provide superior on-target weapon delivery but are limited in SWaP and in their ability to handle dynamics. The Strategic Inertial Guidance with Matterwaves Grand Challenge LDRD developed a sensor on path to 0.3L at a cost of less than $300k and a bias stability of 0.25 micro-g and a 20-foot circular error probability at the end of a 20-minute mission or an error growth rate of ~0.1 nautical mile/hour. The project team developed:

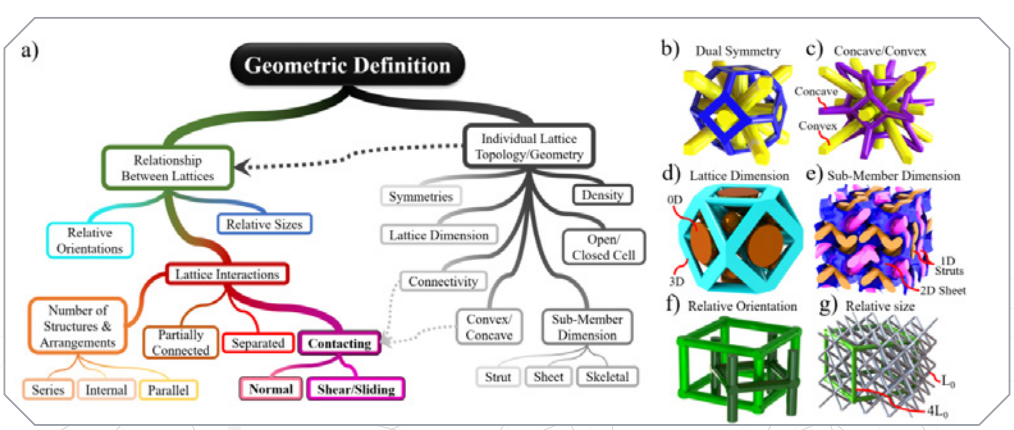
- The first atom interferometer with a grating magneto-optical trap having a data rate of 6.7 Hz and uncertainty of ~25 micro-g.
- An optical-alignment-free sensor head design, techniques to operate the atom interferometer accelerometer in a dynamic environment, and a passively pumped ultra-high vacuum package, demonstrating no degradation of the vacuum for three months and counting ... a world's first.
- A photonic integrated circuit that can provide the required control, which, when integrated with the chip-scale optical amplifiers and frequency doublers (also under development), will provide the world's first integrated laser system for an atom interferometer.

(PI: Grant Biedermann)



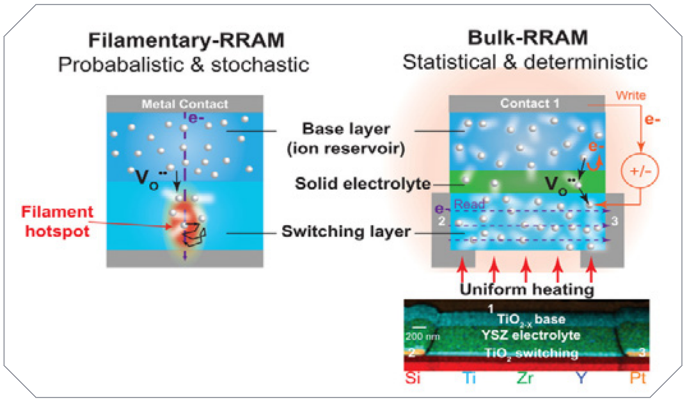
(Left) View of grating chip mountain within the draft prototype. (Right) Test fit of draft prototype into the sensor assembly within the magnetic shielding chamber.

Bringing Euclid's imagined concept to life: Interpenetrating lattice metamaterials. Around the year 300 BC, the Greek mathematician, Euclid, imagined the geometric concept of a dual polyhedra: one 3D shape perfectly intercalating through the interstices of another without touching. Now, using modern 3D printing capabilities, an LDRD team turned these geometric concepts into reality. By tiling dual polyhedra in 3D space, these new "metamaterials" possess an array of strange and potentially useful properties, including a remarkable resistance to fracture, and an ability to electromechanically measure stress with far better sensitivity than existing sensors. The work has resulted in a provisional patent application (filed) and a paper (accepted for publication in *Additive Manufacturing*). (PI: Brad Boyce)



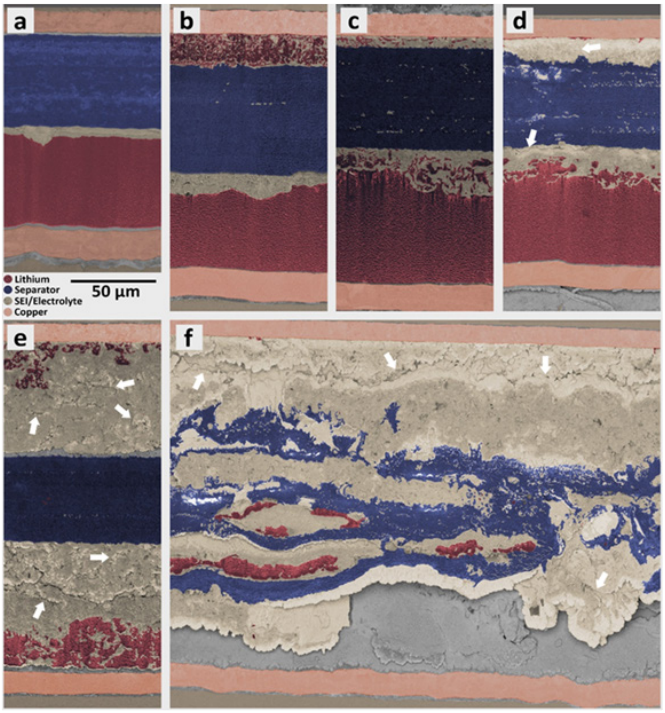
(a) Geometric features that define interpenetrating structures, (b-f) examples of interpenetrating structures demonstrating key geometric features, (g) four body-centered cubic cells nested inside a larger tetragonal cell.

An interfacial synaptic transistor for fast neuromorphic computing. A novel electronic memory device called an electrochemical random-access memory (ECRAM), which is ideally suited for energy-efficient brain-inspired computing, was the outcome of this innovative LDRD project. The ECRAM device is based on fast, low-voltage manipulation of oxygen vacancies in a nanoscale, transition metal oxide channel. By tuning the bulk vacancy concentration within the 3D bulk of the channel, the team solved the challenge of stochastic switching that has plagued filament-based memristors. This provides a compelling artificial synapse for energy-efficient training of deep neural networks, which are then used to process information such as rapid and accurate recognition of images and sounds. The work resulted in a filed patent application and a paper published in the *Advanced Materials*). (PIs: Yiyang Li, Alec Talin)

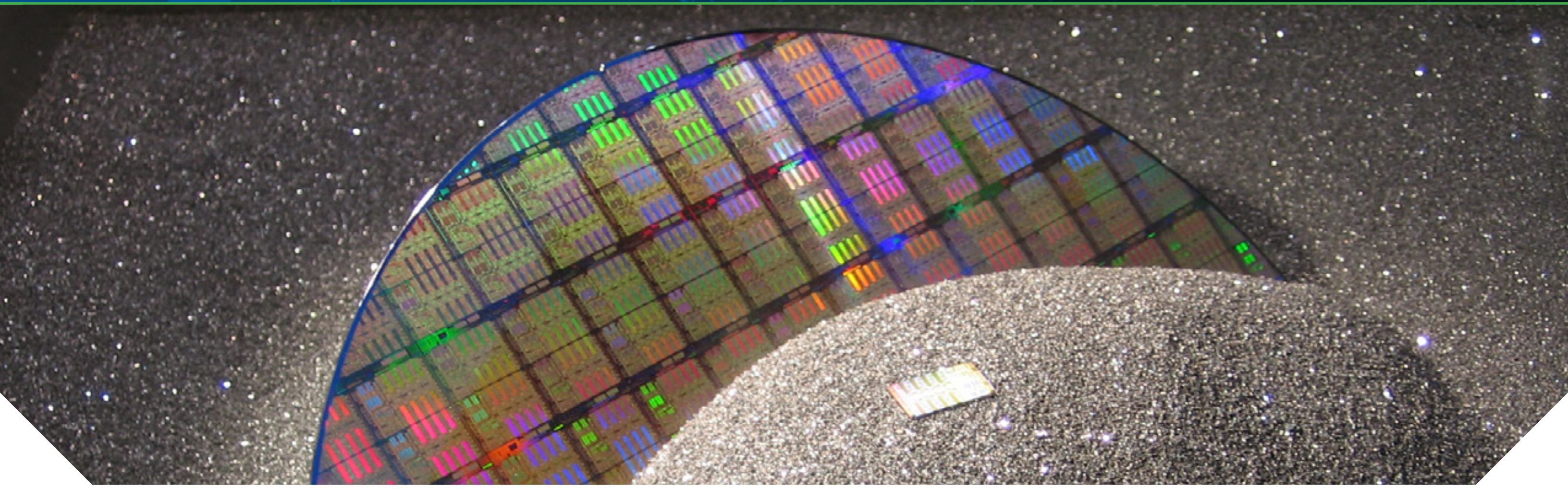


Filamentary-Resistive Random Access Memory (RRAM) compared to Bulk-RRAM.

The relationship between electrochemistry and mechanics in batteries. Lithium metal is the "holy grail" anode material to enable the next-generation of high-energy-density batteries. Because lithium metal anodes undergo large volume and morphology changes during cycling, this project focused on studying the effects of applied interfacial stress on lithium metal anode cycling. The team found that interfacial stress can significantly affect performance and volumetric energy density, which led to a patent application and two papers in preparation. Sandia successfully partnered with ThermoFisher to develop a new technique for imaging entire coin cell batteries without disassembly using ThermoFisher's new Tribeam scanning electron microscope. Ultimately, the project demonstrated that bulk electrodeposited lithium can bear residual stress and showed for the first time that the residual stress can be characterized by X-ray diffraction, resulting in a journal article published in *Powder Diffraction*. (PI: Katie Harrison)

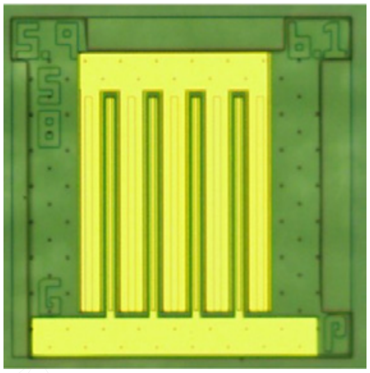


Scanning electron micrographs of intact angled-sections of high-rate cycled Li-metal coin cell batteries. (a) uncycled cell, including: stainless-steel cap, Cu current collector (salmon), stack of two Celgard 2325 separators (blue), Li metal (pink), bottom Cu current collector (salmon), and lower stainless-steel disc, (b) 1st Li cycle plating, (c) 1st Li cycle stripping, (d) 11th cycle plating, (e) 51st cycle plating, and (f) 101st cycle plating step. The battery cycling process causes destruction of the separators.



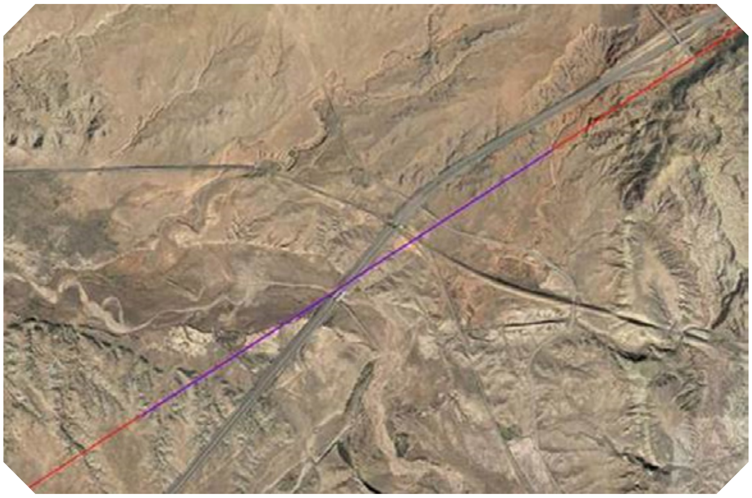
Mitigation of point defects in wide-bandgap semiconductors. Wide-bandgap (WBG) semiconductors represent today's state-of-the-art materials for high-performance power electronics and are being developed for the electric grid and other critical applications. However, the performance of WBG devices, such as gallium nitride (GaN) vertical power diodes, is presently limited by native crystalline defects and impurities that incorporate during materials growth. This project demonstrated that above-bandgap, ultraviolet (UV) excitation of GaN during materials growth can significantly reduce the density of carbon impurities that limit device performance by compensating intentional dopants. This UV-induced reduction in compensating defects was shown to improve GaN electronic transport properties by increasing both electronic carrier densities and mobilities. Through defect-aware drift-diffusion modeling, the project predicted that compensating defects at the sample surface can be converted to benign defects by UV-induced electronic carriers over a reasonable range of growth parameter space, revealing a viable mechanism by which compensating defects are reduced. (PI: Mary Crawford)

Compact solid-state high-voltage switch. Researchers at Sandia developed a semiconductor-based high-voltage switch, with experimental results showing potential for enhanced radiation hardness, for use in several power conversion applications. Gallium nitride (GaN) metal-oxide semiconductor field effect transistors (MOSFETs) were modeled using commercial and Sandia's Charon software to understand their performance and for prediction of future device operation in radiation environments. Fabrication of the GaN MOSFETs required development of epitaxial materials growth using metal-organic chemical vapor deposition, design and fabrication of the insulating gate structures using atomic layer deposition, and high-voltage edge termination designs. This technology laid the path to eventual replacement of traditional vacuum switches with GaN MOSFET switches for improved timing performance, lower cost, and faster redesign cycle time to accommodate evolving requirements. (PI: Gregory Pickrell)



Prototype 4-finger GaN MOSFET chip before packaging and subsequent technology maturation. Current scaling would increase chip size to ~5.5 mm x 5.5 mm and would require a package size similar to a traditional vacuum switch for comparable performance.

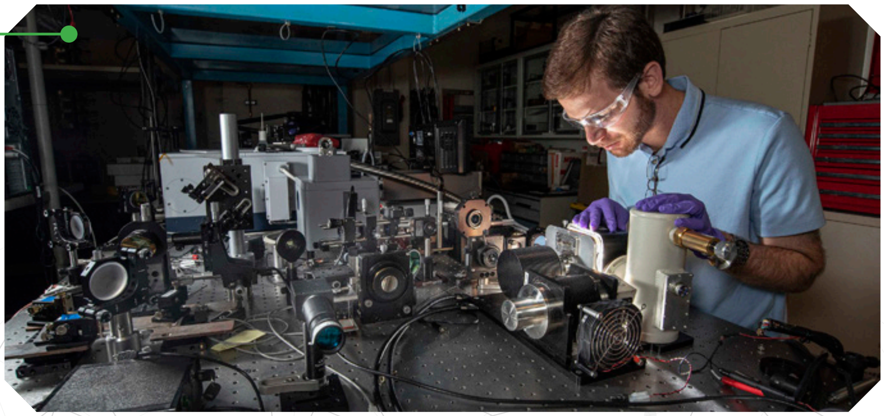
Enhanced positional awareness and jammer resistance for radar fuzing. A novel variant of terrain-aided location estimation was developed and validated by Sandia researchers to facilitate greater positional awareness using a beam-sharpened altimeter (vertical Synthetic Aperture Radar – SAR). This technology can provide future delivery systems with improved positional and trajectory awareness in flight to fuze the weapon at the correct time and location. This provides additional safety, while avoiding the additional equipment and processing complexity of a more complicated directional altimeter or conventional broadside SAR. Some of the technical enhancements achieved relate to ranging resolution, terrain references, trajectory flexibility, ranging altitude, along-path fixes, and counter-measure response. The technique has been validated in flight with a test-bed radar installed on a manned aircraft, demonstrating improved predicted versus measured range differences and resulting in high-quality navigational updates, while flying at over 2,000 m above ground level. (PI: George Sloan)



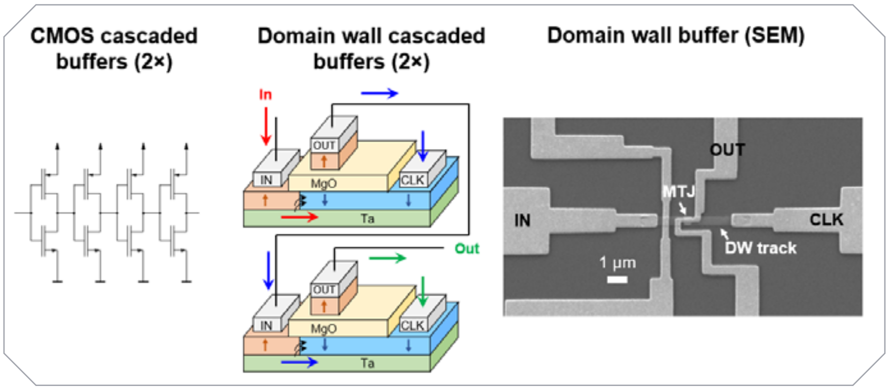
Test flight path, with 3.2 km measurement tail (in purple).

Optical property sculpting with phonon laminates improve national security capabilities. Tunable infrared (IR) plasmonic devices offer utility unavailable with traditional optical components. They are hamstrung, however, by dielectrics that either offer optical or electrical performance but not both. In this project, the team leveraged emergent phonon phenomena — originally developed within thermal physics — to tailor the infrared response while also efficiently mediating electrostatic doping of underlying tunable optical materials. Tunable IR materials, with enhanced ability for detection and sensing, will improve national security capabilities. This project identified mechanisms affecting phonon and infrared responses of superlattices and then investigated these mechanisms for engineered functionality which led to a technical surprise with photoelectron emission. During this work, the project led to three graduate students mentored/recruited to internships, two postdoctoral fellows hired at Sandia, and one postdoctoral fellow converted to staff. In addition, four papers have been published to date. (PI: Thomas Beechem III)

A team of researchers developed a nanoantenna-enabled detector that can boost the signal of a thermal infrared camera by up to three times and improve image quality by reducing dark current, a major component of image noise, by 10 to 100 times. (Photo by Randy Montoya)

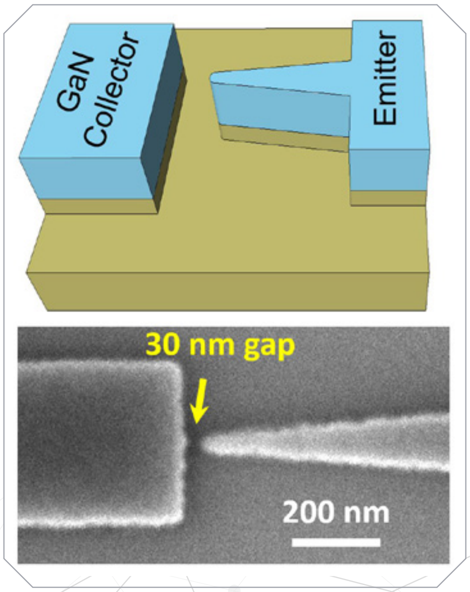


Radiation-hard nonvolatile memory and logic based on magnetic tunnel junctions. State-of-the-art computer processors using electric-charge-based devices have drawbacks including fundamental limits on energy efficiency and sensitivity to radiation. Changing the state variable from charge to magnetization can overcome these limitations. Magnetic memory, which represents the stored memory state by two parallel ferromagnetic layers, is now commercialized. In addition, ferromagnetic layers were recently extended to form logic devices using magnetic domain walls (MDW), replicating complementary metal oxide semiconductor (CMOS) logic. In these devices, logic states are delineated using the separation of magnetic domains that are polarized in different directions (see figure). For the first time, Sandia and the University of Texas at Austin demonstrated MDW logic gates using the efficient spin orbit torque (SOT) effect, that are cascadable, electrically controlled, and demonstrate a record 164% separation between logic states. Furthermore, a device-circuit codesign model predicts power efficiency beyond CMOS limits using SOT MDW logic. Finally, initial radiation measurements on SOT devices confirm resilience to these effects. These results pave the way for low-power, radiation-resilient magnetic computing. (PI: Matthew Marinella)



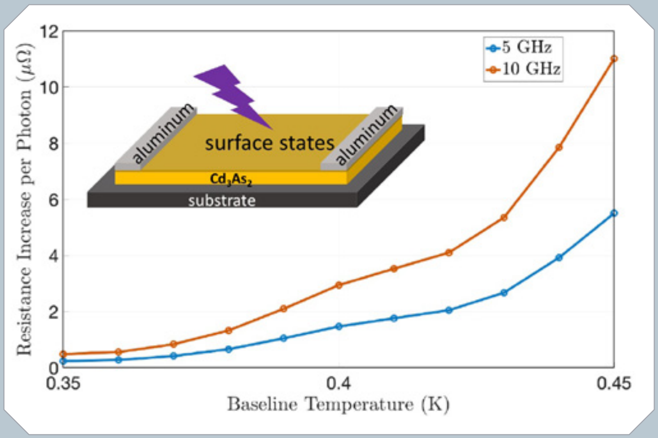
Traditional CMOS cascaded buffer circuit (left) next to the equivalent magnetic domain wall buffer circuit (center) representing the device demonstrated by the Sandia-UT Austin LDRD project. (Right) A scanning electron image of the device is shown.

GaN vacuum nanoelectronics: A new platform for radiation-hard devices and beyond. Sandia developed a new type of on-chip, nanoscale vacuum electronic device that combines the advantages of modern, solid-state devices with "old-school" vacuum tubes. Vacuum tubes are still prized for applications requiring very high frequency and power as well as operation in harsh environments, where even modern silicon-based solid-state electronics are lacking. However, traditional vacuum tubes are large, power hungry, and require a vacuum environment to operate, greatly limiting their use. The new, solid-state "nano-vacuum tubes" were fabricated from gallium nitride (GaN), due to its optimal properties for this technology. Recent GaN devices demonstrated ultra-low turn-on voltages that are an order of magnitude lower than competing silicon- or silicon carbide-based devices. Additionally, due to the nanoscale dimensions of the vacuum channel, the GaN devices achieve this performance in air, without the need for vacuum packaging. Future devices that can be enabled by this novel technology include radiation- and EMP-resistant electronics and photonics that can operate at high speeds and with low power consumption. (PI: George Wang)

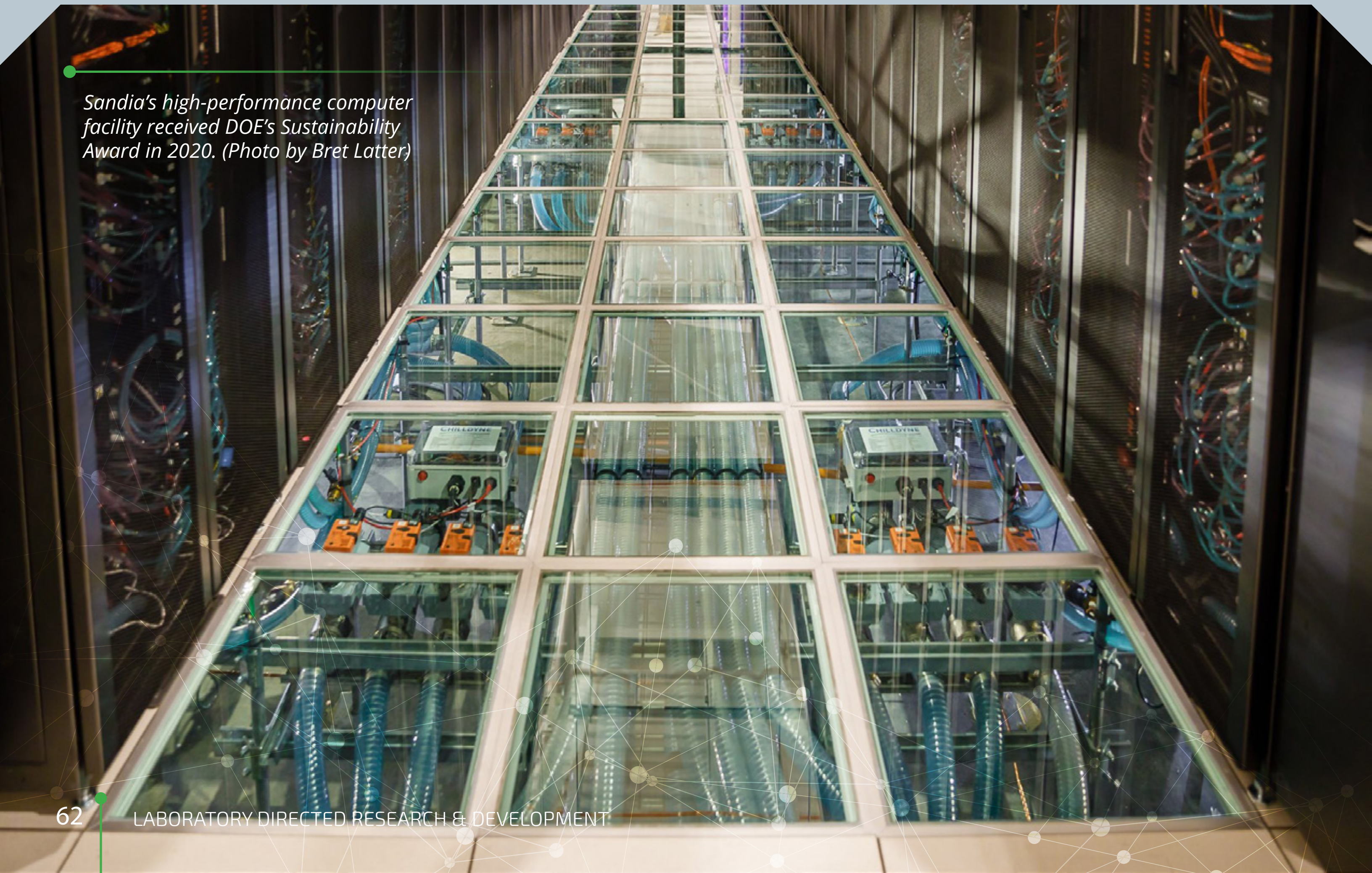


Schematic (top) and electron micrograph (bottom) images of an on-chip, integrated GaN nanoscale vacuum "tube" (diode) with gap size below 30 nm and operable in air.

Single photon detection with on-chip, number-resolving capability. A novel single photon detector (SPD) that operates at microwave frequencies with the potential for deterministic photon number resolving capability is a new development at Sandia. Photon number resolving detectors are highly desired due to their potential to enable major advances in applications including quantum communications and quantum sensing. Existing SPDs do not provide this photon number resolving capability at microwave frequencies due to the low energy of each individual photon. To overcome this challenge, the LDRD team employed topological quantum materials for which the zero-gap superconducting surface states allow for deterministic, number-resolving microwave photon detection. They developed a detailed theoretical model based on their microwave absorption experiments and showed that their approach can lead to a new method for microwave single photon detection suitable for quantum information science applications. The project has further fostered fruitful collaborations with Georgia Tech and the College of William & Mary. (PI: Wei Pan)

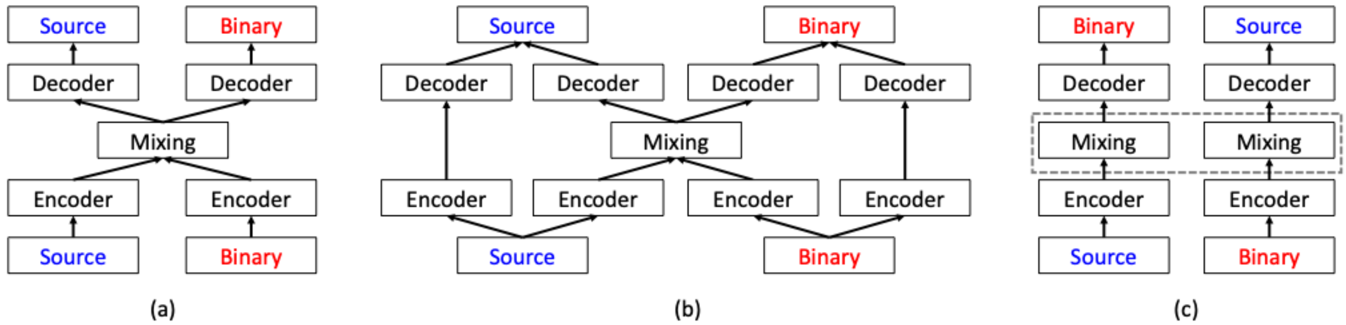


Single photon detection in topological quantum materials. The inset depicts a Josephson junction based on Cd_3As_2, a topological quantum material. The main plot shows the bulk resistance gain (in microohms) due to absorption of a single photon vs. baseline temperature for photon frequencies f = 5; 10 GHz.



Sandia's high-performance computer facility received DOE's Sustainability Award in 2020. (Photo by Bret Latter)

Multimodal deep learning models improve automatic identification of security flaws in software. Sandia and its customers will operationalize machine learning-based methods that simultaneously leverage both source code and machine binary representations of software programs to identify security flaws, thanks to a recent LDRD project. Typically, software developed and used in national security missions is audited and tested before deployment by analyzing source code or reverse engineering a program's binary representation. These newly developed machine learning models, based on multimodal deep learning approaches, were designed to model and analyze both representations simultaneously. Results of applying these models to the Juliet Test Suite, a benchmark used by researchers to demonstrate the efficacy of new methods, and a version of the Linux operating system kernel containing synthetically injected flaws, illustrate a marked performance improvement over existing state-of-the-art machine learning methods. (PI: Daniel Dunlavy)

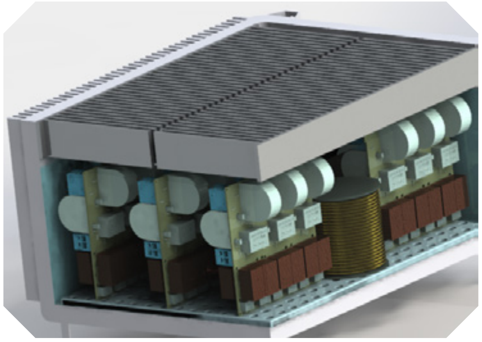


Multimodal deep learning models, based on (a) correlation networks, (b) joint autoencoders, and (c) bidirectional deep neural networks, can accurately model security flaws in software by leveraging both source code and machine binary representations of programs.

Capability development for prediction and optimization of engineered anisotropic thermal barriers. Advanced barriers are needed to protect components from mechanical, thermal, electrical, chemical, electromagnetic, and radiation insults. Multi-layered or composite barriers may be used to manage different environments. The team developed new experimental capabilities to measure the anisotropic thermal properties of advanced thermal barriers. This capability will be the foundation for any further development of thermal model and material designs for advanced thermal barriers. (PI: Karla Reyes)

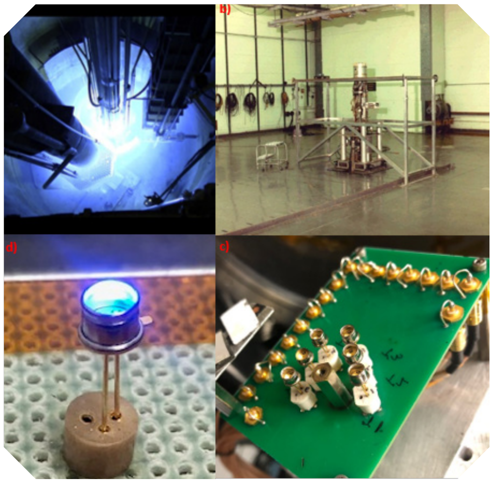
Next-gen high-power electronic systems to be enabled by first AlGaN-based vertical power-switching transistors. The first aluminum gallium nitride- (AlGaN) based vertical power-switching transistor was the product of this Sandia research. The team developed a mechanistic understanding of how crystalline defects at a regrown p/n junction interface influence reverse electrical leakage in AlGaN-based diodes. This understanding enabled selective-area-regrown p/n junctions with low leakage current and will be used as the core element necessary to demonstrate the first AlGaN-based vertical power-switching transistor, an enabling capability for next-generation high-power electronic systems. (PI: Andrew Allerman)

Distributed computational algorithms focusing on modeling and demonstration of transformer cyber resilience. The current power system depends on thousands of generators working in unison (phase and frequency must match) to meet the nation's ever-increasing power demands. This synchronization requirement makes large AC electrical grids vulnerable to cascading failures. The transition to an ever-more interconnected and "smarter" grid has made the electrical grid vulnerable to cyberattack. Solid-state transformers (SST) have the potential to prevent/reduce cascading failures. This one Sandia Resilient Energy Systems LDRD project, done in collaboration with Purdue, resulted in an innovative SST that will enable energy system security and resilience. (PI: Karina Munoz-Ramos)



Solid-state transformer devices achieve 100 kW output and electromagnetic-interference compliance.

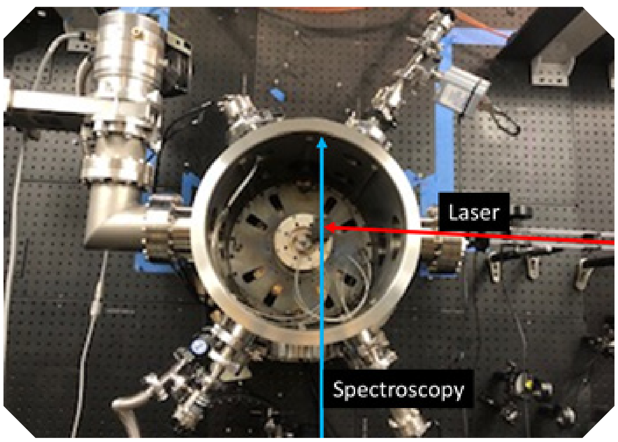
Response of GaN-based semiconductor devices to ion and neutron irradiation. Novel radiation-hardened electronics are based on gallium nitride (GaN), so it's critical to understand their damage mechanisms and response to multiple radiation environments. The research team used ion and neutron irradiations to study the effects of ionization and displacement damage on GaN-based semiconductor devices. The results provided knowledge on the radiation hardening levels of GaN-based devices, ion-to-neutron damage equivalency, and knowledge about temperature and current injection annealing of GaN. The radiation effects community working to develop devices used in strategically radiation-hardened systems across Sandia are benefitting from the project findings. (PI: Brandon Aguirre)



GaN-based semiconductor devices were exposed to ion and neutron radiation environments at (top left) Annular Core Research Reactor, (top right) White Sands Missile Range, and (bottom right) Ion Beam Laboratory to explore the damage mechanisms responsible for device degradation such as light output in (bottom left) high-intensity InGaN LEDs.

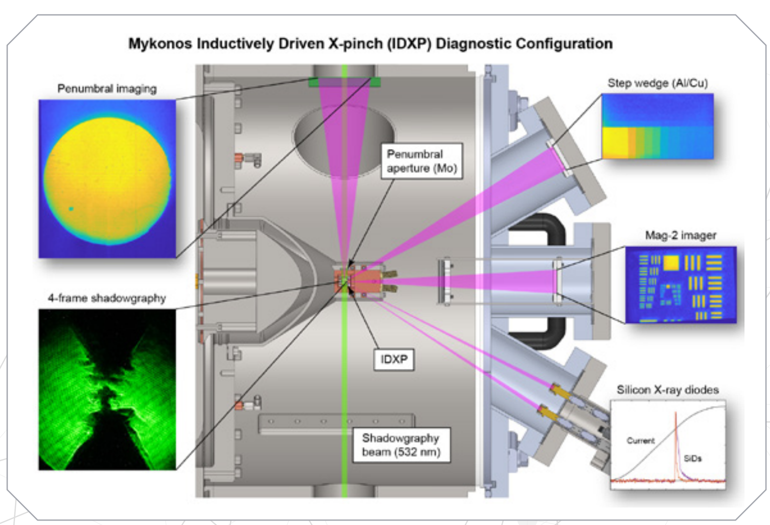
GaN-based power devices are targeted for some applications – for example, Raytheon GaN HEMT technology provided a major boost to Navy radar systems.

Next-gen pulsed power machines benefit from research on diagnosing field strengths and plasma conditions in magnetically insulated transmission lines using active dopant spectroscopy. Accurate estimates of plasma parameters and field strengths in power flow regions using active dopant spectroscopy will inform theory and simulation efforts are needed to design next-generation pulsed-power machines, and improve optical spectroscopy efforts to diagnose load conditions, such as feed plasmas and magnetic and electric fields. The team developed and demonstrated a laser-activated dopant diagnostic on a Mykonos linear transformer driver, obtained spectral measurements of field strengths and electron densities within the anode-cathode gap, and showed that its implementation does not appreciably affect current delivery, as a precursor to similar measurements on the Z machine. Measurements on Mykonos showed that expansion of the ablation plasma is the primary mechanism that drives loss, which can be controlled by timing the laser within 150 ns of peak current. Within this time frame, no noticeable current loss is measured, and the ablation plasma may be used to diagnose magnetically insulated transmission line conditions. As a result of this LDRD, Sandia is planning to implement this diagnostic on the Z machine to measure localized electric and magnetic fields. (PI: Sonal Patel)



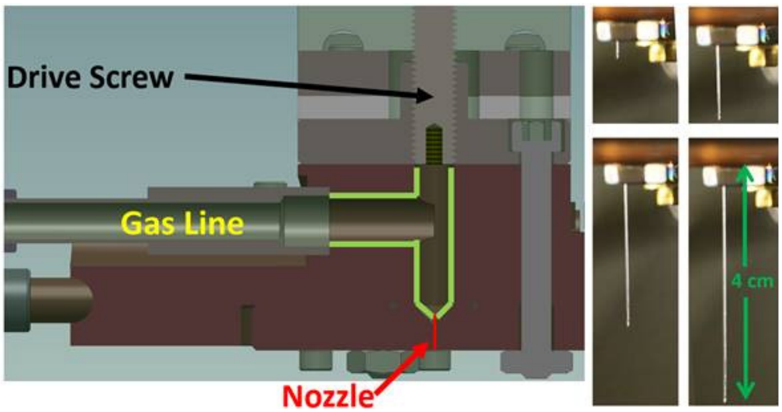
Mykonos linear transformer driver hardware used during the active dopant project.

Developing inductively driven diagnostic X-ray sources to enable transformative radiography and diffraction capabilities on Z machine. Penetrating X-rays are one of the most effective tools for diagnosing high energy density experiments, whether through radiographic imaging or X-ray diffraction. To expand the X-ray diagnostic capabilities at the 26-MA Z Pulsed Power Facility, Sandia developed a new diagnostic X-ray source called the inductively driven X-pinch (IDXP). This X-ray source is powered by a miniature transmission line inductively coupled to fringe magnetic fields in the final power feed. During this LDRD, the team carried out a multistage development of the IDXP concept through experiments both on Z and in a surrogate setup on the 1-MA Mykonos facility. The creation of a radiography-quality X-pinch hot spot was verified through a combination of X-ray diode traces, laser shadowgraphy, and source radiography. The success of the IDXP experiments on Mykonos recently enabled the first-ever diagnostic X-pinch to be fielded on Z. (PI: Clayton Myers)

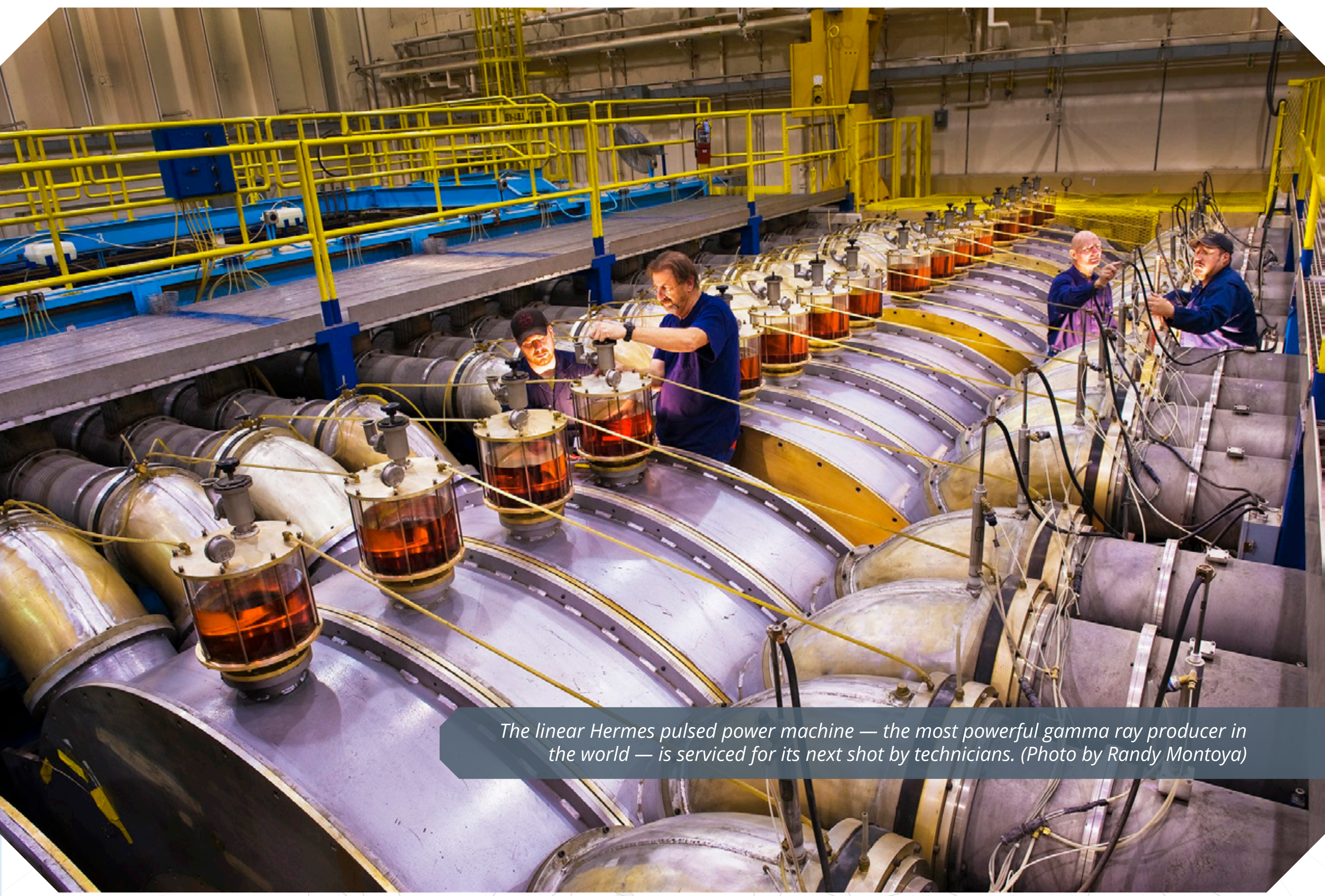


The line-of-sight diagnostic suite developed for inductively driven X-pinch experiments on the 1-MA Mykonos facility. These data are used to verify the formation of a radiography-quality X-ray hot spot in the IDXP.

Development of a deuterium-ice extruder for advanced fuel configurations in inertial confinement fusion experiments at the Z Facility. Deuterium is a critical isotope needed to study fusion in the laboratory, and a variety of deuterium fuel configurations are needed to optimize the fusion conditions that can be achieved at the Z Facility. One configuration of interest is a frozen-rod of deuterium ice, which has now been demonstrated using a screw-type extruder. Extruder testing occurs in Sandia's Pulsed Power Sciences Center Cryogenics Test Laboratory (CTL). The CTL supports cryogenics R&D and is used for pre-experiment testing of all cryogenically-cooled Z-Facility targets. (PI: Thomas Awe)



(Left) Schematic of deuterium-ice extruder for inertial confinement fusion experiments. (Right) Four images of the initial extrusion of a rod from a 300-μm diameter nozzle.



The linear Hermes pulsed power machine — the most powerful gamma ray producer in the world — is serviced for its next shot by technicians. (Photo by Randy Montoya)

Project Highlights - Workforce Development

To execute Sandia's diverse missions, it takes motivated staff with deep expertise who are committed to advancing the frontiers of science and engineering. The individuals and LDRD teams listed below are just a few of the stellar examples that make up Sandia's fabric and just a few of the people who work to change the world.

Former Energy Secretary Rick Perry thanked Sandia employees for their contributions to science and issues of national and international security, equating research to public service during a visit to the Labs in 2018.

International Awards

Sandia wins six 2020 R&D 100 Awards, three with LDRD roots

Sandia won six 2020 R&D 100 Awards, three of which were enabled in part by LDRD projects. The R&D 100 Awards are one of the most prestigious recognitions of innovation in the world. The winning lists are created by teams of examiners identifying the 100 most technologically significant products each year from an international pool of submissions sent in from government labs, universities, and private corporations. The contest is sponsored by R&D World Magazine, the successor to R&D Magazine. With six wins, Sandia surpassed its own record set in 2017 and also highlights Sandia's continuing ability to benefit the nation and the world through the depth of technical expertise, and also the breadth of work done in fundamental science and science-based engineering R&D.

In 2020, three Sandia teams were sole winners and all had roots in Sandia LDRD projects. The other three were achieved with partner organizations — bringing Sandia's total to 140 awards since 1976.

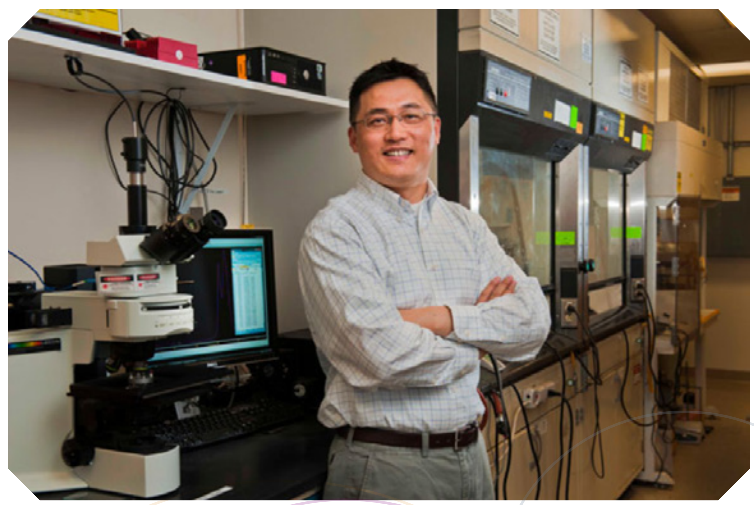
HECATE: High-density Evaluator of Commercial-off-the-shelf Applications for Trust and Efficacy.

The number of software supply-chain attacks has grown to an unprecedented degree over the past decade. HECATE, a software supply chain and assurance platform, reduces risks for commercial and open-source software users. The platform addresses these threats by creating virtual machinery modified to resemble physical devices. Selected software, along with patches and updates, are then installed and automatically observed in performance from the virtual machine. The platform distinguishes between benign, anomalous, and suspicious behaviors. Intruders set off an alarm if they include an unrequested update that changes a program's behavior or requests access to privileged features in the user's system. HECATE provides a testing ground that attackers can't detect and therefore can't lie to, offering a yardstick to determine how much trust to accord a new addition. (PI: Vince Urias) Watch the YouTube video.

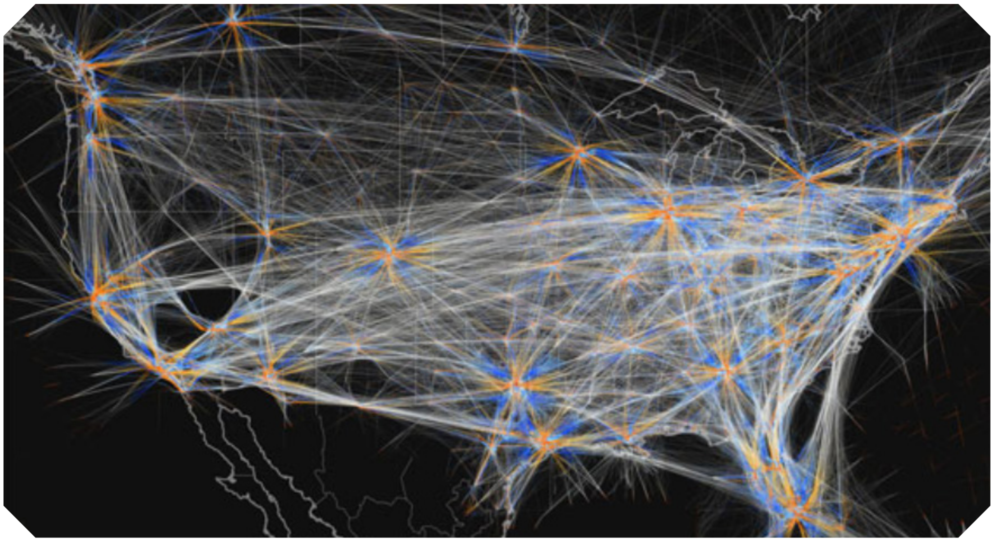
Sandia computer scientist Vince Urias and his team earned a 2020 R&D 100 Award for developing HECATE, a software supply chain and assurance platform. (Photo by Randy Montoya)

Binary Solvent Diffusion for Fabrication of Large Nanoparticle Supercrystals.

Researchers used nanotechnology and chemistry to self-assemble gold nanoparticles into millimeter-sized supercrystals that are very sensitive to chemical traces. Electromagnetic fields within the supercrystals produce superior sensing that correlates to the shape, size, and density of packing. An inexpensive, large-scale production method uses a simple solvent diffusion process for seeding and growth. The supercrystals obtained through this process also proved to have superior qualities in optoelectronics, photovoltaics, and surface catalysis. (PI: Hongyou Fan) Watch the YouTube video.



Sandia materials scientist Hongyou Fan and his team earned a 2020 R&D 100 Award for using nanotechnology and chemistry to turn gold nanoparticles into supercrystals for optoelectronics, photovoltaics and surface catalysis. (Photo by Randy Montoya)



This color map shows take-offs (red ends) and landings (blue ends) for all the flights in the U.S. from a single day. A Sandia team earned a 2020 R&D 100 Award for creating Tracktable, a technology that uses machine learning to analyze large data sets. (Image courtesy of Andy Wilson)

Tracktable.

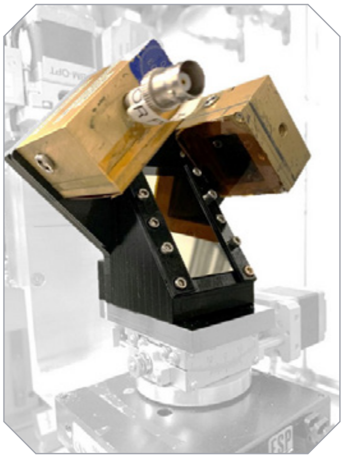
Tracktable applies advanced machine-learning techniques to large trajectory data sets, searching for shapes and patterns in space and time by providing a mathematical framework. The method organizes, searches, and quickly analyzes millions of patterns, grouping similar shapes and extracting unusual trajectories without first requiring a definition of the term "normal," which might eliminate from consideration shapes worth studying. By treating time as a variable similar to space, Tracktable enables searches for collective behavior and patterns over long periods of time. Fast search techniques predict paths and destinations of moving objects by comparing observed paths to historical databases of trajectories. (PIs: Danny Rintoul, Andy Wilson, Chris Valicka) Watch the YouTube video.

Sandia partnered with other organizations on the 2020 R&D 100 Award-winning Legion programming system. Mechanical engineer Jackie Chen was Sandia's lead researcher on the project.

Legion: A Data-centric Programming System.

Legion is a supercomputing programming system that boosts application performance and speed by automating task scheduling and data movement. This type of automation is a basic need for computing at the exascale — performing a billion billion operations per second. At Sandia, scientists used Legion to boost the performance of a complex multiscale physics simulation known as S3D, a turbulence-reacting flow solver used to develop predictive models of better internal combustion engines. Legion enabled calculations capturing turbulence-chemistry interactions that were previously out of reach for S3D as well as scaling to over 10,000 nodes on the Titan supercomputer at the Oak Ridge Leadership Computing Facility, reducing the time to achieve results. (Sandia lead researcher: Jackie Chen) Watch the YouTube video.

Legion lead organization: Los Alamos National Laboratory. Partner organizations: NVIDIA, University of California, Davis, Sandia National Laboratories, Stanford University, SLAC National Accelerator Laboratory

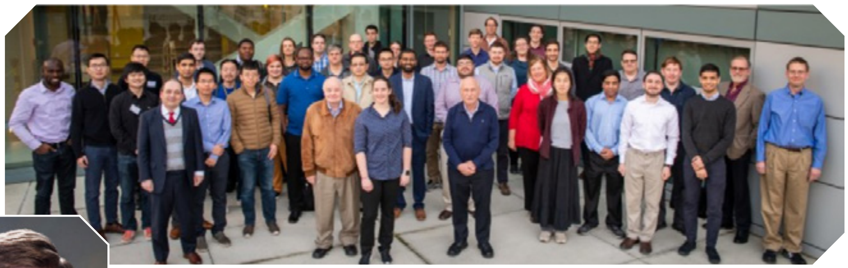


XRPBS, a joint effort led by the Nevada National Security Site, won a 2020 R&D 100 Award. (Image courtesy of Matthew S. Wallace, Nevada National Security Site)

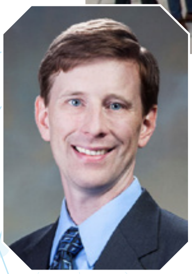
XRPBS: X-ray Polarizing Beam Splitter.

XRPBS is the first X-ray polarizing beam splitter. It separates an X-ray beam in two in order to measure each polarized beam simultaneously, a unique feature because it eliminates reliance upon source stability or repeatability. This diagnostic can be used for high-energy-density plasma investigations in addition to weapons-related work. It also can be used for material studies and X-ray beam manipulation on synchrotrons. Measuring the polarization of X-rays provides information about electron beams and magnetic fields in X-ray emitting plasmas. The same process can analyze the magnetic properties of materials probed with radiation from advanced X-ray sources. XRPBS was developed by Radu Presura at the Nevada National Security Site in collaboration with Sandia, and its development was supported by Argonne National Laboratory. Sandia collaborators, led by Ming Wu, participated in the discussion of applications and in the crystals' characterization. (Sandia lead researcher: Ming Wu)

Lead organization: Nevada National Security Site
Partner organizations: Sandia National Laboratories, Argonne National Laboratory, EcoPulse



A Sandia-led partnership has earned a 2020 R&D 100 Award for the IDAES computational framework. Members of the team from several organizations gathered in February for a group photo. (Photo courtesy of Lawrence Berkeley National Laboratory)



Computer scientist John Siirola was Sandia's PI on the 2020 R&D 100 Award-winning IDAES project.

IDAES: Institute for the Design of Advanced Energy Systems Process Systems Engineering Computational Framework.

This framework is a comprehensive set of Process Systems Engineering (PSE) tools supporting the design, modeling and optimization of advanced energy systems. By providing rigorous modeling capabilities, the IDAES Modeling & Optimization Platform helps energy and process companies, technology developers, academic researchers and DOE to design, develop, scale up, and analyze new and potential PSE technologies and processes to accelerate advances and apply them to address the nation's energy needs. John Siirola, Sandia project lead, said the IDAES Integrated Framework is based on and extends a Sandia-developed open-source modeling environment called Pyomo. IDAES has taken the core optimization capabilities in Pyomo and not only built a domain-specific process modeling environment, but also expanded the core environment into new areas, including logic-based modeling, custom decomposition procedures and optimization algorithms, model predictive control and machine learning methods. (Sandia PI: John Siirola)

Partner organizations: U.S. Department of Energy, National Energy Technology Laboratory, Carnegie Mellon University, Lawrence Berkeley National Laboratory, University of Notre Dame

Sandia's Joint Computational Engineering Laboratory (Photo by Randy Montoya)

National/Federal Awards

2020 DOE Secretary of Energy Achievement Awards. On January 20, 2021, DOE announced winners of the Secretary of Energy Achievement Awards, and Sandia Labs researchers were recipients of one of the highest honors a DOE employee or contractor can receive. These awards recognize the achievements of those who have gone above and beyond in fulfilling DOE's mission and serving the nation. A new group of awards for 2020 reflect DOE responses to the coronavirus pandemic.

- **DOE National Laboratories' COVID-19 Clinical Testing Teams**. These national laboratory teams developed on-site testing capabilities to keep the workforce safe and allow for safe resumption of work, while in turn helping reduce the spread of the novel coronavirus.
- **National Virtual Biotechnology Laboratory Team.** This team, including Sandia's Anup Singh, Joseph Schoeniger, Mark Rintoul, was honored for accomplishments to harness and mobilize the formidable scientific facility and research capabilities of the DOE national laboratories to meet the challenges posed by the COVID-19 pandemic.
- **High-performance Computing Resource Team.** This team, including Sandia's Corey Hudson, Joel Stevenson, and Stephen Monk, facilitated optimal mobilization of the nation's supercomputing capabilities to meet the multiple challenges of the pandemic. This team rapidly organized an effective infrastructure for the selection of research projects and their assignment to supercomputing facilities.

2020 Federal Laboratory Consortium Impact award rooted in LDRD

Sandia secured four Federal Laboratory Consortium Tech Transfer awards in 2020, ranked as some of the most prestigious honors for federal laboratories and industry partners. The Impact award has its roots in a Sandia LDRD project focused on detecting biological and chemical threats. The Trak Male Fertility Testing System is based on Sandia's SpinDx portable lab-on-a-disc diagnostic technology. Former Sandia inventor Greg Sommer realized there could be multiple commercial applications for SpinDx technology, so he pursued Sandia's Entrepreneurial Separation to Transfer Technology program. He was joined later by former Sandia inventor Ulrich Schaff, and the two started Sandstone Diagnostics, a company that specializes in producing medical products and research tools to improve health care. They continue to refine and develop the technology in Trak, which they now call CentriFluidics.

Prestigious Fellowships, Appointments and Memberships

Sandia Fellows and Senior Scientists

At Sandia, outstanding researchers from across technical fields can be appointed to the position of Fellow or Senior Scientist. Appointment as a Sandia Fellow recognizes a career of significant accomplishment for the Labs and for the nation. Fellows help to inform strategic directions and serve as ambassadors to organizations such as DOE, other government agencies, academia, and technical societies. Likewise, Senior Scientists, with their wealth of exceptional technical experience and broad mission impact, act as trusted advisors on technical topics and influence change at Sandia. Fellows are provided with LDRD funding allowing them to invest in strategic research projects and develop outstanding talent. In FY20, Lab Fellows and Senior Scientists helped to define and direct the COVID-19 response and winnow the outstanding ideas submitted by new and experienced researchers at the Labs.

Susan Seestrom named American Association for the Advancement of Science Fellow

Susan Seestrom, associate laboratories director for Advanced Science and Technology and CRO at Sandia, was named a Fellow of the American Association for the Advancement of Science by her peers – and is only the fourth presently active Sandia scientist to have that distinction. The physicist was cited "for her pathbreaking work in nuclear physics, especially using ultra cold neutrons, and her leadership, both in her [physics] community and at national laboratories." Seestrom, who oversees Sandia's LDRD program, envisions enhanced agility. "We need to be able to move our research resources quickly, as we did for a problem like the COVID-19 global pandemic," she said.

Gil Herrera appointed to U.S. National Quantum Initiative Advisory Committee

Gil Herrera, Sandia Labs Fellow, joins 20 others from government, industry, and academia tasked with advising the nation's highest offices on matters concerning quantum information science. His appointment is for three years. Herrera was the PI on the Earth Science Research for COVID-19 Pandemic LDRD project.

Jacqueline Chen named DOE Office of Science Fellow

Jacqueline Chen, whose work on fundamental turbulence-chemistry interactions in combustion helped advance the design of automotive, gas turbine and jet engines, was selected by the Department of Energy's Office of Science as a Distinguished Scientist Fellow — one of only eight researchers in the nation to hold the distinction.

Jacqueline Chen and Justin Smith elected as American Institute of Aeronautics and Astronautics Associate Fellows

Jacqueline Chen and **Justin Smith**, two LDRD researchers, were elected Associate Fellows of the American Institute of Aeronautics and Astronautics in 2020. The designation of Associate Fellow recognizes those "who have accomplished or been in charge of important engineering or scientific work, or who have done original work of outstanding merit, or made outstanding contributions in the field."

Tina Nenoff elected as American Association for the Advancement of Science Fellow

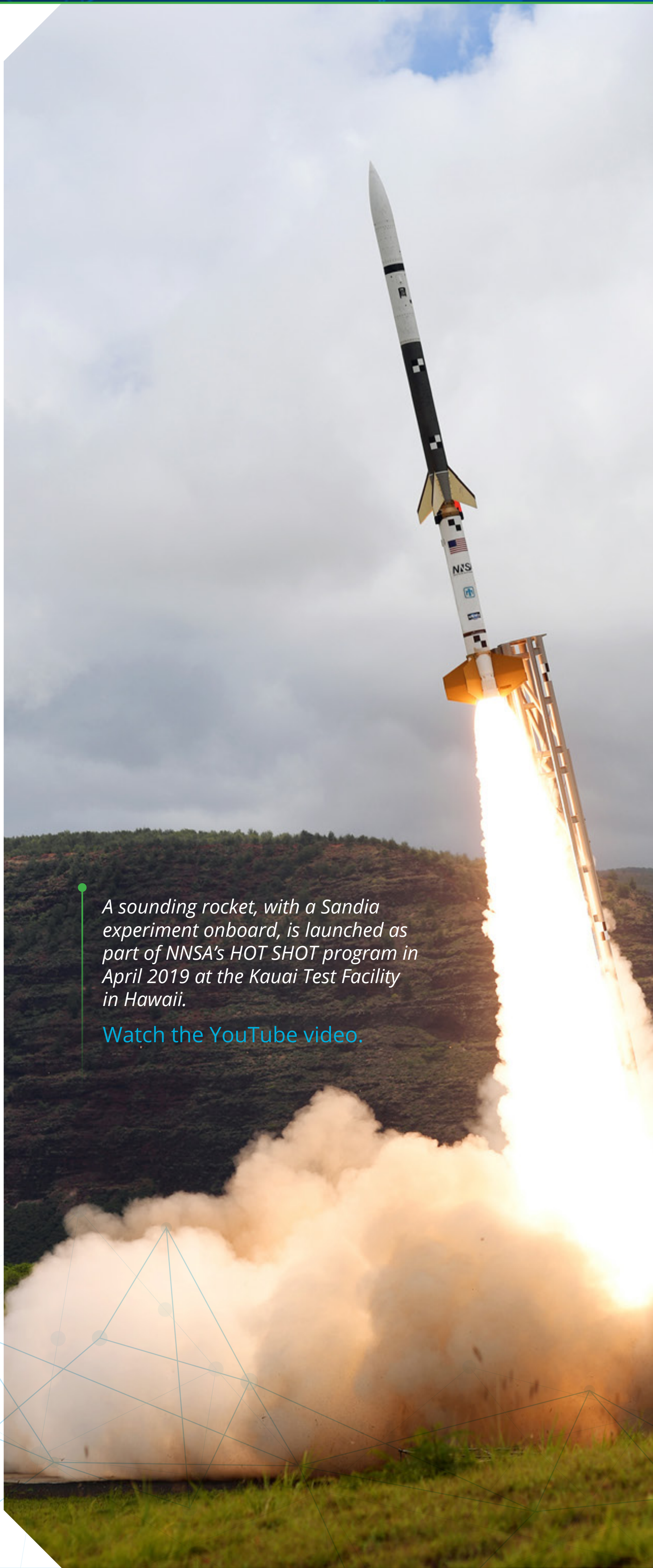
Tina Nenoff, perennial inventor of advanced materials, was elected Fellow of the American Association for the Advancement of Science. She received the honor for advancement of science "in service to society" and "for outstanding accomplishments in nanoporous materials and technology through research and group effort leadership, particularly in ion and gas separations for energy and environmental applications." Nenoff is currently leading an LDRD project creating a breakthrough in optoelectronic materials.

Tamara Kolda admitted to National Academy of Engineering

Tamara G. Kolda, Sandia mathematician and LDRD researcher, is one of the few mathematicians admitted to the National Academy of Engineering. Kolda was selected in part for her groundbreaking contributions to design software, including tensor decompositions and multilinear algebra.

Ganesh Subramania elected Fellow of the International Society for Optics and Photonics

Ganesh Subramania was elected Fellow of the International Society for Optics and Photonics, a not-for-profit international society advancing emerging technologies through interdisciplinary information exchange. Subramania is currently PI on an LDRD project focused on femto-second imaging camera systems that will provide the ability to observe and capture ultra-fast phenomena with high temporal resolution.



A sounding rocket, with a Sandia experiment onboard, is launched as part of NNSA's HOT SHOT program in April 2019 at the Kauai Test Facility in Hawaii.

Watch the YouTube video.

FY20 Hruby and Truman Postdoctoral Fellowships

The LDRD-funded Jill Hruby Postdoctoral Fellowship was established in 2017 to encourage women to consider leadership in national security as scientists and engineers. Jill Hruby served as Sandia's director from 2015 to 2017 and was the first woman to lead a national security laboratory. Each Hruby Fellow is awarded an LDRD-funded three-year postdoctoral fellowship in technical leadership, comprising national-security-relevant research with an executive mentor.

Sandia established the LDRD-funded President Harry S. Truman Postdoctoral Fellowship in National Security Science and Engineering to attract the best nationally recognized new PhD scientists and engineers. Truman Fellows conduct independent groundbreaking research that supports Sandia's national security mission. Fellows choose their own research topics and benefit by having access to Sandia's state-of-the-art facilities and collaborating with some of the nation's best scientists and engineers. A member of Sandia's technical staff mentors each Truman Fellow.

Learn more about our fellowships at Sandia.

Hruby Fellows

There were three Hruby Fellows working in research at Sandia in FY20.

Kelsey DiPietro: As an applied mathematician, DiPietro proposed a way to make computer models more efficient – improving accuracy without increasing time or resources to run them. DiPietro is applying her method to climate research, working with Sandia's supercomputer-powered Energy Exascale Earth System Model, which already has one of the finest resolutions ever achieved for simulating aspects of the planet's climate.

Mercedes Taylor: Taylor's research is focusing on the development of new porous plastics that purify water by soaking up ions, with an emphasis on negatively charged ions, called anions. As climate change and population growth are projected to make drinking water scarcer globally over the coming decades, Taylor hopes her work will provide relief and security.

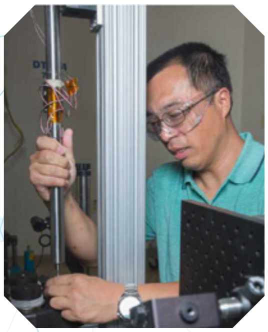
Chen Wang: Chen Wang is analyzing soot precursor molecules with microscopy and designing computational models for cleaner-burning combustion engines at Sandia. "My understanding of LDRD projects definitely helped in the application process," said Wang. "As an inaugural [Hruby] Fellow, I've had a great degree of freedom in my research, as well as many leadership opportunities."

Josh Rackers and Thomas Hardin – FY20 Truman Fellows

Josh Rackers is a computational biophysicist designing new models for describing molecular dynamics in biological systems. Prior to joining Sandia, he earned a doctorate from Washington University in St. Louis. He has insights on modeling important classes of soft materials at the atomic scale with high accuracy, which will extend the methods Sandia uses for modeling other kinds of materials. He plans to use computer simulations to understand how ion channels work.

Thomas James Hardin is a materials scientist with expertise in the molecular dynamics of glass. He comes to Sandia from the Massachusetts Institute of Technology, where, in the process of completing his thesis, he discovered how little is understood about the structure and properties of glassy materials on the nanoscale. His three-year assignment focuses on filling in those gaps by systematically enumerating the fundamental structural building blocks of glassy materials.

Professional Society and Conference Awards



Most Promising Asian-American Engineer of the Year

Bo Song, Sandia mechanical engineer, was recognized as a 2020 Asian-American Engineer of the Year by the national DiscoverE Program for his groundbreaking work in experimental impact mechanics and the dynamic response of materials and structures. Song developed the Experimental Impact Mechanics Lab, the most active dynamic material test facility at Sandia and one of the top Hopkinson bar labs in the world.

Black Engineer of the Year (BEYA): Most Promising Scientist in Government Award

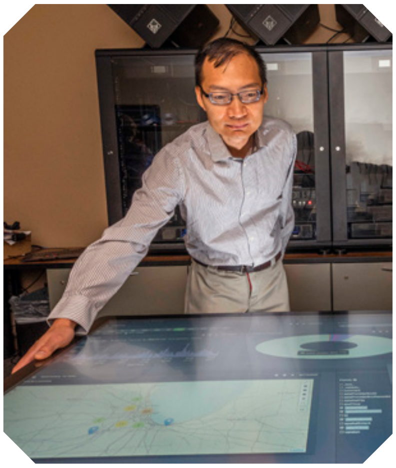
LaRico Treadwell received the Most Promising Scientist in Government Award at the BEYA STEM Virtual Global Competitiveness Conference. This conference acknowledges Black leaders for their incredible contributions in STEM. Treadwell is currently an LDRD PI for the Materials Science and Radiation, Electrical & High Energy Density Science research areas.

A researcher examines a parabolic trough module at Sandia's National Solar Thermal Test Facility in Albuquerque. (Photo by Randy Montoya)

Society of Women Engineers Achievement Awards

Christina Beppler, an analytical chemist in explosives technologies, is Sandia's first recipient of SWE's Work/Life Integration Award, recognizing her "leadership and initiative in establishing a program of forward-looking benefits that demonstrate an understanding of work and life integration." Beppler is currently participating on an LDRD that directly supports NNSA while also providing valuable tools for geosciences, energy, and biosciences.

Anne Grillet earned SWE's 2020 Prism Award for "charting her own path in the STEM fields by demonstrating a variety of outstanding career leadership activities in a technical field." Grillet's technical collaborations span Sandia's mission space from materials science, geosciences and energy to explosives and nuclear deterrence. Currently, Anne is working on an LDRD project looking at how stress is formed in materials during phase changes. This fundamental research will impact new physical models.



Society of Asian Scientists and Engineers Professional Achievement Award

Tian J. Ma, computer scientist, engineer and dedicated LDRD researcher, received the prestigious Professional Achievement Award by the Society of Asian Scientists and Engineers (SASE). SASE's 2020 Professional Achievement Award is given to mid-career professionals who have made significant discoveries and important advances in their chosen career paths and are acknowledged as leaders of large initiatives. Ma was nominated by James Peery, Sandia Labs Director. In 2020, SASE also named Sandia Labs as Organization of the Year in the government category.

Laser Focus World 2020 Innovators Award – Optics Platinum-Level Honoree

MIRaGE: Multiscale Inverse Rapid Group-theory for Engineered-metamaterials (MIRaGE) uses scientific knowledge developed from molecular spectroscopy on how the symmetry of a natural molecule affects its optical behavior and properties to design a metamaterial with comparable properties. By making the comparisons that molecules in chemistry are analogous to metamolecules in electromagnetics and that molecular modes of vibration are analogous to the fundamental resonant electrical current modes in a metamaterial, the principles of symmetry and point groups can be translated to electromagnetics. Serving as a basis for metamaterials design, MIRaGE facilitates the quest for unusual electromagnetic behaviors that can be associated with optical properties. MIRaGE has its roots in a metamaterials science and technology Grand Challenge LDRD project. (PI: Ihab El-Kady; team members: Charles Reinke, Denis Ridzal, Bart van Bloemen Waanders, David Fitzpatrick, Mehmet Fatih Su, Ryan Chilton, Tony Wilson) Watch the YouTube video.

Brimacombe Medal Award

Brad Boyce, materials scientist, received the Brimacombe Medal from the Minerals, Metals & Materials (TMS) Professional Society in 2020 for sustained excellence and achievement related to minerals, metals, or materials science and engineering. Boyce is currently leading an LDRD project that employs both computational optimization and experimental validation to create novel architected metamaterials that can be tailored to mitigate a complex combination of insult environments.

EARLY CAREER AWARDS AND HONORS

Nathaniel Trask, Sandia researcher, received two Early Career Research Awards in 2020 – one from DOE and another from the Office of Advanced Scientific Computing Research for his proposed project, aimed at helping scientists use the laws of physics to view multiscale physical events at a new level of clarity. The design of microelectronic devices, resilient energy storage systems, and the study of discrete fracture networks in subsurface flows, could benefit from increased accuracy.

Thomas O'Connor, a 2019 Truman Fellow, was appointed Inaugural Early Career Officer within the Division of Polymer Physics (DPOLY) of the American Physical Society. In 2020, he published four papers, co-organized the 2021 DPOLY short course on the "Macromolecular Engineering of Formulations," and was invited to give seven talks.

Jessica Rimsza, Sandia materials science researcher, was recognized at the 7th World Materials Research Institutes Forum Workshop for Early Career Scientists. Her work focuses on the molecular scale modeling of glass and ceramic materials, with a particular focus on surface properties.

Kevin Young, named by DOE Office of Science to their Early Career Research Program, received a grant to continue his work improving the performance of modern quantum information processors. Young co-leads Sandia's Quantum Performance Laboratory and performs research focused on modeling, assessing, and improving the performance of quantum computers. His winning proposal was titled, "Quantum Performance Enhancement."

Mike Hamel received a 2020 Mission Innovator Award for technical impact, leadership, and innovative research for Sandia's radiation detection program. His award noted that Hamel seeks to advance the field by generating new concepts and LDRD projects and works across the Labs to unleash Sandia's capabilities.

Honors and Distinctions

Vince Urias, Sandia computer scientist and LDRD researcher, earned national recognition for cybersecurity platforms he conceived – Cloud Hypervisor Forensics and Incident Response Platform, and High-fidelity Adaptive Deception and Emulation System. Urias was invited to pitch his software to investors, entrepreneurs, and prospective customers at a special 2020 virtual event sponsored by DOE to accelerate the commercialization of federally developed technologies.

Seema Singh, one of Sandia's Office of Science program leads and Joint BioEnergy Institute scientists, received recognition from PLoS Biology for being in the top 2% of biotechnology researchers and top international scientists based on publication citations by the Public Library of Science. Singh, who acted as PI on several Sandia LDRD projects, was also announced as joint editor-in-chief for *Biotechnology for Biofuels*.

Thomas Beechem, a materials science researcher, was named a Center for Integrated Nanotechnologies (CINT) affiliate. CINT is a DOE Office of Basic Energy Sciences nanoscale science research center operated as a national user facility by Los Alamos and Sandia national laboratories.

Rupert Lewis and his team demonstrated the first working superconducting qubit at Sandia through their LDRD project focused on fast-cycle charge noise measurement for better qubits.

Dorina Sava Gallis' research article, "Encoding Mulitlayer Complexity in Anti-Counterfeiting Heterometallic MOF-Based Optical Tags" made the cover of *Angewandte Chemie*, a journal of the German Chemical Society.

Exploratory Express LDRD Strategic Initiative funds 21 early career staff during FY20.

Exploratory Express (EE) is a unique LDRD Investment Area (IA). Often a researcher conceives an idea with the potential to become important for one of Sandia's strategic missions, but the idea is technically risky, and requires some maturation and testing before it is ready to serve as a basis for further R&D or for technology transition. EE specializes in funding these short-term projects (six months to a year in duration with a cost under $125K). The PIs must scope their project to obtain a concrete result by the end of the cycle, the results of which will determine the direction of additional investments. The EE IA runs on a different call cycle than the standard annual LDRD call. There are three "speed networking" events where researchers can pitch their idea and obtain feedback from multiple EE committee members before ultimately submitting their idea for consideration.

Many early career staff at Sandia have brilliant concepts that fit this description. Their burgeoning and focused ideas are risky but could have a significant impact on one of Sandia's mission areas. For example, Jessica Rimsza, materials science researcher, got her first LDRD as a postdoc in 2018 through EE. Her successful project, "Computational and Experimental Characterization of Intermediate Amorphous Phases in Geological Materials," helped her to step out as a researcher at Sandia. She converted to staff, is a successful PI in other investment areas, and a recognized expert in her field.

In FY20 alone, EE funded 21 early career staff with promising, yet technically risky, ideas.

ABSTRACT

This report provides an assessment of the value of the LDRD program to Sandia National Laboratories during FY20.

FY20 LDRD ANNUAL REPORT TEAM

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