SAND2020-3752R

FY19 LDRD Annual Report

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Where innovation begins

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LDRD

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Laboratory Directed Research and Development 2019 Annual Report

From the Chief Research Officer

Sandia National Laboratories' LDRD program provides transformational innovations that support the Nation's national security enterprise. Sandia's researchers, in collaboration with our partners, apply their knowledge and creativity to answer today's challenging questions and provide solutions for tomorrow's problems.

Sandia LDRD research teams work on transformational science, technology, and engineering projects. They focus on national security with an emphasis on the safety, security, reliability and agility of our nuclear deterrence capabilities, energy security and reliability, nonproliferation, counterterrorism, and defense. Our researchers deliver methods of protecting our grid, provide high-quality intelligence of world events, maximize energy outputs of devices, and demonstrate the value of our research through advanced prototypes. Through their innovation, they discover new ways to use, fabricate, and harden materials and microelectronics to withstand a variety of challenging environments, and improve high-performance computing, simulation and modeling via fundamental discovery and advanced diagnostic methods. LDRD teams are working year-round to capitalize on what they know now to achieve what they believe to be possible.

The LDRD program expands Sandia's capabilities and contributes to our nation's long-term vitality. It also enables Sandia to recruit and retain highly talented scientists and engineers. Each year, researchers submit hundreds of proposals for leading-edge research & development projects with the potential to provide significant impact to a mission. Their ideas are preceded by the strategic priorities articulated by leadership and supported through Sandia's internal LDRD processes and NNSA guidance. Together, these provide the framework for review and selection of Sandia's LDRD portfolio. In the 2019 fiscal year (FY) process, 675 short idea proposals were submitted. Of those, 283 were invited to submit full proposals, and 178 were funded. When added to ongoing projects and late-start projects (which are also reviewed), 404 projects were active in FY 2019. Many of these contributions were showcased through technological advances, awards, patents, and a variety of publications.

The LDRD program expands Sandia's capabilities and contributes to our nation's long-term vitality.

The 2019 LDRD Annual Report provides an update on some of the significant accomplishments achieved by the forward-looking LDRD teams who have their eyes on the horizon

Susan Seestrom

Chief Research Officer
Associate Laboratories Director
Advanced Science and Technology

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INTRODUCTION

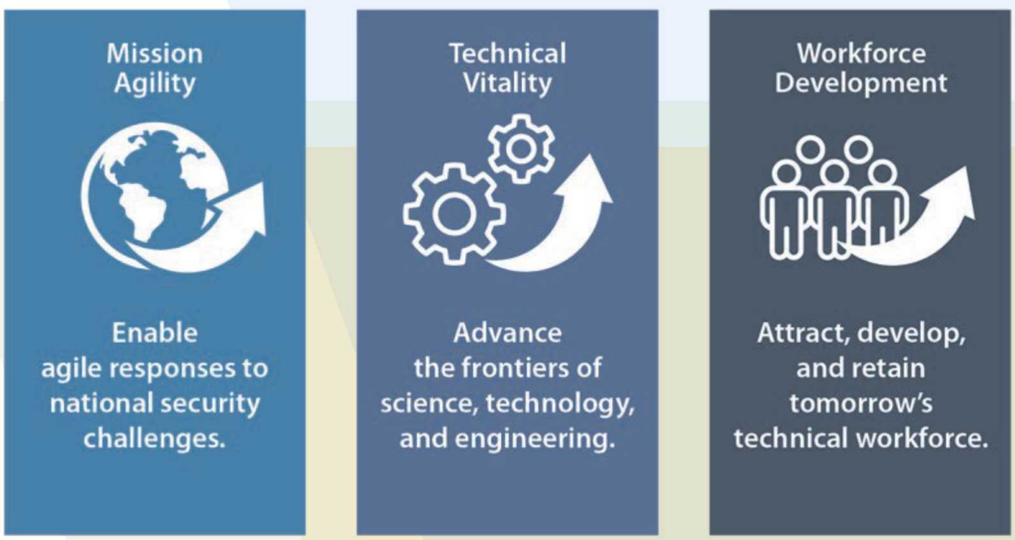
LDRD Program Overview

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 universities and companies.

Sandia's LDRD program aims to maintain the scientific and technical vitality of the Labs and to enhance the Labs' ability to address future national security 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.

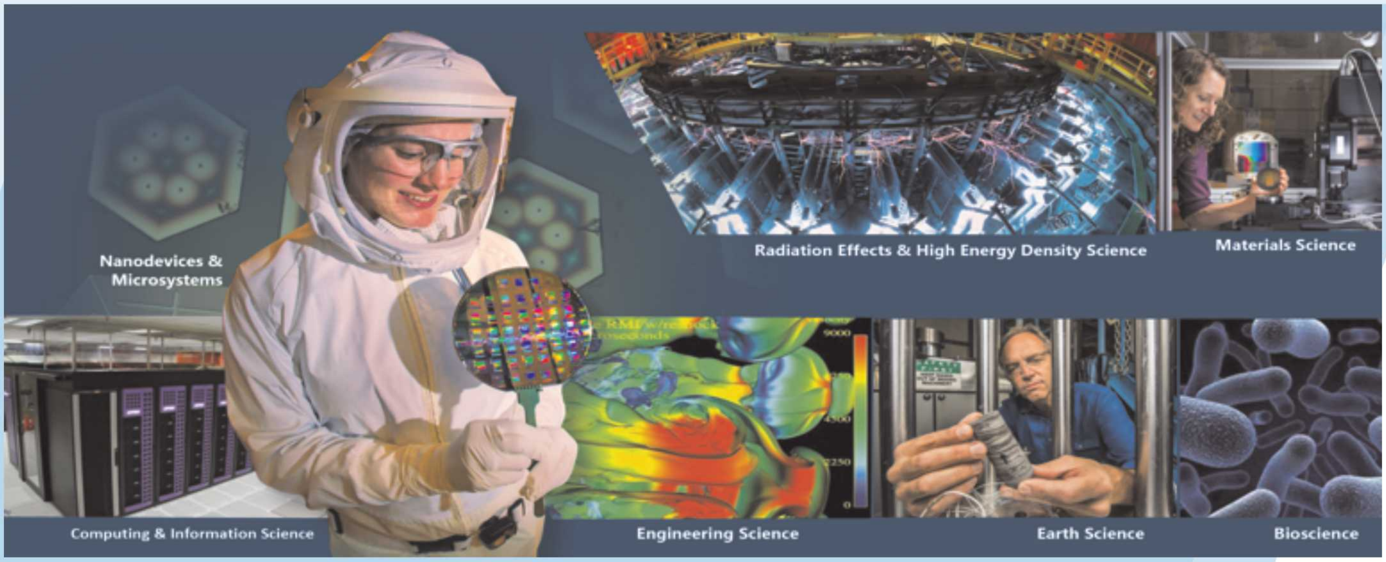


Sandia's LDRD Program Structure

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



Mission Foundations: Sandia oversees five major portfolios that address national security mission challenges. LDRD Mission Foundations align with the 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 (104 LDRD-supported university collaborations in FY2019), and the Truman and Jill Hruby Postdoctoral Fellowships.

Program Metrics

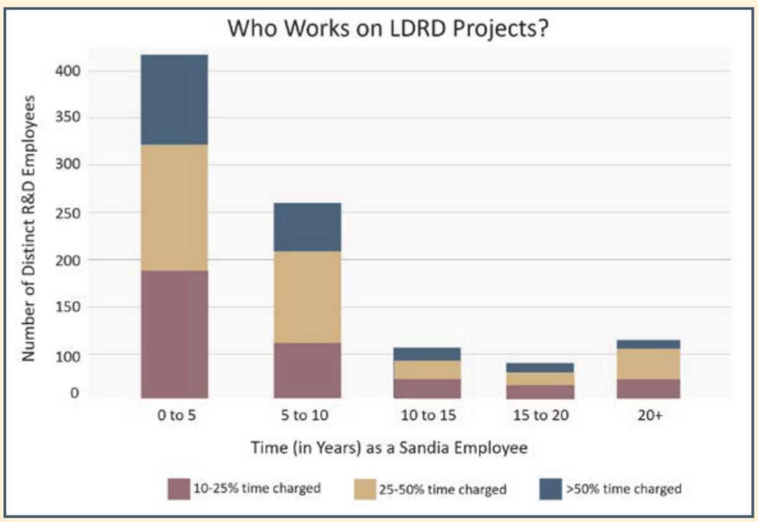
While the FY2019 LDRD program represented only about 5.2% of Sandia's total lab costs, the metrics shown below highlight how LDRD has a much larger relative impact on Key Performance Indicators and metrics for the lab. The bar graph demonstrates the large percentage of early career staff and postdocs 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.

LDRD provides a clear advantage to Sandia's technical vitality and to the development of its workforce. Approximately 67% of Sandia's DOE Early Career award winners and around 88% of PECASE winners have prior LDRD experience. The LDRD advantage continues for Sandia's experienced workforce where 78% of American Physical Society Fellows and 67% of Sandia Fellows have prior LDRD experience.

FY 2019 LDRD Program Statistics

$177.7M	$371K	404	216
Total Program Cost (not including PM costs)	**Median Project Size**	**Total LDRD Projects**	**New Projects in 2019**

LDRD Participants



LDRD-Supported Postdocs	**148**	38% of Sandia total
LDRD-Supported Postdoc to Staff Conversions	**34**	50% of Sandia total
Refereed Publications	**363**	31% of Sandia total
Technical Advances	**112**	44% of Sandia total
Patents Issued	**76**	48% of Sandia total
Software Copyrights	**20**	18% of Sandia total
R&D 100 Awards	**3**	75% of Sandia total

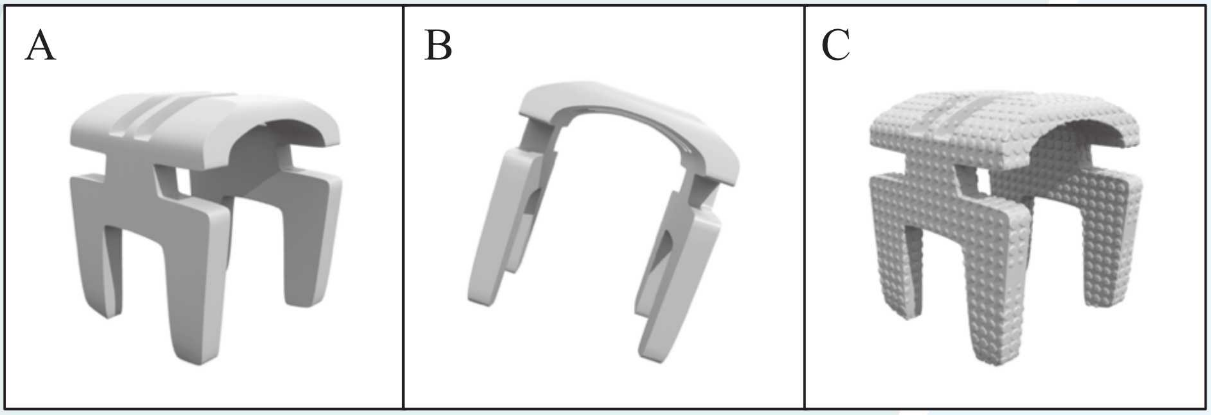
LDRD PROGRAM ACCOMPLISHMENTS

The following sections highlight some of the accomplishments of Sandia's LDRD program, organized around the three themes of mission agility, technical vitality and workforce development. Unless otherwise noted, these highlights are for projects that ended in FY19. Some of these highlights are for projects that ended prior to FY19, but whose impact is still being realized across the mission and the nation.

Enabling agile responses to national security missions (technology/capability affecting the mission)

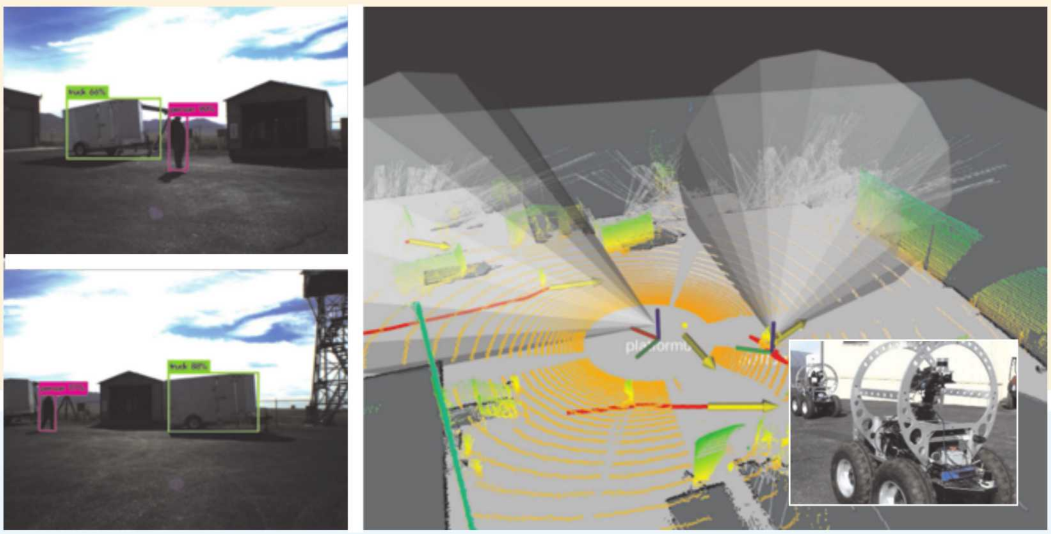
It takes innovative STE to create and enhance the capabilities needed to ensure that the U.S. is ready to respond nimbly to national security mission needs. LDRD is a critical resource at the heart of what it takes to lead into the future.

Using cognitive information environments for international safeguards. For the first time, a team of Sandia researchers has applied cognitive science principles to the international nuclear safeguards' domain. The project garnered international attention at the International Atomic Energy Agency (IAEA) and the European Safeguards Research & Development Association for its sound experimental design and scientific principles, as well as its novel approach of using human performance testing to document the impacts of information visualization on safeguards inspectors working in the field. The follow-on work funded by the Intelligence Advanced Research Projects Activity will explore the cognitive impacts of erroneous response from machine learning models, and on cognition-informed safeguards best practices. The findings were published in the proceedings of the Institute for Nuclear Materials Management Annual Meeting, the European Safe-guards Research and Development Symposia, and the Human-Computer Interaction International Conference.



Example stimuli from a human performance experiment assessing the impact of safeguards inspector note-taking methods on change-detection tasks. The use of abstract stimuli allowed the team to reduce bias based on technical expertise. (Images used with permission from the IARPA/MiCRONS project.)

Mobile sensors find the best data to identify threats. Researchers at Sandia developed information-driven control techniques allowing mobile robotic sensors to determine and collect the data most likely to help identify threats. Distinguishing potential threats from other alarm sources like animals and weather is a central physical security challenge. Sensors that can reposition themselves without human action can "get the information they need to make threat determinations faster, more efficiently, and more reliably" than traditional security systems, Steve Buerger, the LDRD principal investigator (PI) said. The team developed algorithms that fuse detections and object identification from multiple sensors and make optimal plans to acquire new data that drives down threat uncertainty, all in real-time. Initial experiments used teams of ground and airborne platforms and intelligently fused data from sensors including color, thermal, and LIDAR range. The technology is expected to form an important pillar of future high-value physical security systems.



Two mobile ground sensors (inset) autonomously identify potential threats in a security scene. Sensors detect unfamiliar objects and identify them using classifiers running on LIDAR, color, and thermal imagery.

Sandia scientists begin to unlock the optical emission characteristics of plutonium. A collaboration leveraging expertise in uranium oxide formation at Sandia and in laser-produced plasmas at Pacific Northwest National Laboratory (PNNL) measured what is thought to be the first-ever reported electronic spectra for Pu-oxides. The team is analyzing historic electrodeless discharge lamp Pu-240 spectra for quantitative emission strength analysis. Spectra were collected using an experimental laser-induced breakdown spectroscopy (LIBS) on Pu-239 metal, characterizing the spectral, spatial, and temporal dynamics of the laser-produced plasma. The data demonstrate an enabling capability that places Sandia and PNNL as national leaders in the field of actinide optical spectroscopy.

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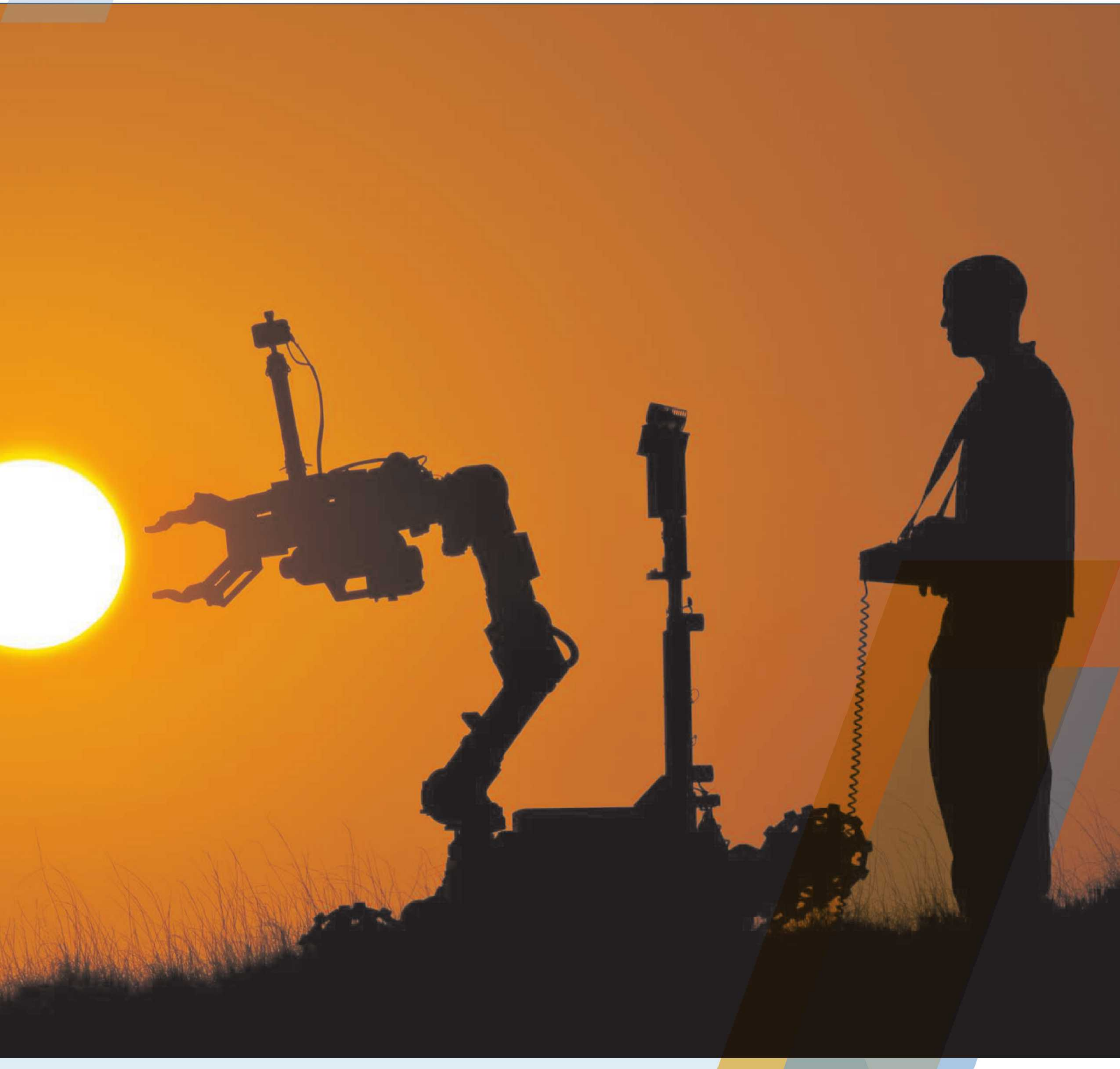
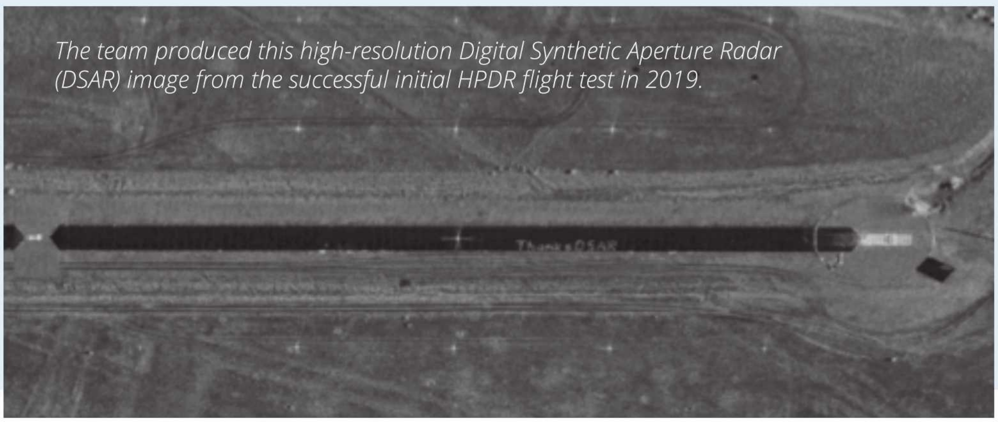
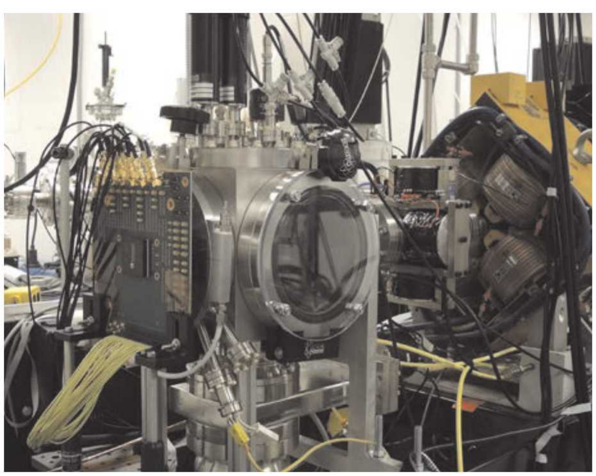


High-performance digital radar for multi-mission intelligence, surveillance, and reconnaissance. Sandia researcher Jacques Loui and his team demonstrated an ultra-wide-band (UWB), multi-mission modular digital radar architecture that overcame limitations of single-application analog radar designs by leveraging commercial-off-the-shelf (COTS) hardware, existing/new firmware/software intellectual properties, and available radio frequency (RF) apertures. The team demonstrated several Sandia firsts in real-time ultra-wide-band sensing, including multi-channel 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. The innovations resulting from the HPDR project are already having significant impact, with funding for follow-on development from an important national security program and potential application in several projects within the radar intelligence, surveillance, and reconnaissance mission space.



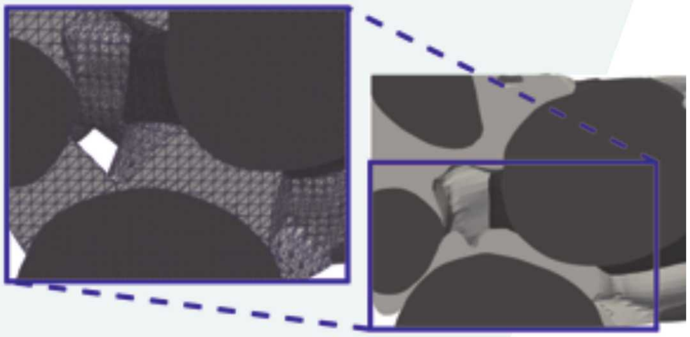
The team produced this high-resolution Digital Synthetic Aperture Radar (DSAR) image from the successful initial HPDR flight test in 2019.

Adopting advanced commercial CMOS technology for rad-hard applications. The performance of Nuclear Deterrence (ND) systems could be improved by adopting advanced commercial complementary metal-oxide-semiconductor (CMOS) technologies. However, the radiation hardness of these systems must be assured. This project quantified dose-rate upset thresholds, allowing the team to evaluate whether advanced commercial technologies could be used in rad-hard applications, to evaluate the susceptibility of advanced commercial technologies to neutron displacement damage and single-event effects, and to develop hardness assurance methods. As a result of the work, Sandia is collaborating more closely with DoD agencies and their contractors to understand and improve the radiation hardness of advanced commercial technologies. Sandia capabilities (SPHINX, Ion Beam Lab, and field programmable gate array test capabilities) were developed and are now being utilized by other programs, and staff were trained to perform radiation survivability testing. One of the external collaborators includes Georgia Tech. This project received the Best Paper award at the 2019 Hardened Electronics and Radiation Technology (HEART) Conference.



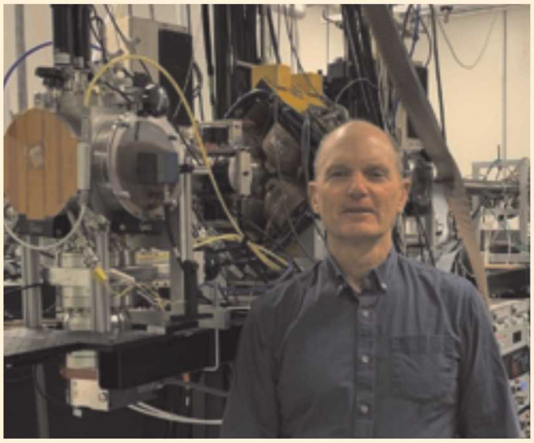
Circuit boards, such as the one on the left, were irradiated with neutrons at the Sandia Ion Beam Laboratory's new 14 MeV neutron facility, which provides a capability recently developed under LDRD funding (see page 12), to investigate neutron displacement damage and single-event effects. Experiments like these revealed the radiation failure levels and failure mechanisms in cutting-edge commercial CMOS technologies.

Speeding up model development for improved mission agility. Sandia researchers designed and prototyped a numerical method capable of efficiently producing high-quality mechanical predictions using automated meshing processes. "As an analyst, I was spending an average of 30 hours per week meshing CAD models for use in my simulations. I wanted to change this to 30 minutes," said Jacob Koester. Jacob teamed with Michael Tupek and researchers at the University of California, San Diego to create the conforming reproducing kernel (CRK) method, which leverages aspects of both mesh-free and finite element methods, resulting in observed numerical efficiencies of up to 1000x greater than current techniques when starting from an automatically produced mesh containing low-quality elements. Jacob and Michael are continuing to advance CRK for use in rapid design-to-analysis, micro- and meso-scale material simulations, and mass conserving fracture predictions. The work has been published in Computer Methods in Applied Mechanics and Engineering.



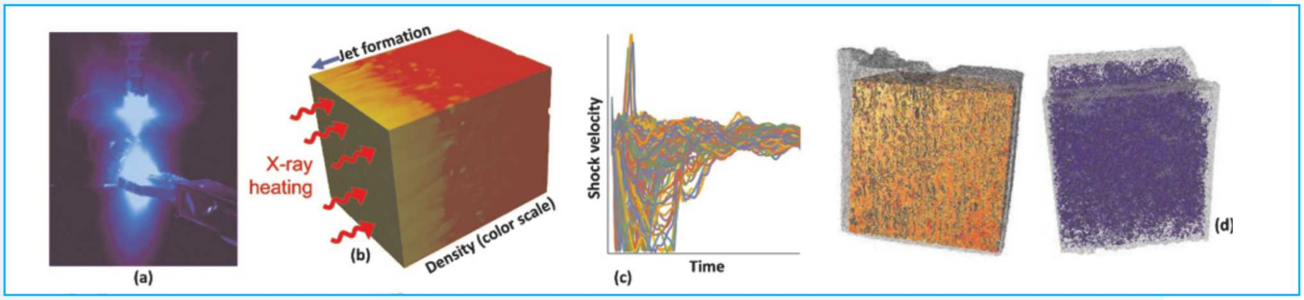
The conforming reproducing kernel method, developed by Sandia researchers Jacob Koester and Michael Tupek, is capable of predicting large deformation (left) using a mesh generated from x-ray computed tomography (CT) images and containing very low-quality elements (right). (Photo courtesy of Jacob Koester)

14 MeV DT Neutron Test Facility at the Sandia Ion Beam Laboratory. A recently completed LDRD project provided a new facility at Sandia for testing effects of energetic neutrons on electronic components. Fourteen MeV neutrons are produced with a deuterium ion beam onto a thin-film tritide target. The project's goal was to increase the neutron fluence to levels needed for radiation effects testing and qualification, and this was achieved through two technical advances. First, a new multilayer target concept was developed to reduce the rate of tritium loss from the target by isotope exchange, thereby reducing tritium usage and increasing target lifetime. The second advance was the construction of a new test chamber designed to maximize neutron flux at test locations. Together, these advances increased the available neutron fluence by several orders of magnitude. This new capability is being used in tests for Sandia nuclear weapon programs; evaluation of commercial parts such as highly scaled CMOS static random-access memory (SRAM) integrated circuits; tests of new devices under development at Sandia such as III-V heterojunction bipolar transistors and gallium nitride high-voltage diodes; and fundamental studies of physical mechanisms of device failure.



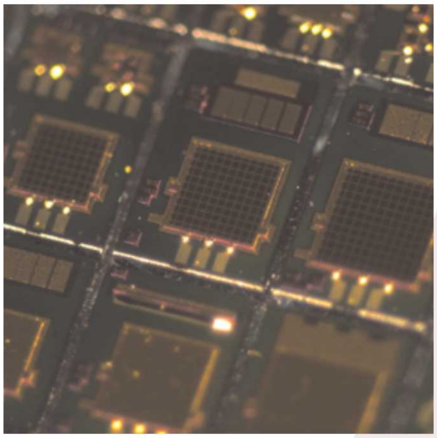
New 14 MeV DT neutron test facility at the Sandia Ion Beam Laboratory with LDRD PI Bill Wampler.

Stochastic shock in advanced materials. Many new materials being developed for defense applications require high resilience to heating, radiation, and shock environments. Predicting their behavior is often complicated by porosity and anisotropy from emerging fabrication methods, such as additive manufacturing. In this project, the team developed experimental and computational tools for predicting stochastic material responses in spray-formed metals. They developed methods to irradiate and recover samples following x-ray heating at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL), allowing study of micron-scale morphological changes using the synchrotron at the Advanced Photon Source at Argonne National Laboratory. Also developed were methods for multi-point sampling of shock velocity during plate-impact experiments. Based on these detailed investigations, the team developed fast algorithms for generating computer representations of spray-formed microstructures, enabling rapid exploration of the effects of material variability. Models in the ALEGRA finite element code were then expanded to allow the first three-dimensional (3D), fully coupled, radiation-hydrodynamics simulation of heterogenous materials. The capabilities enable assessment of a wide variety of complex architectures, such as porous materials, composites, additively manufactured components, ablation plumes, and other 3D articles subjected to mechanical and radiation environments. The Sandia project involved collaboration with three other DOE laboratories (LLNL, Los Alamos National Laboratories (LANL), and Argonne National Laboratories) and researchers spanning the materials, radiation, physical, computational and engineering sciences.



Many new materials have random behavior from microscale features. Here, the first NIF shot to generate x-ray shock (a), 3D simulation of a porous material (b) showing stochastic heating and shock across a specimen (c) resulting from complex, 3D microstructures (d). (NIF photo courtesy of LLNL)

High-energy x-ray detectors using fast, high-Z semiconductors. The development of warm x-ray sources at the Z machine pulsed power accelerator requires fast x-ray diagnostics with sensitivities significantly higher than what is commercially available. This need was met through a collaboration between the Microsystems Engineering, Science and Applications (MESA) Complex and Z to fabricate gallium arsenide (GaAs) x-ray detectors. The delivered detectors were fielded in several Z shot series and are providing hard x-ray data to physicists at Z. In addition to improved time response and hard x-ray sensitivity compared to commercial detectors, the devices fabricated at MESA show much more consistent device-to-device signal levels. This improved repeatability gives researchers at Z new quantitative data for source development efforts and will help support national security missions.

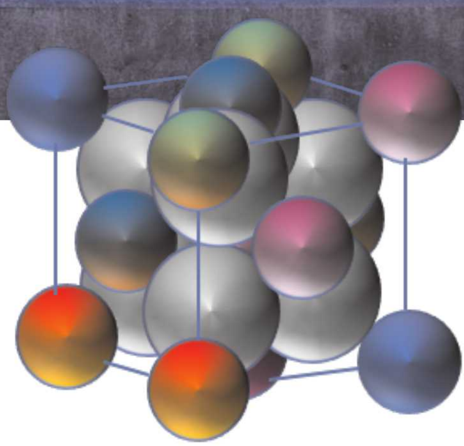


Angle view microscope image of microfabricated GaAs x-ray detectors. These detectors' absorber layer thickness and aperture sizes are customized to support mission needs for sub-nanosecond time response and good sensitivity to >10 keV x-ray signals. (Photo by Sandia staff member Michael Wood)

Sandia's MESA labs at sunrise

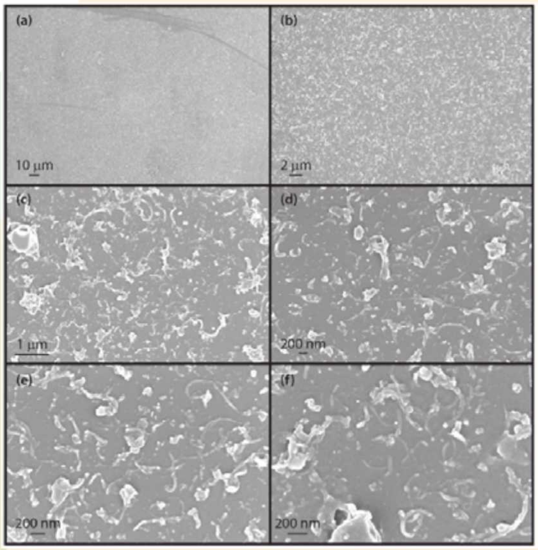
Generating hypersonic flight plans with Georgia Tech. Researchers at Sandia collaborated with Georgia Tech to develop an autonomous mission-planning solution that reduces the time to generate hypersonic flight plans from months to minutes—enabling rapid response to time-sensitive threats. Flight plans generated using this method are realistic, feasible, and satisfy and validate current constraints for flight. New projects with Georgia Tech and Purdue University are looking to advance this capability to develop a scrimmage tool for realistic engagements.

—enabling rapid response to time-sensitive threats.



Gram scale synthesis route for high entropy oxides, with chemical control over particle composition and size. Sandia researchers, Stanley Chou and Beth Paisley, developed a gram scale synthesis route for high entropy oxides, with chemical control over particle composition and size. Since high entropy materials are stabilized by configurational entropy, increasing the number of elements in the system creates stability and allows for unique combinations of atoms within one material. These materials are tailorable in composition and fabrication method, allowing for mechanical and thermal response design considerations. The specific material created has the potential for enhancing radiation insult resilience and fault tolerance with a coating that can be applied during part fabrication, or as a coating added to existing or COTS parts. The ability to synthesize ceramics as designed will serve as a materials discovery building block for several of the Labs' mission areas.

Avove: This concept image depicts an atomically modular ceramic for thermal-radiation barrier, and composites.



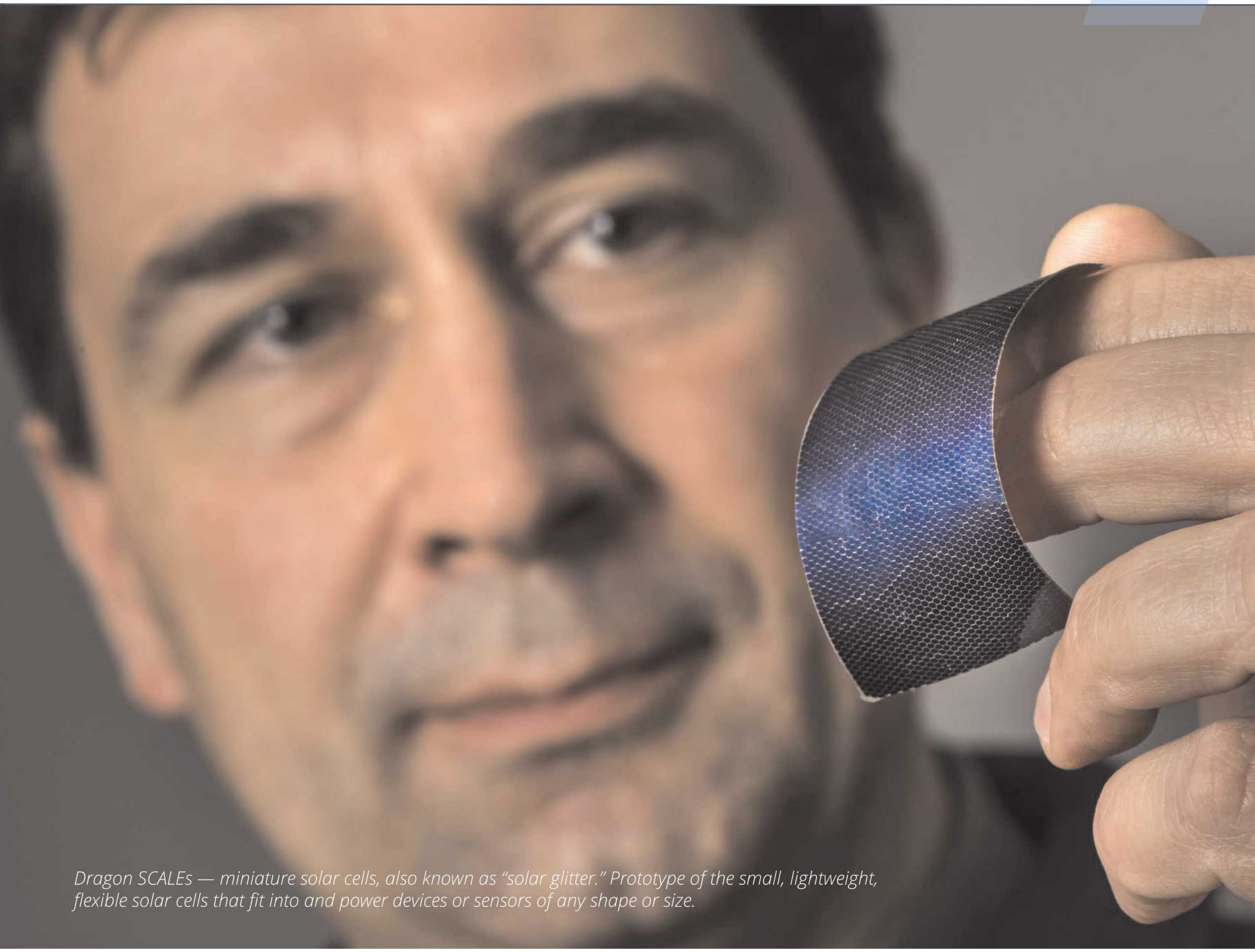
Surface treatment methods for activating the surface of polymers. Andrew Vackel and a team of Sandia researchers developed surface treatment methods for activating the surface of polymers to allow for metallization or, for the first time, the ability to chemically bind carbon nanotubes (CNTs) to the surface of polymers. This work creates a pathway for plasma-spraying high Z materials onto polymers with the use of a robustly bonded interlayer. Additionally, the method to pattern CNTs onto polymer surfaces has implications for applications in electronics and may offer an alternative pathway to plasma etching as a surface treatment method for applying chemically bonded metallic films to polymer surfaces.

Pre-dispersed CNTs after surface treatment showing no large cluster formation.

Creating an electromagnetic pulse (EMP)-resilient electric grid. Members of the EMP-Resilient Electric Grid for National Security Grand Challenge (GC) (FY18-FY20) received $2.3 M in its second year from the Advanced Research Projects Agency-Energy (ARPA-E) to develop a GaN-based, sub-nanosecond EMP surge arrestor. Initial work on the surge arrestor technology under the GC was completed and sufficiently promising for ARPA-E to pick it up for further development as part of its Building Reliable Electronics to Achieve Kilovolt Effective Ratings Safely (BREAKERS) program. The program seeks to create a new set of technologies and capabilities for next-generation utilities that are more resilient to EMP produced by high-altitude nuclear explosions and low-frequency geomagnetic disturbance threats. Work done during the GC and at ARPA-E positions Sandia to become a leader in addressing these complex problems of critical national security.

The program seeks to create a new set of technologies and capabilities for next-generation utilities...

Rapid screening of CRISPR gene editing therapeutics. The NanoCRISPR LDRD Grand Challenge (GC) project (FY17-18) developed key capabilities related to rapidly screening for CRISPR gene editing therapeutics for emerging or engineered diseases and the novel cellular delivery systems for CRISPR comprised of a lipid coating that can contain groups to target specific types of cells and a porous nanoparticle to contain the therapeutic material. The team hosted a workshop last July on CRISPR for Biodefense Applications, and that plus the project overall, has established Sandia capabilities in the rapidly evolving CRISPR arena. The NanoCRISPR GC resulted in a key role on the Defense Advanced Research Projects Agency (DARPA) Safe Genes project led by Jennifer Doudna at UC Berkeley, one of the discoverers of CRISPR, and is generating significant interest from other potential customers including the Defense Threat Reduction Agency.

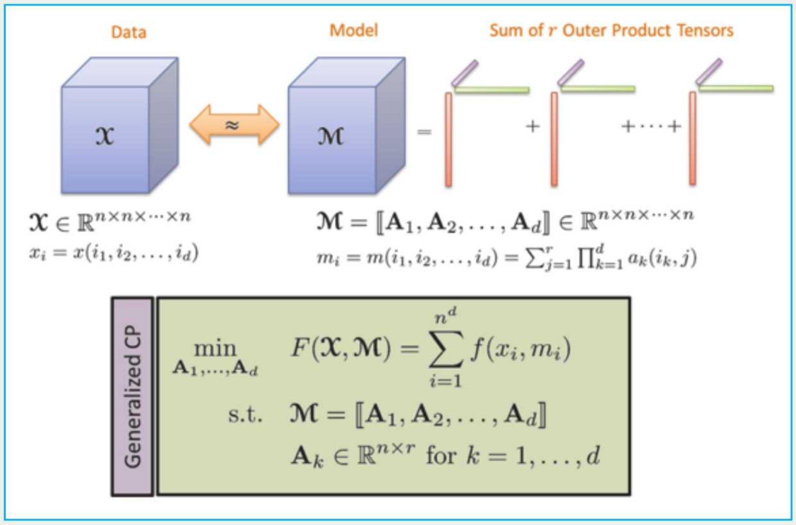


Dragon SCALEs — miniature solar cells, also known as "solar glitter." Prototype of the small, lightweight, flexible solar cells that fit into and power devices or sensors of any shape or size.

Power Bus Grand Challenge (GC) capabilities could reduce time/cost of nuclear system upgrades. The Power Bus GC resulted in the development of key technologies to enable power distribution and conversion in extreme environments. In particular, the Power Bus team developed power conversion circuits using custom semiconductor devices, fabricated at Sandia, that can operate at higher voltages while maintaining an intrinsic resilience to high temperature and intense radiation. The new technology was designed for power distribution in national security applications and other high consequence systems. Partnerships will continue with the Office of Naval Research on electric ship applications, DOE Vehicle Technologies Office's Electric Drive Train Consortium on electric vehicles, the ARPA-E, and two R&D Certification and Safety projects.

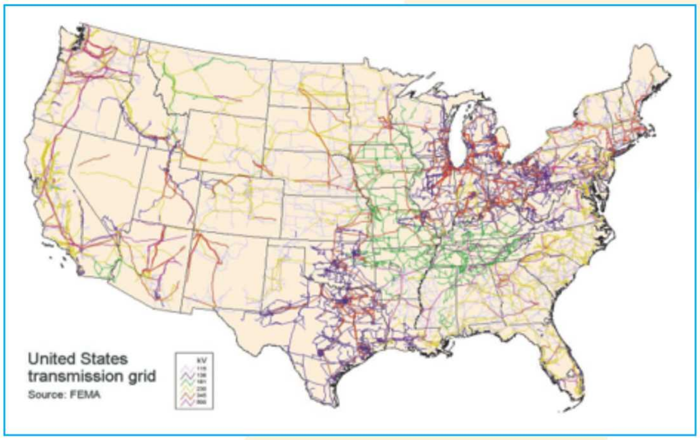
...designed for power distribution in national security applications and other high consequence systems.

Parallel tensor decomposition for massive, heterogeneous, incomplete data. Tensor decomposition is a fundamental tool for unsupervised machine learning and understanding complex data sets. Unlike deep neural nets and related tools, tensor decomposition can identify structure in data in a way that's transparent to users and can work with very limited data. The LDRD-developed Generalized Canonical Polyadic (GCP) tensor decomposition is especially unique in its ability to handle binary, count, and nonnegative data, in contrast to standard approaches geared to normal-distributed data. Sandia recently developed GenTen, *open source C++ software* for GCP tensor decomposition, that achieves high performance on multiple platforms including many-core central processing units and graphical processing units. Data science applications for this software include sensor monitoring, cyber security, treaty verification, and signal processing, where it identifies latent structure within data, enabling anomaly detection, process monitoring, and scientific discovery.



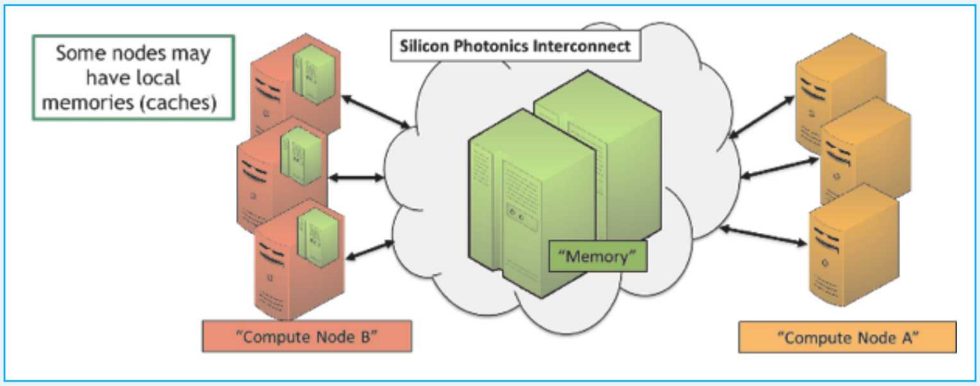
GCP tensor decomposition enables alternate objective functions and more analysis options including binary and nonnegative data. (Image by Tamara Kolda)

Stochastic optimization to enhance resiliency and response strategies in critical infrastructure. The loss of critical infrastructure services, such as electric power grids, water systems, and communication networks, can be caused by natural hazards or intentional acts. The U.S. critical infrastructures must be designed so that they are robust under abnormal conditions such as line faults, generator failure, water contamination, and computing network intrusions. Sandia developed software for optimal design and operation of critical power systems that considers uncertainty, discrete decisions, and nonlinear physics associated with the critical infrastructure. These techniques have been published in six journal articles, and the capabilities for mixed-integer nonlinear programming and electrical grid optimization have been incorporated into two open source software packages based on Pyomo (*CORMIN and EGRET*). Follow-on work is being funded by ARPA-E and the DOE Office of Fossil Energy (FE).



The CORMIN and EGRET software was applied to two exemplary problems including the design and operation of nonlinear power systems and stochastic sensor placement. (Image by Carl Laird)

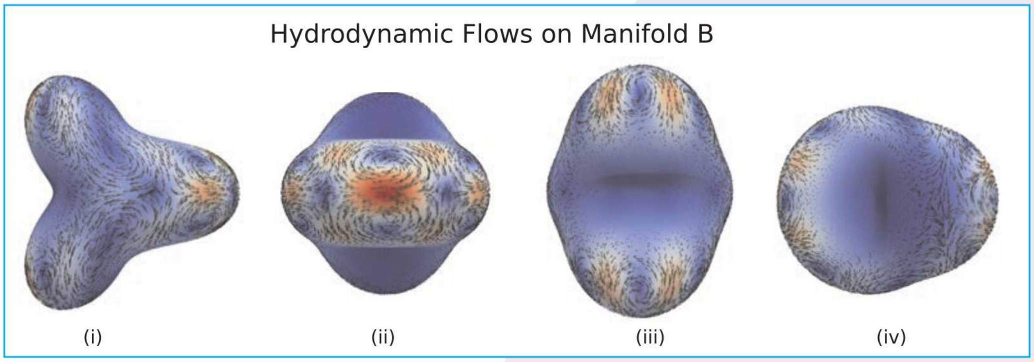
Disaggregated memory architectures for future High Performance Computing (HPC). Low-cost, high-bandwidth, silicon photonics-based networks have the potential to significantly disrupt the design of future HPC systems by dramatically changing the cost function (both energy and speed) for data movement. To enable design exploration for future DOE and DoD Exascale HPC systems, Sandia developed several tools that will allow the HPC community to evaluate the impact of these technologies on mission-critical applications. One-sided and atomic communication models were introduced into Sandia's Structure Simulation Toolkit (SST), allowing for entirely new simulation and modeling capabilities of silicon photonic networks. In addition, an "OpenFAM" application program interface (API) was developed in collaboration with Hewlett Packard Enterprise. Using these tools, the first mixed-fidelity, on-node models were created to evaluate communications and local memory access performance impacts.



Silicon photonic networks could create a disruptive capability in future Exascale Computing architecture designs. (Image by Simon Hammond)

Compatible particle methods. In many mission applications, the simulation workflow is dominated by the CAD-to-mesh task that can consume up to 75% of the full design-to-solution process. Meshfree and particle methods bypass the meshing process and can enable automated, rapid simulations of complex mission applications. Unfortunately, up until now, meshfree methods lacked the rigorous mathematical foundations and the associated software tools for compatible discretizations that we expected of mesh-based discretizations. To close this gap, Sandia developed a mathematical framework and software implementation for compatible meshfree discretizations based on the Generalized Moving Least Squares (GMLS) regression approach. This framework provides the first computationally efficient construction of a conservative and consistent meshfree method. A modern, performant software library (*Compadre Toolkit* V. 1.0, DOI 10.11578/dc.20190411.1 for meshfree and particle methods) was implemented on different HPC architectures and is now available.

Numerical solution of hydrodynamic flows using GMLS from the Compadre Toolkit to implement a compatible meshfree discretization of the surface partial differential equations. (Figure credit: N. Trask, P. Kuberry, A Compatible meshfree discretization of surface PDEs, Computational Particle Mechanics, 2019. DOI: 10.1007/s40571-019-00251-2)



Controlling the activity of gene-editing tools. Sandia developed a pipeline to discover clinically useful CRISPR-Cas9 genome-editing inhibitors to ensure the safety of CRISPR-based gene therapies and provide an antidote in the event of unwanted exposure. In collaboration with the University of California, Berkeley, a high-throughput fluorescence resonance energy transfer (FRET)-based assay was developed with low background noise and high sensitivity. A phage display assay was also developed to identify small peptides with high affinity binding to Cas9, and has identified peptides that selectively block SpyCas9 activity and peptides with activity across Cas9 variants. This represents the first identification of broad-spectrum anti-CRISPR therapeutics that block multiple Cas9 variants from phylogenetically CRISPR-Cas systems.

Novel zoned wasteforms for high-priority radionuclide waste streams. A new negative thermal expansion (NTF) material, that readily incorporates radionuclides of interest, including Pu and Tc, was discovered and characterized in the process of synthesizing a phase-pure $Zr_2P_2WO_{12}$. The project successfully showed that NTF materials that shrink upon amorphization are viable wasteforms. Because of their resistance to long-term radiation damage, these materials can maintain radionuclide isolation more effectively than standard wasteforms, and may represent ideal solutions to prevent remobilization of radionuclides.

Nuclear Fusion Award

Sandia Fellow Keith Matzen received the 2019 Distinguished Career Award from Fusion Power Associates, a national nonprofit research and education foundation, for his many contributions to the Labs' development of nuclear fusion. The foundation annually brings together senior U.S. and international fusion experts to review the status of fusion research and consider ways to move forward. The goal is to provide timely information on the status of fusion development and other applications of plasma science. Keith views this particular award as a recognition of the large team of people who made tremendous progress on many very difficult problems during his time as senior manager and director in the Pulsed Power Sciences Center. Within this context, LDRD investments had a large impact on the overall success of the program.

Technical vitality and frontiers of S&T

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 enable national security impacts, can transfer to industry, be commercialized under licensing agreements, and then brought to market for the U.S. public good.

Credible image meshing enables as-built computational analysis. A Sandia LDRD research team developed new technologies to automatically and credibly convert 3D images of materials or components arising from imaging techniques such as x-ray computed tomography (XCT) into high-quality computational meshes for multi-physics simulation. Deep Bayesian neural networks identify parts, materials, or phases of interest in the images. New facet-based meshing algorithms create high-quality and computationally efficient meshes. The uncertainty that is inherent in each of these processes is quantified and propagated, providing impact of geometric uncertainty on physics predictions. "Robust image-based meshing introduces a new paradigm for computational simulation, enabling enhanced surveillance of as-built components and direct feedback on the impact of manufacturing variability on component performance, each of which enhances mission agility," said PI Scott Roberts. The newly developed workflow has already been applied to a variety of Sandia mission applications, including thermal protection systems, battery materials, detonators, thermal sprays, and laser welds.

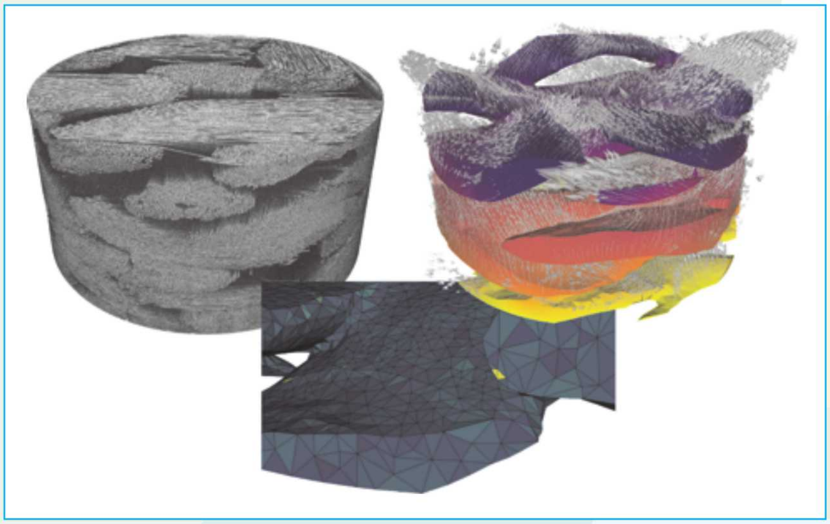
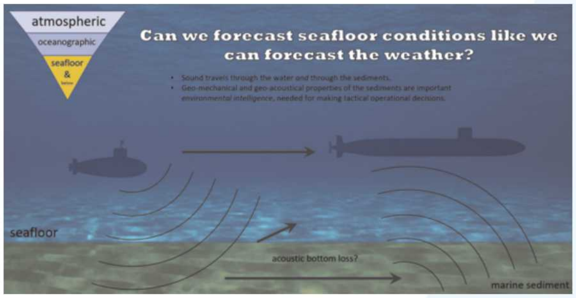
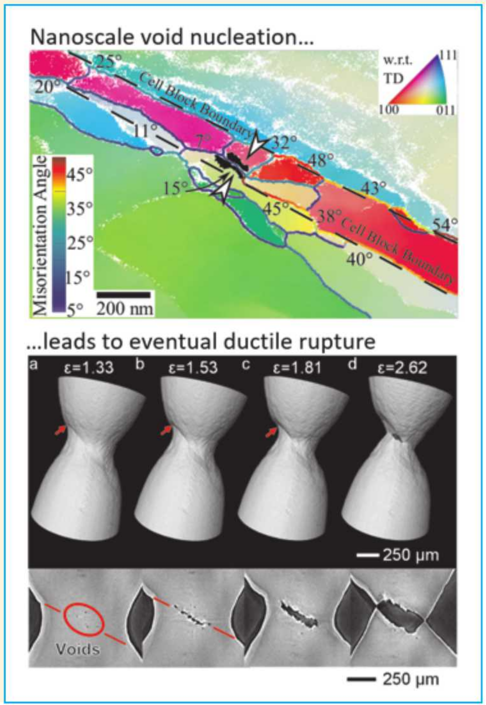


Image-based simulation of a woven composite material showing greyscale XCT (top left), a high-quality tetrahedral mesh (bottom), and a thermal-mechanical simulation (top right). (Images courtesy of Lincoln Collins)

Forecasting marine sediment properties on and near the Arctic shelf with geospatial machine learning. This LDRD team proposed a combination of geospatial machine learning prediction and sediment thermodynamic/physical modeling to create probabilistic maps of geoacoustic and geomechanical sediment properties. This new technique for producing reliable estimates of Arctic seafloor properties will better support naval operations relying on sonar performance and seabed strength and can constrain models of shallow tomographic structure that are important for nuclear treaty compliance monitoring/detection. By gaining more complete awareness of the battlespace environment through the development of seafloor forecasting capability, it will provide an assessment tool to support decision-making by warfare commanders. Such a tool can be made to automatically ingest data to produce a battlespace-assessment calculation that will improve blue force status awareness. It also benefits Sandia's energy security mission areas, because it will provide a means to estimate the resource potential of seafloor petroleum systems. Two of the most important geologic parameters that determine seafloor acoustic properties are free gas and methane gas hydrate (natural gas). The project results were presented at the National Geospatial-Intelligence Agency's Maritime Community of Practice Meeting in November 2019, the American Geophysical Union Annual Fall Meeting in December 2019, and the Gordon Research Conference on Natural Gas Hydrate Systems in February 2020.

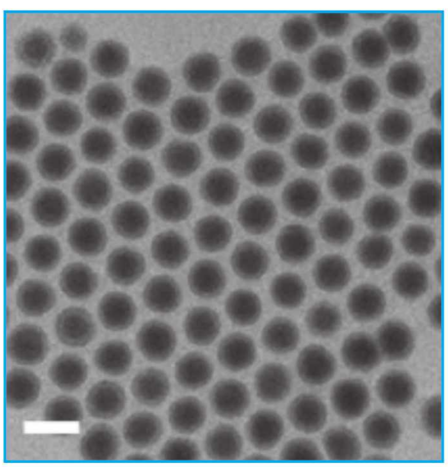


Understanding ductile rupture of metals. Sandia-designed hardware is expected to withstand numerous mechanical environments ranging from crush to shock. However, our ability to engineer such structures relies on a fundamental understanding of how the constituent materials break. The ductile rupture of metals has always been difficult to predict, in part due to a lack of understanding of the basic mechanisms of damage formation. This LDRD utilized state-of-the-art experimental tools including high-resolution electron backscatter diffraction and transmission electron holography, combined with state-of-the-art materials modeling tools to investigate the incipient conditions that give rise to the onset of material failure. As a result, Sandia discovered that the previous formulation of failure processes under tension and shear, developed largely in the 1970s, is far too narrow. The results were published in a series of nine journal articles in top materials journals, including four in *Acta Materialia*. One article on "The Mechanisms of Ductile Fracture" was independently highlighted by an editor at *Materials Today*, in a summary article titled *New Understanding for Metallic Failure*, who stated, "This work is an important step forward as it introduces a new approach for interpreting ductile failure and can lead to a resolution to the problem of reported discrepancies in strain-to-failure predictions."



During deformation of pure metals, incipient void formation was found to occur at sites of intense localized plasticity known as cell block boundaries, ultimately leading to coalescence of multiple voids and catastrophic failure.

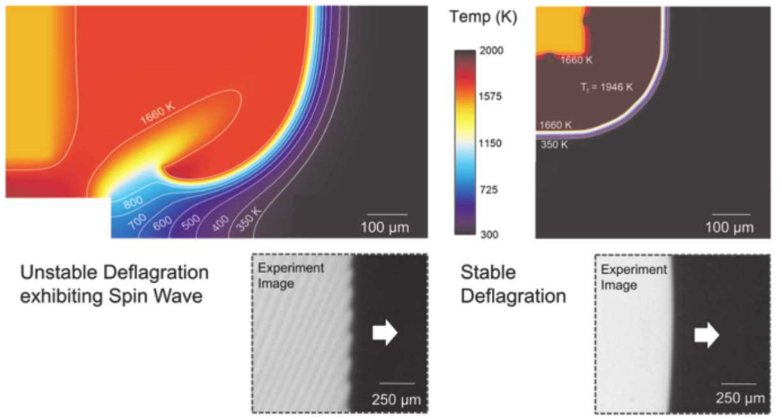
Discovering new ways to make magnetically soft materials. An LDRD-funded team, led by Dale Huber, discovered new ways to make magnetically soft materials. The work started with a simple idea. Since magnetic nanoparticles can align with magnetic fields very quickly and with little energy input, a composite made from those particles that could retain the magnetic properties of the individual nanoparticles would produce improved, soft magnetic materials. Those materials could change their magnetization faster than conventional materials and with lower energy losses. Materials like this could find use in areas of interest for Sandia like pulsed power or enhancing the energy efficiency of switching power supplies in everything from the nation's electrical grid to weapons systems or cell phone chargers. The team studied every aspect of the design and fabrication of these nanocomposites from synthesizing new precursors to designing new synthesis methods with unprecedented control over the nanoparticles' sizes, simulating interactions between magnetic particles, and fabricating soft magnetic materials with particles precisely spaced to avoid those interparticle interactions. The team successfully made nanocomposite magnets with dramatically lower, high-frequency energy losses, and the body of work resulted in 10 published papers and three patent applications.

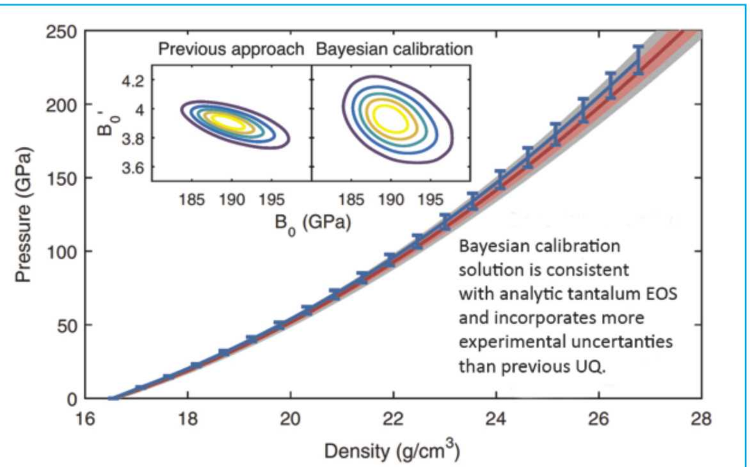


A key development for designing the soft magnetic nanocomposites was a synthesis approach that allows for precise tailoring of both the size and spacing between magnetic nanoparticles. Iron nanoparticles are pictured, and the scale bar is 25 nm. (Micrograph courtesy of Grant Bleier)

Design/fabrication of reliable, reactive multilayer coatings/foils to release stored chemical energy as light/heat. A Sandia-led team discovered the thermal and chemical factors underlying stable deflagration in reactive nanomaterials. These discoveries enabled the design and fabrication of new, more reliable reactive multilayer coatings and foils that can be stimulated by an external source to promptly release stored chemical energy as light and heat. The developed heterogenous solids have tailorable ignition thresholds and calorific output – important for envisioned heat source applications such as joining and power sources. Critical to function, these materials also avoid unstable reaction modes including 2-dimensional spin instabilities. The predictive, 3D reaction-diffusion model established for this LDRD project provides opportunity for rapid assessment of emerging reactive materials and optimization for future applications. Details were also published in the *Journal of Applied Physics*.

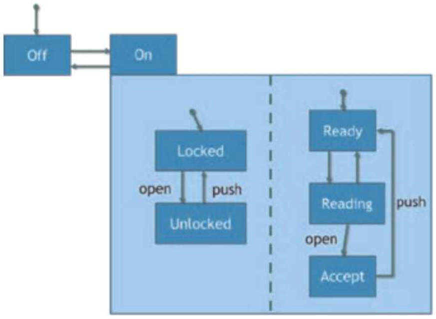
Snapshots showing propagating reaction waves in Co/Al nanolaminates after point ignition. Unstable and stable propagating waves develop in thick and thin period multilayers, respectively. Temperature maps on top are results from predictive thermal model simulations with the ignition zone positioned in the left, upper corner (in orange). The gray-scale, high-speed videographic images, included at the bottom, show similar behavior in experimental test samples. Multiple spin waves are evident in the unstable example on the left. Reacting material is bright in these images due to light emission.





Statistical uncertainty quantification for multivariate physical parameter estimation with multivariate outputs. Sandia recently developed algorithms quantifying uncertainty in computer model inputs by diagnosing and reducing overfitting in model calibration when the input is functional in nature. These methods were applied to the calibration of dynamic material properties in Z-machine experiments. Elastic shape analysis is used to calibrate misaligned functional data, and power-likelihood models are used to discount the statistical information associated with model discrepancy. Additionally, this method has found interest in the calibration of sea ice models by the monitoring of cracks in the ice shelf. The method is being actively applied in that domain.

Above: Improved uncertainty quantification and data fitting is achieved using elastic functional data calibration and power likelihood models in the Tantalum Equations of State (EOS) exemplar problem. (Figure by James Tucker)



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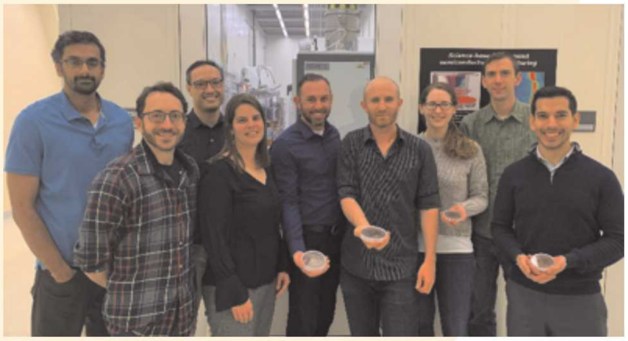
A domain-specific language for high-consequence control software. Formal methods approach the verification of digital systems using the mathematics by which, and for which, they are created—formal logic. This approach is particularly valuable for the design and verification of embedded digital systems in high-consequence control systems such as nuclear weapons. Under a Sandia LDRD, a formal specification language was developed and implemented within the Q formal verification toolset. The formal semantics enables machine-checked proofs of key properties, including real-time functionality, and correct-by-construction techniques important to affirming the safety, security, and reliability of the device. This capability is now being successfully applied within the Nuclear Deterrence program generally, and current life extension programs specifically.

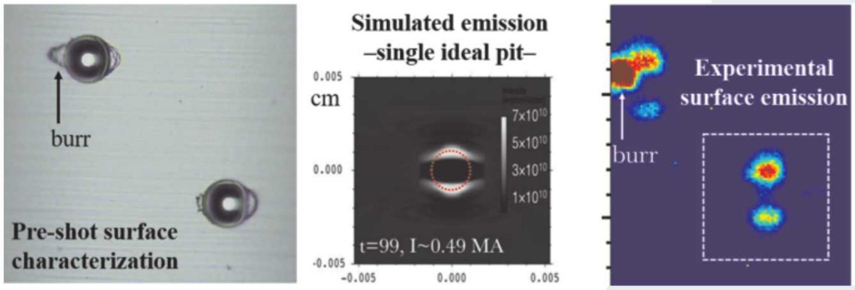
Example of a formal specification using the language developed through the LDRD. (Image courtesy Robert Armstrong)

State-of-the-art operation of an RF acoustic amplifier technology. Researchers at Sandia, led by PI Matt Eichenfield, demonstrated state-of-the-art operation of an RF acoustic amplifier technology. These devices operate by the acoustoelectric effect, wherein direct current electrons injected into a semiconductor on the surface of a piezoelectric substrate can transfer their energy to an acoustic wave traveling on the surface of that piezoelectric substrate, providing amplification. The technology platform is constructed using a novel heterogeneous integration of epitaxial semiconductors and lithium niobate surface acoustic wave devices, which required a large, multidisciplinary team to devise and build prototype devices. While passive RF acoustic devices are ubiquitous in wireless RF communications, incorporating active and nonreciprocal functionalities could have significant impact in areas such as radar and secure communications. The developed platform shows a 10x improvement in gain per unit length and an 89x improvement in required power consumption over the previous state-of-the-art operation.



A team of Sandia researchers stands in front of the microfabrication cleanroom utilized to fabricate wafers of acoustoelectric devices. The material platform developed during this LDRD program yielded surface acoustic wave amplifiers with state-of-the-art performance in terms of gain per acoustic wavelength and reduced power consumption.

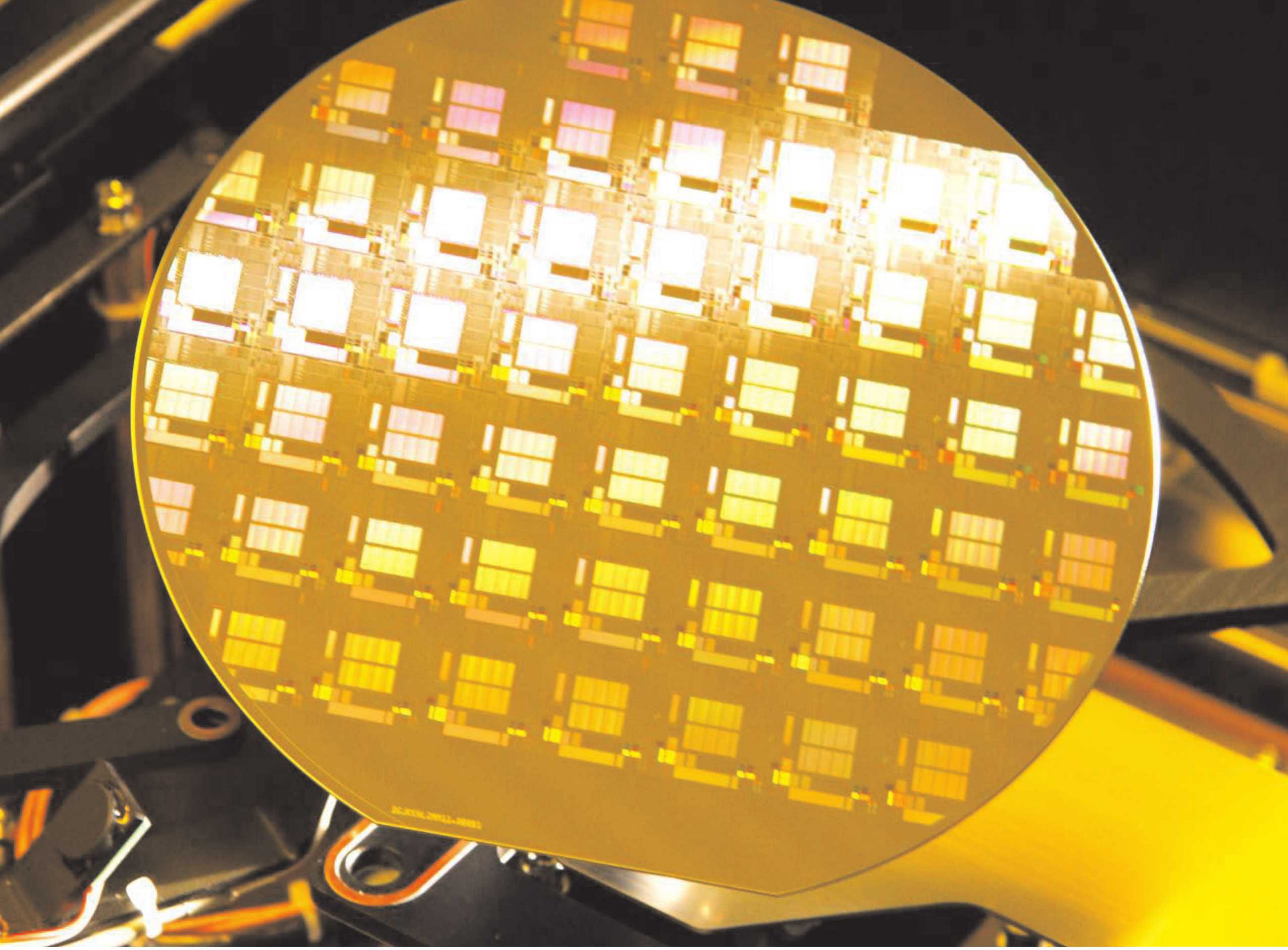
3D-magnetohydrodynamic simulations of electrothermal instability growth by studying Z-pinches with engineered defects. Electrothermal instability (ETI) is driven by Joule heating and arises from the dependence of resistivity on temperature. When a metal is Joule-heated through the boiling point, ETI drives azimuthally correlated surface density variations or "strata," which provide the dominant seed for subsequent growth of the Magneto-Rayleigh-Taylor (MRT) instability. MRT erodes implosion symmetry in magnetically driven liners, reducing their ability to compress and inertially confine fusion plasmas. Data and simulations suggest that reducing the growth of ETI meaningfully reduces MRT. Data on ETI can be difficult to interpret due to the complexity of inhomogeneities present in the metal (inclusions, surface defects, grain boundaries, etc.). To reduce such complexities, experiments have examined ETI growth from 99.999% pure aluminum, 800-micron-diameter Z-pinch rods driven to 800 kA in 100 ns. Rod surfaces are diamond turned to extreme smoothness, and then further machined to include carefully characterized "engineered" defects—designed lattices of micron-scale pits. Such defects are assured to be the largest current density perturbation in the system, enabling clear comparison with simulation. Visible-light emissions from the rod surface were captured with high-resolution gated imaging. Experiments confirmed two theory/simulation predictions. First, this shows that even for 100-nm-scale surface roughness, the surface will heat more rapidly than the larger defect if the curvature of the roughness (amplitude/wavelength) is sufficiently large. Second, when emissions from the defect do dominate, perhaps counterintuitively, the first plasma emissions are observed from above and below the defect.



(Left) Pre-shot surface characterization of two engineered defects machined into an otherwise ultra-smooth 5N aluminum surface. (Middle) Simulated emission from a single pit at the experimentally measured current. (Right) Experimental surface self-emission from engineered defects. Overheating and plasma formation above and below the pit qualitatively match simulation prediction. Impact of the micron-scale machining burr is also observed.

How to see what's happening inside a battery without disturbing it. Materials science researcher Eric Sorte focused on fuel-cell components, working on new ideas for energy-storage-device components, such as fuel cell membranes and batteries. The focus of the LDRD project was to develop new in-situ nuclear magnetic resonance technologies to monitor and diagnose batteries during charge and discharge cycles without having to tear them apart. That work continues via a new Grand Challenge LDRD, focused on customized lithium batteries, that started in the fall of 2019.

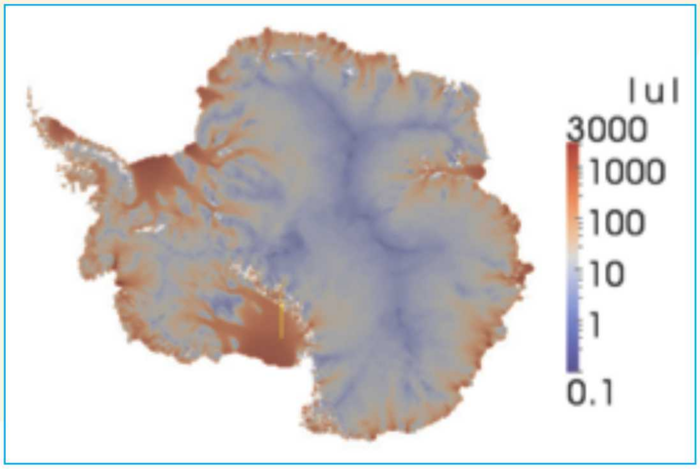
Below: Sandia materials scientist Eric Sorte is working to help battery researchers understand what goes on in a battery during operation.



Passive magnetoelastic smart sensors for a resilient energy infrastructure. A novel, passive, autonomous, and affordable microsensor for indirect detection of μA currents was developed. When integrated near current-carrying conductors, these wireless magnetoelastic smart sensors (MagSens) can detect small changes in their magnetic field via frequency shifts and thus detect leakage currents, arc faults (AF), ground faults (GF), transmission and distribution faults, and assist with asset health monitoring. The adoption of a sensitive and reliable fault detection system will ensure improved safety and integrity in complex grid, energy generation, conversion, and storage systems.

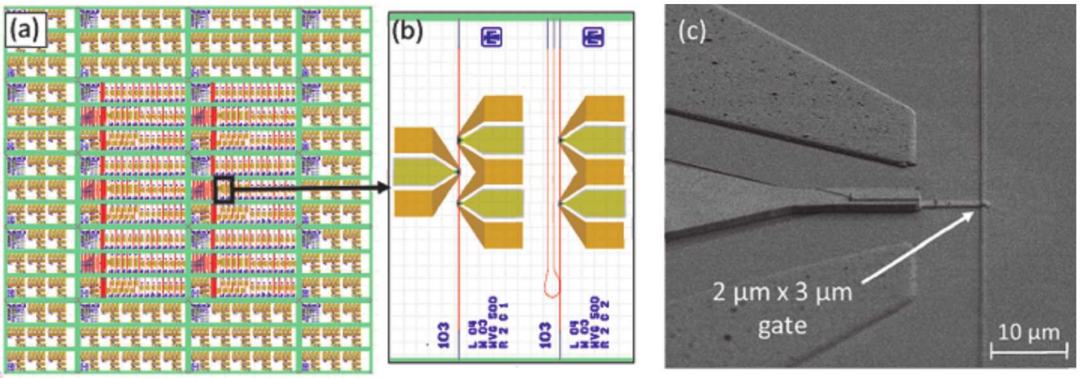
An exascale computational simulation capability for pervasive fracture and failure of structures. Modeling fracture is a difficult problem based on stochastic material properties throughout a structure. Sandia, together with the Jet Propulsion Laboratories, completed a joint project to develop computational algorithms and software that models the physics of pervasive failure for structures under severe loading, such as the Europa lander crashing into an icy moon of Jupiter. Sandia developed non-local and phase-field regularization algorithms within the Sierra/Solid Mechanics software package that predict the location and extent of fracture in structures under load. Further development of this software is now being funded by the NNSA Advanced Simulation and Computing program.

Fast and robust hierarchical solvers. Sandia and Stanford University created a portable software library for solving ill-conditioned, large-scale linear equations from partial differential equations on HPC architectures. These solvers take advantage of the inherent hierarchical structure of approximate low-rank systems. The software was applied to solving climate simulations for ice sheets. A related solver, developed jointly with University of Texas at Austin through Sandia's Academic Alliance program, was used for solving complex problems in electromagnetics. These solvers are being integrated into the *Trilinos package*.



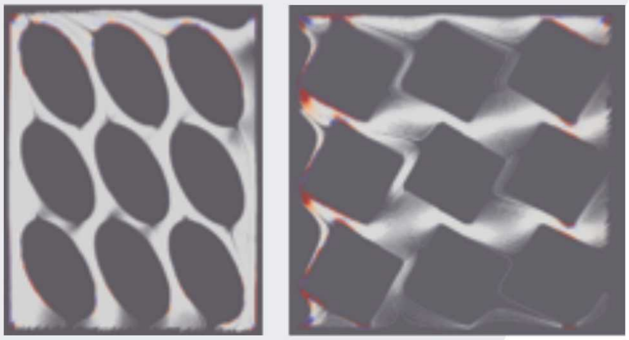
Simulation results obtained from climate modeling thin-ice sheets demonstrate linear scaling for up to 18.5 million elements. (Figure by Mauro Perego)

Near-infrared nanophotonics through dynamic control of carrier density in conducting ceramics. The LDRD project goal was to better understand the operation of epsilon-near-zero (ENZ) modulators through experimentation, material characterization, and modeling, and use that learning to design and demonstrate a new class of devices with improved performance and increased functionality. The experimental and modeling work was well received by the integrated photonics community, generating more than 60 citations by the conclusion of the program, and sparking a new wave of research and development on ENZ modulators. While earlier works developed the concept of ENZ modulation and provided critical early proof of the physics, the demonstration of gigahertz speed modulation in this program acted to bring renewed interest in the promise of Si photonic modulations that break the bandwidth-size tradeoff without requiring exotic or unstable materials. The capabilities developed in this project led to a new ENZ modulator design incorporated into silicon nitride waveguide platform for a more simplistic fabrication process and operation at shorter optical wavelengths. This new design was proposed as part of an ultra-low-power and dense photonic transceiver platform selected for funding under the DARPA PIPES program. This continuation funding will support fabrication of this updated modulator design and work to mature the technology by insertion into a full photonic system.

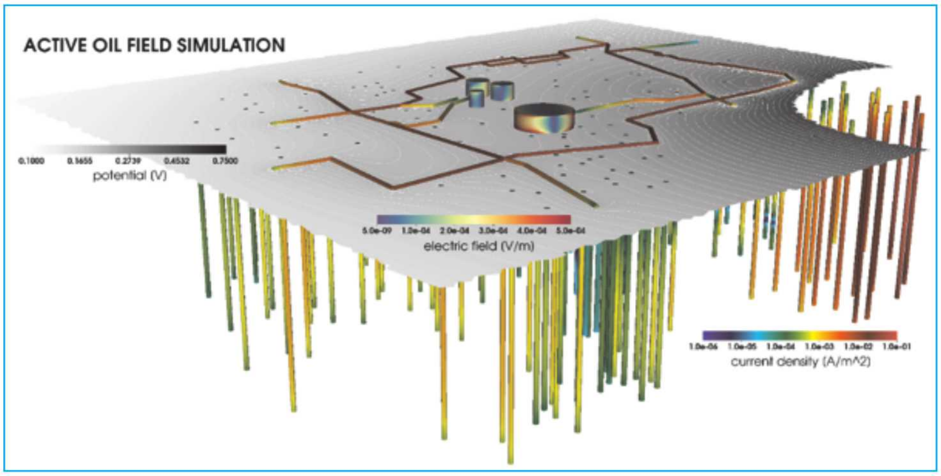


Results of updated mask and fabrication process: (a) Image of new photomask. Outer die are radio frequency test structures and inner die have a variety of waveguide and modulator designs. (b) Close-up view of a pulse amplitude modulation device implemented on the mask set. (c) Angled-view scanning electron microscope image of a fabricated device showing good alignment of the large contacts patterned by photolithography and the waveguide and metal gates patterned with two different e-beam lithography processes.

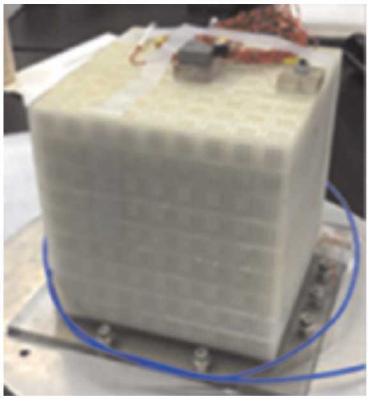
Characterization of ultralow permeability geomaterials using electrokinetics. A team from Sandia, including collaborators from the University of Illinois at Urbana-Champaign, are extending the hydrogeophysical use of electrokinetics to characterize the permeability of key geomaterials. The effort is developing and refining a laboratory apparatus to estimate permeability for rock cores from the electroosmotic and streaming potential coupling coefficients. At Sandia, coupled numerical models and analytical solutions were developed using an eigenvalue uncoupling approach to apply these methods at the laboratory and field scale. The team at Illinois produced pore-scale fully coupled electrokinetic simulations of flow around various shapes (see charge and flowlines in images). Pore-scale results are also being fused into lattices and porous media through machine learning.



Prediction and inference of multi-scale electrical properties of geomaterials. A team of Sandia geoscientists and mathematicians developed a pair of breakthrough algorithms for efficiently simulating the geophysical response of complex, multi-scale systems in the Earth's subsurface critical to Sandia's ongoing efforts in Nuclear Deterrence as well as Energy and Homeland Security. The problem with such complex systems is that for certain classes of geophysical phenomena (electromagnetic, fluid flow, etc.), the fine-scale detail present in real geologic materials can have a massive effect on the overall geophysical signature, yet capturing all the relevant details in a computer model is practically infeasible. Led by Chester J Weiss, the team proposed and implemented two distinct approaches to overcome this limitation: a hierarchical finite element method (HiFEM) to explicitly capture these details, and a fractional calculus method to accurately capture their macroscopic equivalence. These end-member approaches not only allow for a previously unobtainable set of predictive data, but also allow the team to explore the physics of the intermediate meso-scale where the transition from an exquisitely detailed to a "blurred" but equivalent upscaled model resides. Initial applications of the HiFEM software were extended to also account for the effects of man-made infrastructure in geophysical sensing applications, leading to reduction in computer runtime by a factor of 1000 or more. Details of the research were published in *Geophysics* and *Geophysical Journal International*.



Metamaterials science and technology Grand Challenge (GC) project. Multiscale Inverse Rapid Group-theory for Engineered-metamaterials (MIRaGE) software started under the Metamaterials Science and Technology GC (FY09-11), continued development under a DARPA contract, and just received a 2019 R&D 100 Award. The software contains functionality not offered in existing packages including: inverse design, symmetry-aided design, a metamaterial design library, increased scalability and speed by a factor of two, uncertainty quantification, and optical properties. MIRaGE enables designers to create, simulate, and optimize metamaterials having suitable optical behaviors through a process that assembles available information for analysis in minutes rather than months or years. This allows for more rapid cycles of learning and assured real-world performance. Applications where tailoring optical properties are important include cloaking/camouflage of assets and compact aberration-free imaging systems such as a miniaturized Hubble Space Telescope.

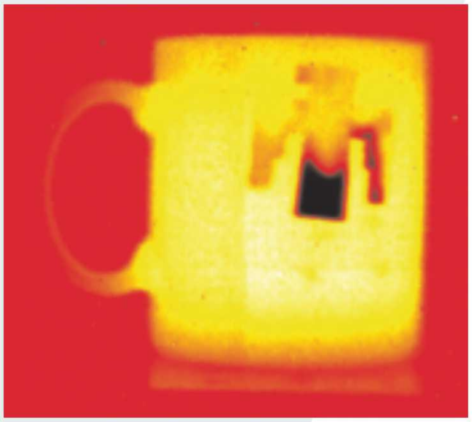


Metamaterial fielded on a 2019 Hot Shot flight. The material is designed to mitigate flight shock and vibration.

Microsystems-enabled photovoltaics. Microsystems-enabled photovoltaics provide a pathway to a solar power system that is cost-competitive with grid power. Flexible photovoltaic technology provides unique energy-harvesting capabilities anywhere there is light and promises 10x improvement in watts/kg over current flexible photovoltaic technologies. A Sandia employee is currently on entrepreneurial leave to commercialize the DragonSCALEs™ solar cell technology in the aerospace market. A total of $2.5M was raised to accomplish this. In December 2019, a $1.1M small business research grant was awarded by the Army Combat Capabilities Development Command Center. The funding will be used to further develop and test solar modules for portable power in remote locations, potentially opening up military markets and commercial sales for outdoor applications. DragonSCALEs has its origins in the Microsystems-Enabled Photovoltaics Grand Challenge that ended in FY14.

Providing high-quality intelligence of world events.

A nanoantenna, which has its origins in ttwo Grand Challenges including Smart Sensors (FY16-FY18) and Metamaterials (FY10-FY12), received a 2019 R&D 100 Award. The work took a concept from infancy and developed the world's first functioning long wave detector that is ready for commercialization. The high-performance nanoantenna-enabled focal plane array detector helps detectors see more than 50% of incident Infrared radiation (current technology can only see 25%). The nanoantenna architecture makes it possible to break through the background noise wall that traditional focal plan array technologies can't move beyond. The technology is on a path to improving detection of noncompliance relating to foreign programs.

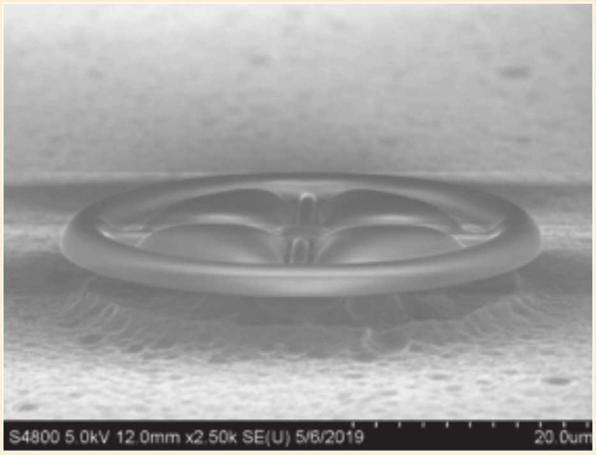


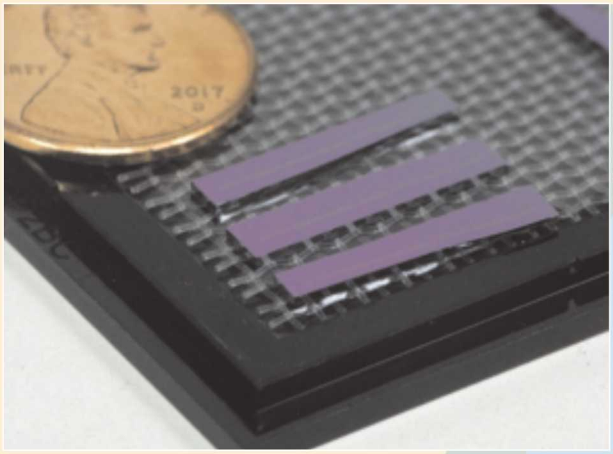
A fabricated nanoantenna-enabled detector array images a warm coffee cup heating a cooled Sandia Thunderbird logo. Nanoantennae can catalyze enhancements in the spectral and noise performance of infrared detectors. This promising new capability is being transformed from theory to reality by Sandia's efforts in the design, fabrication, and characterization of this emerging sensor architecture.

Realistic emulation of automated synthetic biology facilities to prevent risk of unintended manufacture. Sandia researchers are working with the Department of Homeland Security (DHS) and collaborators at LLNL to help protect the global bioeconomy and prevent bioweapons manufacture. Current protections against the manufacture of malicious biological material require DNA and RNA synthesis companies to ensure that the sequences that they produce cannot be used for harm. Sandia is using its Emulytics™ simulation, assessment, and modeling platform to provide a safe and secure environment to assess performance and provide data security assurance. For example, to the team's knowledge, this is the first time that a realistic emulation of synthetic biology lab computer systems was constructed with the goal of yielding insights and associated security recommendations that can be considered for adoption by the synthetic biology community. This work extends Sandia's previous engagements with the DHS and the National Institute of Standards and Technology to provide safe assessments of software and database security and reliability in digital biosecurity.

Assessing seismic analysis and analyst performance using the normalized compression distance metric. This project brought together a multi-center, interdisciplinary team to achieve a cutting-edge technical advance. They successfully applied the normalized compression distance metric (NCD) to seismic waveform data and demonstrated that this technique can accurately identify the onset of seismic events, particularly those caused by explosions and nuclear tests. They compared the peak of the NCD metric to an expert seismic analyst's assessment of the range of possible event onset times for 543 seismic waveforms and found that the NCD peak fell within the analyst's range for 75% of the seismic stations in the data set and was within 0.1 seconds of that range for 87% of the stations. In addition, they compared NCD to the algorithm that is currently used for automatic event detection and found that NCD provides more accurate results than the state-of-the-art method.

A truly micro-scale gyroscope based on optomechanical oscillation. A Sandia-led team designed, fabricated, and tested optomechanical oscillators for gyroscopes. These devices utilize pressure from light stored in a cavity to induce mechanical oscillation of the cavity. Through fabrication improvements, they achieved optical cavity Q greater than three million in free-standing micro-structures and achieved optomechanical oscillation with threshold pumping power less than 200μW. US Patent 10,458,795 was granted for the novel use of optomechanical oscillators as micro-scale gyroscopes. Devices were fabricated on a silicon chip and device radii as small as 20μm were characterized. They experimentally investigated the scaling behavior for both the gyroscope sensitivity and noise and found that the sensitivity is currently limited by residual optical absorption. Improvements are suggested to realize the goal of a micro-scale, gyroscope. They also initiated glass doped with phosphorous as a new foundational optical material capability at Sandia. The team demonstrated process improvements including void-free thermal melting of glass to smooth thousands of optical resonators





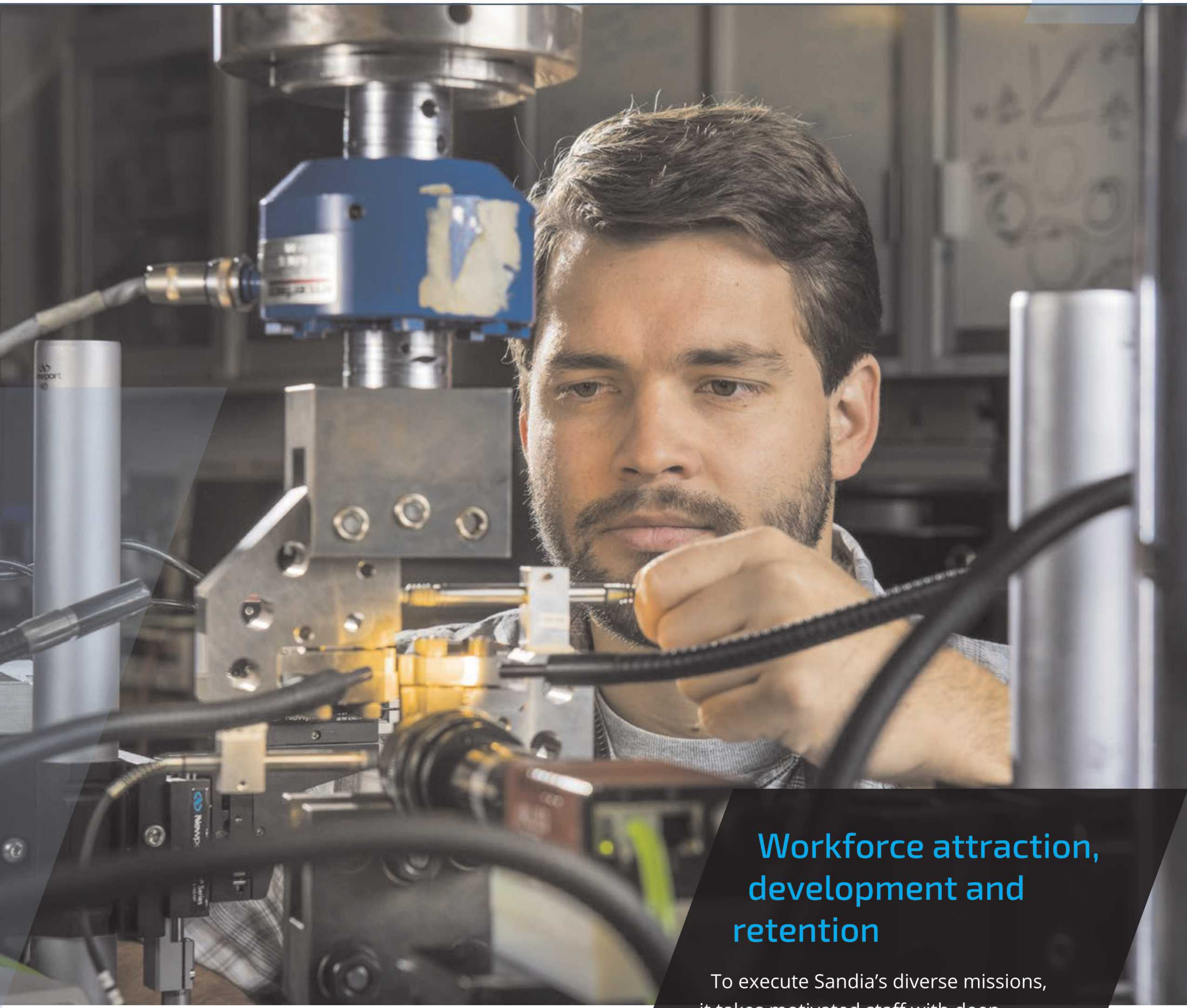
Left: Phosphorous-doped glass device created to be mirror smooth after melting in a furnace
Right: Fabricated chips each containing more than 72 unique devices

Sandia researchers create new ion selective membranes for batteries. Zn is a promising high capacity, multi-electron electrode material for batteries. However, charging and discharging zinc electrodes in alkaline electrolyte leads to soluble zinc [as zincate, $Zn(OH)_4^{2-}$] which redistributes throughout the battery and results in numerous problems that limit the energy density and cycle life that can be realized for alkaline Zn-based batteries. These limitations present technical roadblocks to a promising low cost, energy dense technology for large-scale electrochemical energy storage. Sandia researchers developed selective membranes that limit zinc re-distribution [as zincate, $Zn(OH)_4^{2-}$] throughout the cell and provide for longer cycle life with sustained capacities. "The membrane is really simple to prepare and appears to prevent 100% of zincate transport. Limiting the zincate to the anode only portion of the battery has multiple benefits and could allow for energy densities from zinc-based batteries equal or greater to that of a lithium ion battery with costs lower than that of the lead-acid," says Timothy N. Lambert. Intellectual property for this achievement is currently being sought. The

Zn is a promising high capacity, multi-electron electrode material for batteries.

Sandia's expertise in Emultytics and distributed systems leads to top three placement in competitive workshop. A Sandia team placed 2nd out of 30 international teams in the academic/industry programming competition workshop, "Integrating Data for Analysis, Anonymization, and Sharing" (iDASH). iDASH has pushed the state of the art in applied cryptography in the context of cyberbiosecurity and is stimulating the creation and accumulation of de-facto benchmarks with reference implementations for the cyberbiosecurity community at large. Sandia's team participated in the technical track, "Distributed Gene-Drug Interaction Data Sharing based on Blockchain and Smart Contracts," which leveraged the LDRD team's expertise in Emulytics and distributed systems. Sandia was asked to conceive and run a cyberbiosecurity track in the 2020 iDASH. This opportunity is an important next step in Sandia leveraging the national laboratory perspective to shape the technical landscape and priorities in this important and emerging research area.

Corey Hudson (second from the left) accepts the award for Sandia Team Genigma's submission which earned 2nd place out of 30 teams internationally.



Workforce attraction, development and retention

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.

work will be further developed under Sandia's DOE Office of Electricity program.

Four Sandia researchers win Presidential Early Career Award

Sandia researchers Salvatore Campione, Matthew Gomez, Paul Schmit and Irina Tezaur received the *Presidential Early Career Award for Scientists and Engineers* (PECASE) for 2019.

Salvatore Campione, from Catania, Italy, with a doctorate in electrical and computer engineering from the University of California, Irvine, is an electromagnetic analyst involved in national security projects that include analysis and modeling for lightning, EMP effects and radiation, and fundamental research and design in metamaterials and nanophotonics. He won for "pioneering work in metamaterial and nanophotonic design, capability development in accurately predicting electromagnetic-pulse consequences on the U.S. power grid, and for excellence in engaging with the external scientific community and mentoring junior staff." Salvatore believes that contributing to challenging R&D projects, including the Smart Sensor and the EMP-Resilient Electric Grid for National Security LDRD Grand Challenges, is an exciting aspect of being a Sandian and has certainly contributed to his early career successes by allowing him to interact with world-class experts.

Salvatore Campione
(Photo courtesy of the Marconi Society)

Matthew Gomez, from Hillsborough, New Jersey, with a doctorate in nuclear engineering and radiological sciences from the University of Michigan, is an experimental high-energy density physicist who has progressed in fusion experiments that rely on a combination of electricity, lasers and magnetism. His work was noted "For exceptional leadership and contributions to innovative research in high energy density physics and leadership of the magnetically amplified inertial fusion effort; and for his formidable commitment and exemplary role modeling to develop a community of scientists and engineers." Over the last eight years, Matthew led approximately 100 experiments in several areas of high energy density physics, including inertial confinement fusion, at Sandia's Z machine facility.

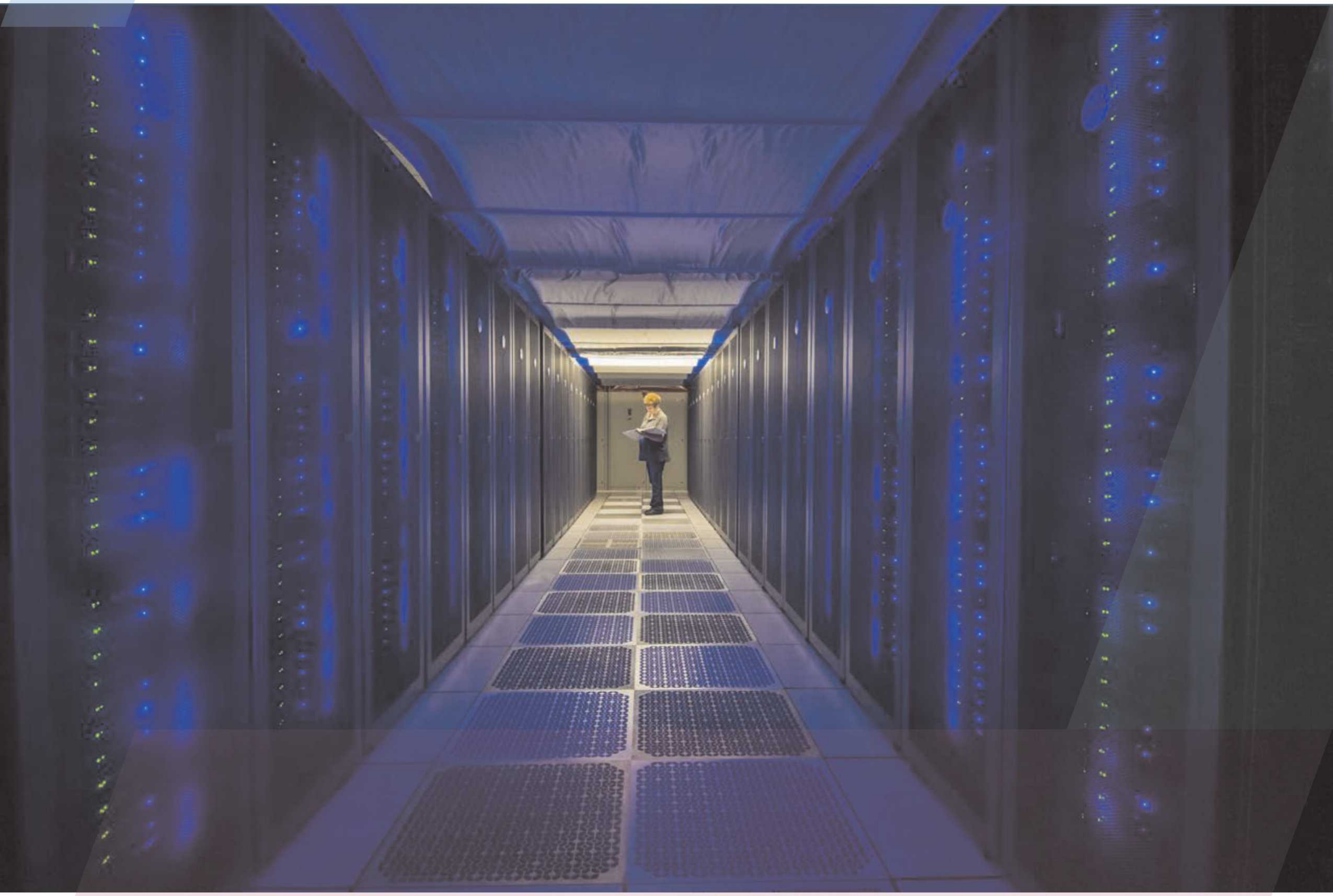
Matthew Gomez
(Photo courtesy of the Krell Institute)

Paul Schmit, from Glendale, Arizona, with a doctorate in plasma physics from Princeton University, uses pulsed-power techniques at Sandia accelerator facilities to advance inertial confinement fusion research through theory, simulation, and design and analysis of experiments. His PECASE award was for "exceptional technical contributions to the fields of inertial confinement fusion, magnetized plasmas, and related science applications in support of the country's national nuclear security mission, and for outstanding leadership and excellence in community outreach and mentoring of graduate students." Paul entered Sandia in 2012 as a President Harry S. Truman Postdoctoral Fellow in National Security Science & Engineering, a highly competitive distinguished fellowship program funded through LDRD. The fellowship provided him extraordinary opportunities to pursue independent research, integrate with established Sandia technical staff, and develop focused expertise in mission-critical scientific domains over a three-year period. Since his conversion to the Sandia technical staff in 2015, he has designed over 50 experiments on the world-leading Z Pulsed Power Facility supporting the inertial confinement fusion and high-energy-density science research thrusts, focusing particular attention on novel approaches to generating fusion-relevant conditions with pulsed power and assessing the physics of how these methods scale at higher coupled energies.

Paul Schmit
(Photo by Randy Montoya)

Irina Tezaur, from West Bloomfield, Michigan, with a doctorate in computational and mathematical engineering from Stanford University, focused on modeling and simulation of complex multi-scale and multi-physics problems using high performance computing impacting a variety of Sandia and DOE mission areas. Her areas of expertise include model reduction and multi-scale coupling methods, both of which enable analysts to simulate more scenarios than existing technologies support. Her award was for "developing new, impactful mathematical methods and computer algorithms to enable real-time analysis, control and decision-making on computationally prohibitive problems relevant to the nuclear security mission, and climate modeling." Irina joined Sandia as a year-round intern in 2007 and has been lead developer of several open-source codes. Since 2012, she has been a lead developer on the land-ice component of DOE's climate model, known as the Energy Exascale Earth System Model. She had an Early Career LDRD (FY12-FY14)on reduced order modeling for compressible flow that funded some of the work that was acknowledged by the PECASE. Irina stated, "The great LDRD program influenced my decision to come to Sandia."

Irina Tezaur



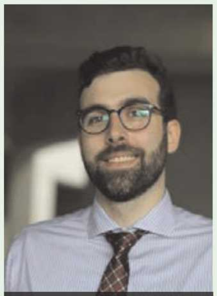
2019 Truman Postdoctoral Fellowship

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. This three-year fellowship is named for President Truman who charged AT&T to manage Sandia in 1949 to provide “an exceptional service in the national interest”— a motto that leads Sandia to excel to this day. 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. Fellows may work at either of Sandia’s principal locations in New Mexico and California. A member of Sandia’s technical staff mentors each Truman Fellow. This emphasis on research mentoring enables Fellows to become integral members of Sandia R&D teams while acquiring unique skills during their early career development.

2019 Truman Fellows


Pauli Kehayias

Pauli Kehayias received his PhD from the University of California, Berkeley in physics in May 2015. He earned his BS from Tufts University, with a double major in physics and mathematics, and has published 17 journal papers to date. His post-doctorate work developing a delicate magnetic sensor for paleomagnetism, the study of ancient-Earth magnetic fields, evolved at the Harvard-Smithsonian Center for Astrophysics. For his Truman Fellowship, "Imaging Microwave Fields with Sub-Micron Resolution Using Nitrogen-Vacancy (NV) Centers in Diamond," Pauli is continuing to develop better NV diamond microscopes and applying NV sensing to novel applications. Possible applications include electronics, materials and sensing in extreme environments.


Thomas O'Conner

Thomas O'Connor received his PhD in physics from Johns Hopkins University in May 2018 and earned his BS in physics from Rensselaer Polytechnic Institute. O'Connor received the Integrative Graduate Education and Research Traineeship Fellowship, was a finalist in the 2018 Frank J. Padden Award for Excellence in Polymer Physics Research, and published eight journal papers. His post-doctorate work focused on solving a decades-old riddle of why polyethylene isn't as strong as it theoretically should be. For his Truman Fellowship, "Modeling the Nonlinear Rheology of Additive Manufacturing," Thomas will work with nanostructure physics researchers at Sandia to develop molecular models that improve industrial processes for additive manufacturing.

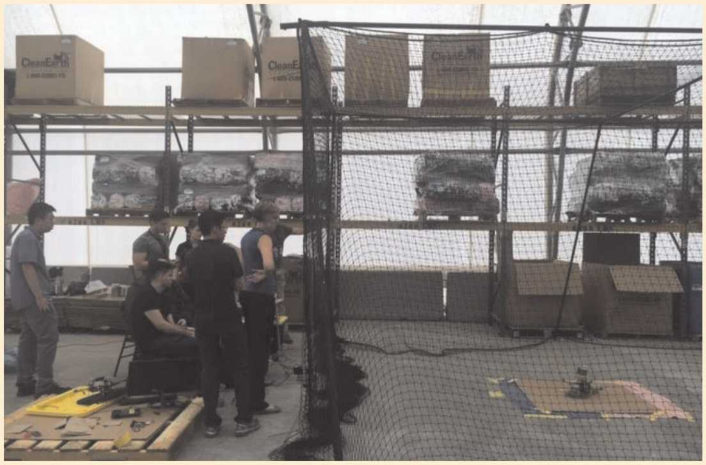
2019 Jill Hruby Postdoctoral Fellow

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. In 2018, Mercedes Taylor and Chen Wang were named as the first Jill Hruby Fellows. **Kelsey DiPietro** was named as a Hruby Fellow in 2019 and started her work in 2020. Each Hruby Fellow is awarded an LDRD-funded three-year postdoctoral fellowship in technical leadership, comprising national-security-relevant research with an executive mentor. Susan Seestrom, Chief Research Officer and Associate Laboratories Director for Advanced Science and Technology, is mentoring Mercedes, Chen, and Kelsey.

Kelsey, an applied mathematician, proposed a way to make computer models more efficient — improving accuracy without increasing time or resources to run them. Her technique changes how often a model makes calculations. If a model using her algorithms were predicting the thickness of an ice sheet over a large area, it would sprint through areas where there's little change from one spot to the next, checking the ground perhaps every half mile, until it gets to an area that starts changing more noticeably. That's when the model slows down and examines the ground perhaps every few feet. Conventional programming only allows researchers to choose between the big picture or the details, but it doesn't let them switch back and forth. DiPietro will use her fellowship to first apply her method to climate research, working with the Energy Department's supercomputer-powered Energy Exascale Earth System Model, or E3SM, which already has one of the finest resolutions ever achieved for simulating aspects of the planet's climate.

AutonomyNM attracts collaborative researchers in Autonomy for Hypersonics



Developing advanced autonomous solutions for hypersonics and other national security missions requires expertise in some of the most sought-after STEM disciplines in the job market. Initiated in conjunction with Sandia's Autonomy for Hypersonics Mission Campaign Investment Area, AutonomyNM was designed to attract collaborative research in artificial intelligence and autonomy and develop a talent pipeline in these critical fields for the Labs. Since its establishment in 2018, the number of interns has grown from six to 24 and is expected to expand even further with an anticipated 36 interns joining the team in the summer of 2020. Last year's interns gained exposure to Sandia's unique national security mission including our hypersonic research and development. They also gained valuable hands-on experience by building the first two drones the Labs will use to try out new algorithms for autonomous navigation, guidance and control, and target recognition. These drones will fly in a new indoor robotarium that is expected to open later this year. The AutonomyNM drones will provide Sandia an agile platform to quickly evaluate algorithms and technologies for autonomous flight before incorporating them into larger flight systems and tests.

Above: AutonomyNM student interns flight test one of the drones they built over the summer of 2019. This new drone will provide a low-cost test platform in AutonomyNM's new indoor robotarium for rapid evaluation of algorithms developed for autonomous flight. (Photo courtesy of Jason Brown)

Sandia's LDRD Program attracts Joel Clemmer to work on challenging Engineering Science projects

Joel Clemmer, who has a PhD in physics from Johns Hopkins University, chose Sandia over other opportunities because of the exciting and challenging opportunities afforded by two LDRDs in Engineering Science. His contributions have already made significant impacts on two projects: "Novel Approaches for Modeling Aluminum Melt and Relocation Supporting Weapon Safety Assessments" (2020 new start -- exploratory) and "Enabling Particulate Materials Processing Science for High-Consequence, Small-Lot Precision Manufacturing" (2019 new start). While recruitment and retainment of top U.S. advance degree holders has been challenging in recent years, the LDRD program and portfolio of projects continues to be a key means of exciting and attracting top talent to deliver innovative capabilities to meet the mission.

New hire postdoc, Joel Clemmer, is making an impact in Engineering Science. (Photo by Taisha Rodriguez)

Sandia LDRD principal investigator, Tamara Kolda, named Association for Computing Machinery (ACM) Fellow

Tamara Kolda was named an *ACM Fellow* for "innovations in algorithms for tensor decompositions, contributions to data science, and community leadership." The work for which Kolda is cited has been supported in large part by the LDRD program, including "Data Mining on Attributed Relationship Graphs" (FY05-07), "Leveraging Multi-way Linkages on Heterogeneous Data" (FY08-FY10), and "Parallel Tensor Decompositions for Massive, Heterogeneous, Incomplete Data" (FY17-19). Most notably, an LDRD supported the initial development of the Tensor Toolbox for MATLAB, which has spurred innovation across many sectors because of its ease of use and good performance. From the ACM announcement, "The accomplishments of the 2019 ACM Fellows underpin the technologies that define the digital age and greatly impact our professional and personal lives. ACM Fellows comprise an elite group that represents less than 1% of the Association's global membership."

New Mexico Legislators' Serial Innovator Awards

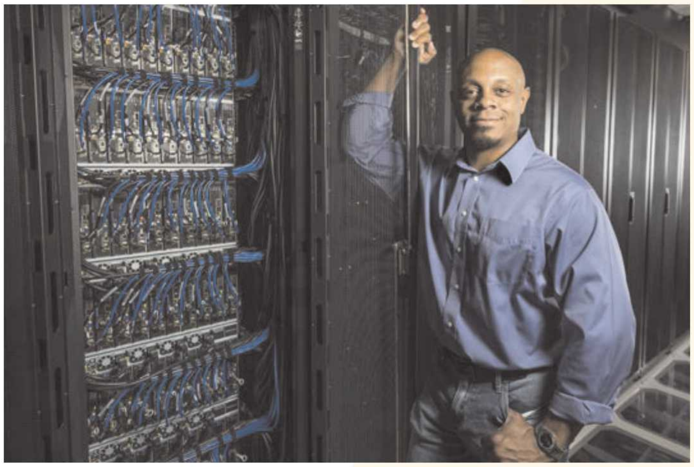
Stan Atcitty and Hongyou Fan received recognition from the New Mexico Legislature recently for their distinguished achievements as serial innovators. Stan works in Energy Storage Technology & Systems and is a member of the Navajo Nation. He was the first American Indian male to earn a doctorate in electrical and computer engineering from Virginia Tech University. He has won six *R&D 100 awards*, as well as the prestigious Presidential Early Career Award in 2012. Hongyou, of the Advanced Materials Laboratory, is also a National Laboratory Professor in the Chemical and Biological Engineering Department at the University of New Mexico. He has four R&D 100 awards and recently became the first researcher from a national lab to receive the Materials Research Society Mid-Career Research Award. Hongyou stated of his awards, "Sandia's LDRD program plays a foundational role for science understanding and serves as the basis for technology invention and further development." *(Photo by Mason J. Martinez)*

Most Promising Asian-American Engineer of the Year

Sandia researcher Stanley Chou selected as one of three most promising 2019 Asian-American Engineers of the Year (AAEOY). Stanley Chou, a leading innovator in materials synthesis and materials chemistry, was highlighted as an expert in the field of graphene-like, two-dimensional materials, and in the engineering of these materials for energy catalysis and sensors. The AAEOY noted, "Stan is at the forefront in their chemistry and engineering. His papers and presentations have been cited over a thousand times." Stan is a committee member of the Materials Research Society. He was chair of the 31st Rio Grande Symposium on Advanced Materials and has served on the board of many educational organizations, including the Albuquerque Association for Gifted and Talented Students, and Campersand, the national mathematical education organization. Support from the LDRD office enabled Stan to establish his lab and pursue exploratory science for stockpile stewardship and global security. It was also a key mechanism in empowering Stan's career development.

Black Engineer of the Year STEM Global Competitiveness Awards

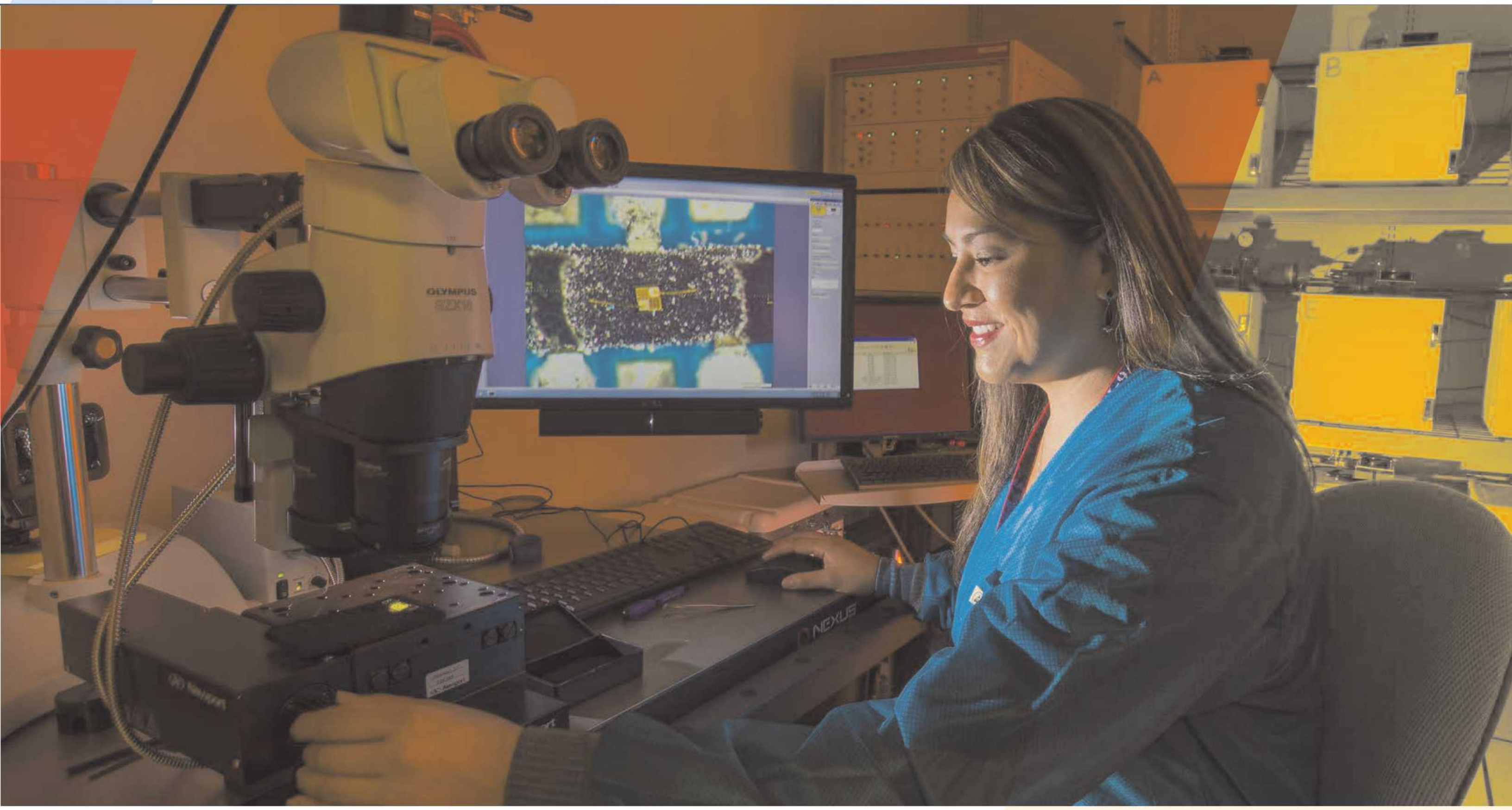
Warren Davis, an expert in machine learning, received the 2019 Research Leadership Award at the Black Engineer of the Year (BEYA) STEM Global Competitiveness Conference for being "a consistent leader in discovering, developing and implementing new technologies," according to the award citation. Warren is also adept at recreating natural, mechanical processes to solve problems in engineering. In these cases, he takes natural phenomena — such as air flowing over a surface or a person taking a step — and uses machine learning to explain them mathematically by way of an equation, also called a function. Machine learning can approximate complex processes much faster than they can be solved numerically, which saves companies time and resources, for example, if the goal is to predict how well a proposed aircraft design will hold up in flight. The savings compound when designers use machine learning to simulate multiple iterations.



(Photo by Randy Montoya)

Black Engineer of the Year (BEYA) STEM Global Competitiveness Awards

Olivia Underwood was honored with a Science Spectrum Trailblazer Award, given to "men and women actively creating new paths for others in science, research, technology, and development." Olivia has bachelor's and master's degrees in metallurgical engineering from the University of Alabama in Tuscaloosa and a doctorate in materials science from the University of Alabama in Huntsville. In 2015, she became the first African-American to earn a materials science doctorate at the Huntsville campus. Olivia started at Sandia as a postdoctoral appointee, and now as a product realization team lead, she manages the technical and programmatic aspects for specialized components. In 2019, Olivia received the 2019 Frank Crossley Diversity Award from The Minerals, Metals & Materials Society and she was inducted into 2019 Class of 40 under Forty by Albuquerque Business First. Olivia also will receive the 2019 Frank Crossley Diversity Award from the Minerals, Metals & Materials Society. When she was a postdoctoral appointee, she worked on a variety of projects. The Additive Manufacturing (AM) Defect Predictions Project was LDRD funded, and it allowed her to correlate defect populations with mechanical performance in AM tensile samples of precipitation-hardened 17-4 stainless steel using 3D reconstructions, which had a huge impact on her career at Sandia. It also allowed her to collaborate and co-author a paper "Corroborating tomographic defect metrics with mechanical response in an additively manufactured precipitation-hardened stainless steel,", with world class scientists across the Labs. She also had the opportunity to present this work at the External Advisory Board for the Born Qualified Grand Challenge LDRD in October 2016. Before coming to Sandia, she never had an opportunity to work on a project of that magnitude. *(Photo by Stephanie Blackwell)*



Hispanic Engineer National Achievement Award

Materials scientist Nic Argibay was honored at the 31st annual *Hispanic Engineer National Achievement Awards Conference* **by Great Minds in STEM, a nonprofit organization that recognizes Hispanic leadership and achievement in science, technology, engineering and math.** Nic Argibay has made outsized contributions to the scientific field of tribology, the study of interacting surfaces in relative motion, including the principles of friction, lubrication, and wear. He has received more than $7 million in scientific grants and awards leading to groundbreaking discoveries such as the in situ formation of diamond-like carbon on platinum-gold substrates and one of the most wear-resistant materials ever tested. LDRD funding was instrumental in enabling the technical achievements for this award.

Society of Women Engineers Achievement Award

Jackie Chen received a *Society of Women Engineers* **Achievement Award for her impact on society and the engineering community.** The award is the highest honor given by the society and recognizes at least 20 years of outstanding technical contributions to the field of engineering. Jackie received an LDRD on simulation of thermal stratification effects on homogeneous charge compression ignition engines that helped establish direct numerical simulations as a tool to understand the coupling between turbulence and chemistry in compression ignition environments encountered in internal combustion engines.

Society of Asian Scientists and Engineers Award

Engineer Alan Mar, who worked at the Labs for 25 years, was honored by the *Society of Asian Scientists and Engineers* with a 2019 Professional Achievement Award. The society recognized Alan as someone who "has made significant discoveries, made important advances in his or her chosen career path and is acknowledged as a leader of large initiatives."

Institute of Electrical and Electronics Engineers' Nuclear and Plasma Sciences Society Early Achievement Award

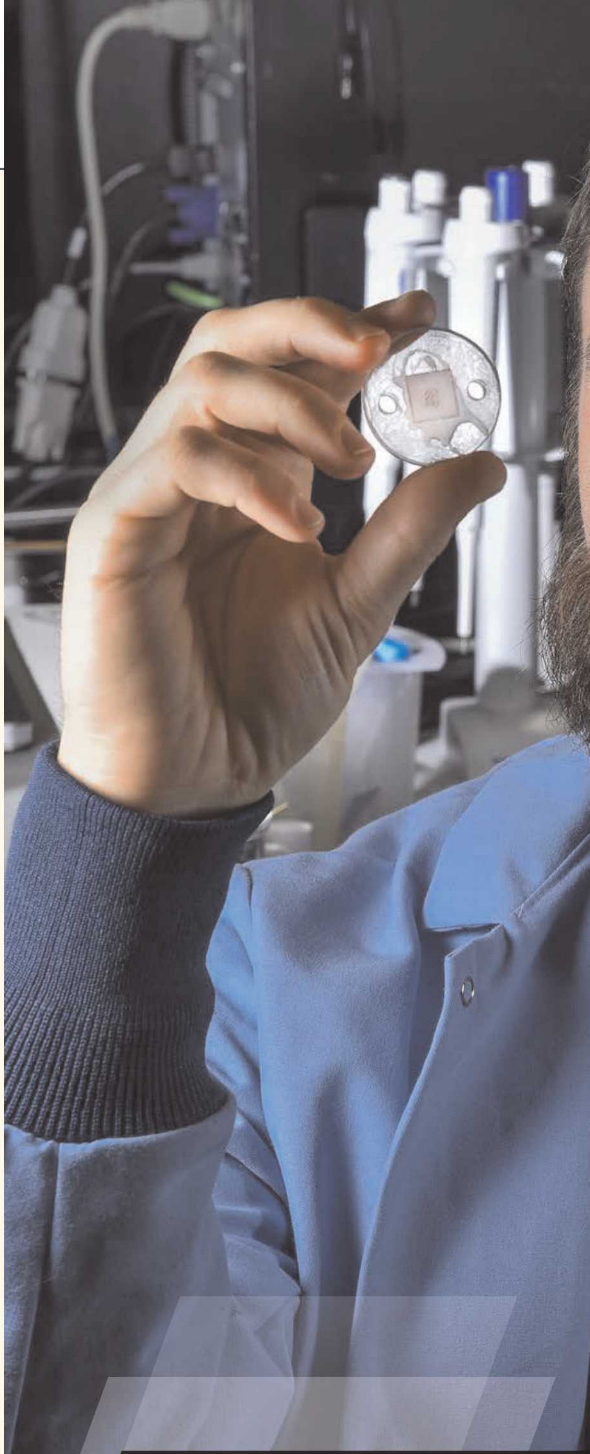
Sandia physicist Matthew Gomez received the 2019 Institute of Electrical and Electronics Engineers' *Nuclear and Plasma Sciences Society* Early Achievement Award. Only one scientist in the world receives the award each year that recognizes excellence in technical contributions to the fields of nuclear and plasma science that take place during the first 10 years after the honoree completes their degree. An experimental high energy density physicist, Matt was honored for contributions to magnetically driven high energy density physics, and for leadership in the experimental demonstration of a magneto-inertial fusion concept with the possibility of scaling to ignition. He led more than 90 experiments at the Z-machine facility and published the first experimental results of the Magnetized Liner Inertial Fusion (MagLIF) concept. His publication on the first MagLIF experiments has received more than 130 citations in the last four years, and he has given 11 invited talks on MagLIF during roughly the same time span.

Society for Industrial and Applied Mathematics Fellow

Michael Heroux, senior scientist at Sandia's *Center for Computing Research*, was selected as a fellow of the Society for Industrial and Applied Mathematics (SIAM). The *SIAM Fellows Program* honored Mike for research, leadership, and building community in software and algorithms for scientific and high performance computing. Mike leads the Trilinos scientific software project for Sandia, which collects open-source software libraries, called packages, used as building blocks for the development of scientific applications. He is also the director of software technology for the DOE's Exascale Computing Project, overseeing efforts to provide key elements of the software stack for the next generation of leadership computing platforms. LDRD funds early in Mike's Sandia career enabled fundamental and collaborative research and development in algorithms and software for advanced high-performance computing systems. The success of these LDRD efforts laid some of the foundation for Mike' contributions to the SIAM community, contributing to his recognition as a SIAM Fellow.

Materials Research Society Mid-Career Researcher Award

Hongyou Fan, Sandia materials scientist, is the sole recipient of this year's Mid-Career Researcher Award from the *Materials Research Society*, the largest U.S. materials society. The distinction is given midway in a researcher's career for exceptional achievements in materials research and for notable leadership in the field. Hongyou was chosen for "outstanding contributions in nanoparticle self-assembly of functional nanomaterials." He is widely recognized for pioneering work that employs stress rather than chemistry — the more conventional approach — to form new materials at the nanoscale. A distinguished member of Sandia's technical staff and a national laboratory professor at the University of New Mexico, Hongyou is the first U.S. national lab researcher to win the mid-career award, which has been presented annually for the last seven years.

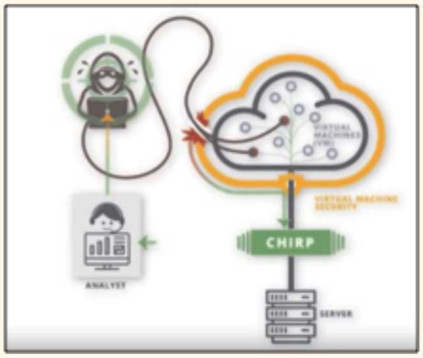


Microneedles

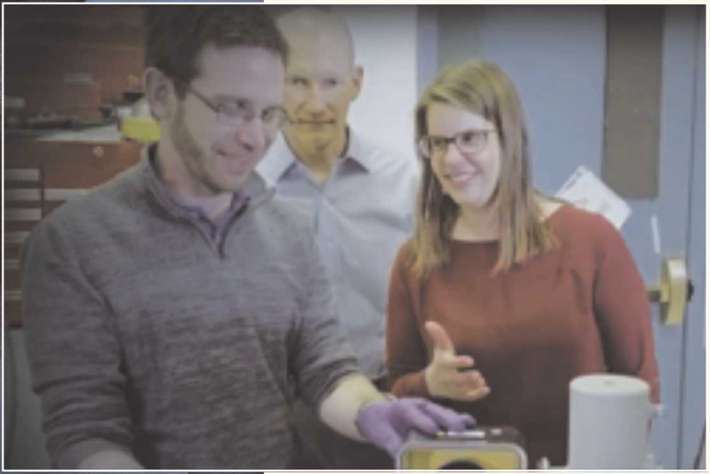
A Sandia-developed technique using microneedles to draw relatively large amounts of interstitial fluid — a liquid just under the skin — opens new possibilities in quickly diagnosing disease, cancer or exposure to chemical attacks.

2019 R&D 100 Awards

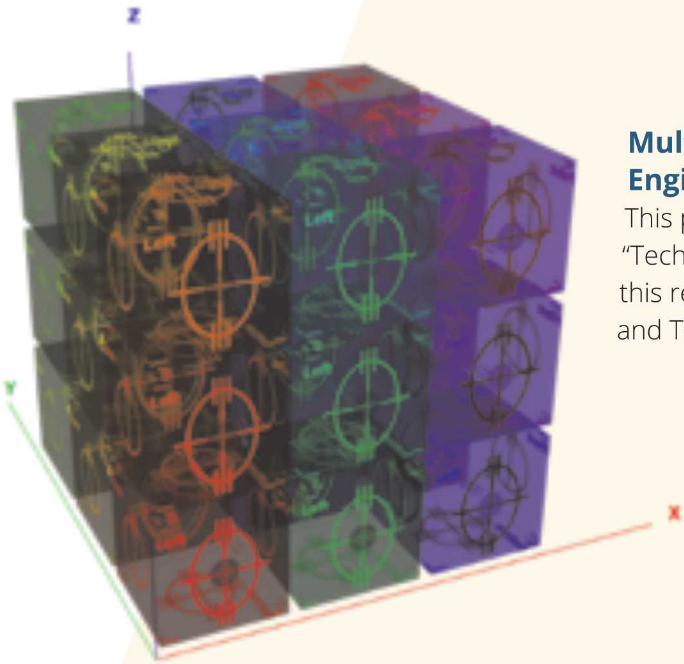
Sandia won four R&D 100 awards in 2019, three of which were enabled in part by LDRD projects. The R&D 100 Awards are one of the most prestigious recognitions of innovation in the world. Since 1976, Sandia has earned 134 awards.



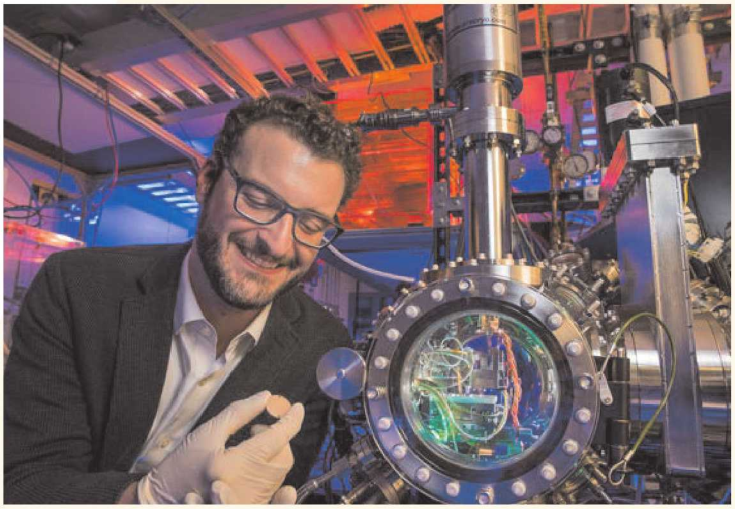
CHIRP: Cloud Hypervisor Forensics and Incident Response Platform. Researchers at Sandia have developed a scalable virtual machine instrumentation and introspection capability that transparently extracts data from cloud infrastructure at an in-depth level. The Cloud Hypervisor Forensics and Incident Response Platform (CHIRP) provides analysts the ability to collect forensics artifacts and evidence as well as incident response materials in real-time without disturbing the user environment. This project has its roots in the Instrumentation Infrastructure for Cyber Emulations LDRD Grand Challenge. *YouTube*.



High-Performance Nanoantenna Enabled Detectors. Researchers at Sandia have developed High-Performance Nanoantenna Enabled Detectors, which will allow for enormous advancements over the current state of the art using an architecture that is independent of detector material and wavelength band. In addition to dramatically improving image quality, this architecture allows for entirely new detector concepts unrealizable with existing technology. This project had its roots in the Smart Sensor Technologies LDRD Grand Challenge. *YouTube*.



Multiscale Inverse Rapid Group-theory for Engineered-metamaterials. This project, discussed in more depth in the "Technical vitality and frontiers of S&T" section of this report, has its root in the Metamaterial Science and Technology LDRD Grand Challenge. *YouTube*.



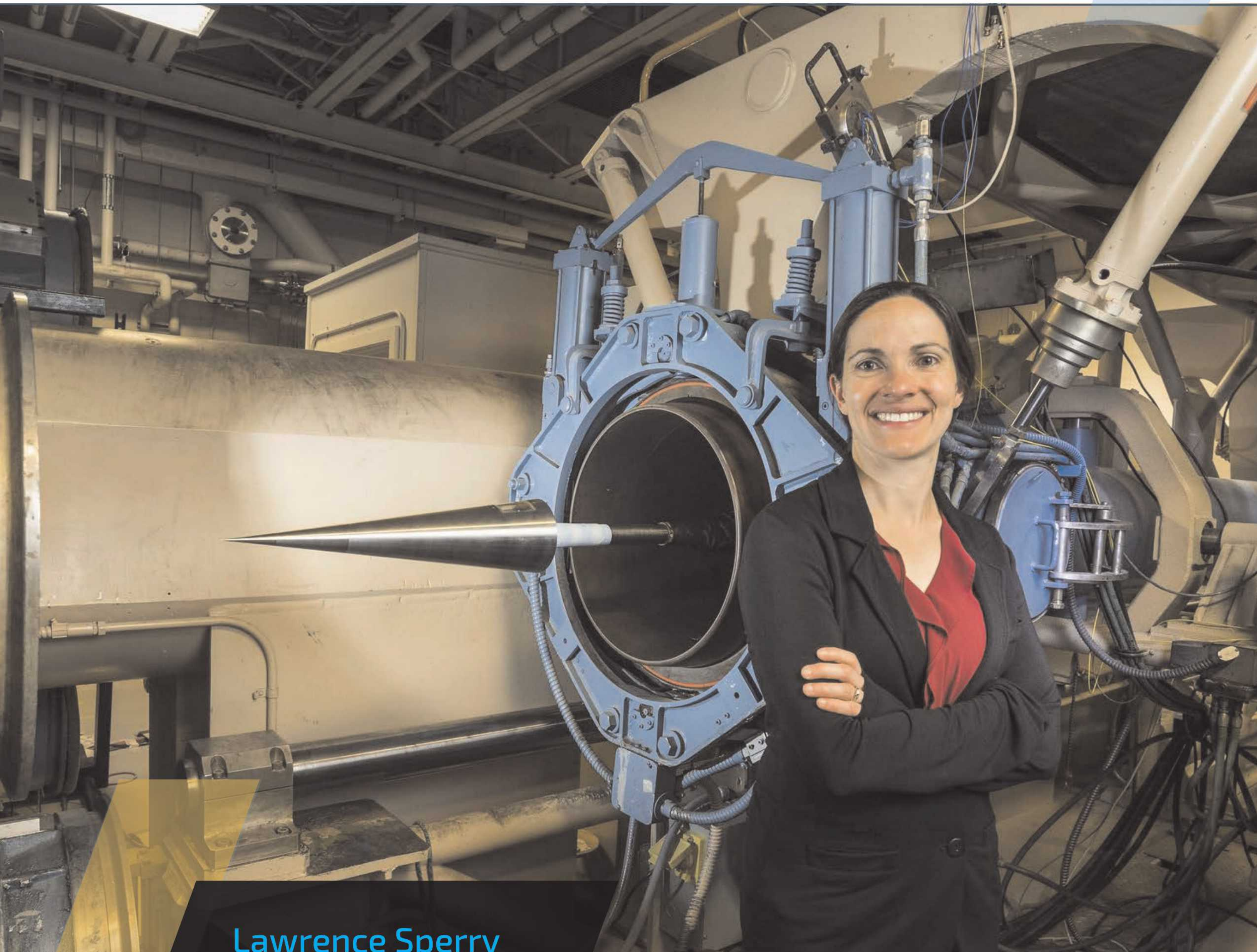
Special Recognition: Market Disruptor R&D 100 Award

BRONZE: Stable Nanocrystalline Metal Alloy Coatings with Ultra-Low Wear, PI Nicolas Argibay. Building on data from an earlier LDRD project, Sandia researchers developed a platinum-based alloy that is extremely wear-resistant, using a technique called grain boundary segregation to create highly stable nanocrystallinity of a minority constituent — in this case, gold. *YouTube*.

Federal Consortium Awards

Sandia won *four regional awards* from the *Federal Laboratory Consortium* (FLC) for its work in developing and commercializing innovative technologies. The FLC Awards are considered some of the most prestigious honors in technology transfer. These new Sandia technologies and partnerships showcase the Labs' talented workforce. LDRD played a critical role in two of these awards.

- The Labs' 25-year partnership with The Goodyear Tire & Rubber Co., which produced many successful projects and advances for the tire industry and the Labs.
- Advances in the science of scintillators — objects that detect radiation — through the development of organic glass.



Lawrence Sperry Award

Katya Casper has become known for her innovative techniques measuring the effects of pressure on hypersonic vehicles at Sandia National Laboratories wind tunnels.

Katya Casper, a principal member of the technical staff at Sandia received the Lawrence Sperry Award, given by the American Institute of Aeronautics and Astronautics (AIAA) for a notable contribution by a young person to the advancement of aeronautics and astronautics. Specifically, she was honored for her "highly significant contributions to the fundamental understanding of boundary layer transition and fluid-structure interactions in hypersonic flows through novel diagnostics with national program impact." Katya noted, "While at Purdue, I learned how to conduct novel experiments in a hypersonic wind tunnel and was also able to intern at Sandia because of Purdue and Sandia's collaborations. That experience led to my research position at Sandia upon graduation."

ABSTRACT

This report provides an assessment of the value of the LDRD program to Sandia National Laboratories during fiscal year 2019.

2019 LDRD TEAM

Susan Seestrom, Grant Heffelfinger, Ben Cook, Greg Frye-Mason, Donna Chavez, Brandon Heimer, Leigh Cunningham, Donna Mullaney, Rachel Leyba, Nicole Seay, Douglas Prout, and Amy Treece

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