The mission objectives of LDRD are mission agility, technical vitality, and workforce development. Articles are assigned with icons to designate the strongest leaning(s) towards these objectives.

LANL HIGHLIGHTS

LDRD researchers apply functional data analysis to new weapons physics tools at Los Alamos

Incorporating cutting-edge science and technology into our weapon designs is essential to national security. The most recent incorporation comes in the form of a groundbreaking Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL)—“Rapid Response to Future Threats,” led by principal investigator Charles Nakhleh. The LDRD researchers applied functional data analysis to streamline and optimize weapons design. The premise is to free up the weapons designer from tasks a computer can perform just as well, so that the designer can focus on human-required decision-making—seeing the big picture in order to guide the future of weapons design.

The LDRD supplied new weapons design tools that extend existing capabilities (focused on classic weapon designs currently in the stockpile) to non-canonical weapons designs and optimization of design for a weapons full lifecycle.

“These tools allow our engineers and scientists to experience every part of a weapon’s lifecycle; this is really valuable in the event we need to design a weapon from scratch,” said LDRD Researcher Matt Tucker, Weapon Stockpile Modernization Division.

Modernization is a must

Weapon design policy has had ups and downs over the decades, with a hiatus on new design concepts since the start of the Stockpile Stewardship Program (except for the Reliable Replacement Warhead and some lower-level paper studies). During that time, generational turnover hit particularly hard, resulting in a new workforce that had never fully designed a weapon from start to finish. It was a vulnerability in our defense posture.
The Stockpile Responsiveness Program mandated a return to weapons design in 2016. The congressional mandate called for a return “to identify, sustain, enhance, integrate, and continually exercise all capabilities required to conceptualize, study, design, develop, engineer, certify, produce, and deploy nuclear weapons.” LDRD, designed to enable agile responses to national security challenges, funded Nakleh and his team as an off-cycle proposal. By the time the Nuclear Posture Review called for weapons modernization in 2018, the Los Alamos LDRD team was well on their way, modernizing weapon design from start to finish.

“We tested our new design tools in July 2019 with an actual experiment: a hydro of a non-canonical design,” Tucker said. “Hydros use surrogate materials to safely test weapons designs. “It confirmed that we were able to predict the behavior very well.”

However, there were also instances when the codes did not work as well as the researchers had expected. But as Tucker explained, it’s important to understand where you can trust your tools and where you can’t. That alone is valuable information.

The production complexes have changed

Another important goal of modernizing our design tools is to improve our ability to actually manufacture the weapons. Production complexes have changed since the time of classic designs, which means it’s becoming more difficult to bring those designs to life as a real weapon. Modernizing the codes will help make new weapons easier to manufacture.

The new design tools developed through this project were briefed to the National Nuclear Security Administration (NNSA). The proven success spurred the Design for Manufacture Program that is now in place.

Optimizing new tools even further

These new tools can be improved. Freeing up designers from tasks that could be performed by a computer is one such optimization.

To get to that point, statistical methods have to be applied to the choices designers make. The computer has to learn about these choices and when to make them. Data has become increasingly complex over the years, including complicated curves and images. Until now, that meant that learning algorithms relied on very large datasets for learning. This new functional data analysis removes that dependency, reducing the parameter search space for learning algorithms. *(LA-UR-20-22531)*
Los Alamos researchers develop restartable rocket motor to maneuver satellites in space

Los Alamos LDRD researchers developed what is believed to be the first motor for solid rockets that is restartable an arbitrary number of times. With the patented design, the scientists and engineers were able to demonstrate restarting the motor at least six times in succession. All other known solid rocket motors in use are a “one and done” scenario for maneuvering in space.

“We developed an aerospike nozzle at Los Alamos with an actuated cowl,” said Nicholas Dallmann, lead LDRD research engineer. “Once a burn has achieved the desired velocity change, the cowl would rapidly open, decompressing the chamber and extinguishing the burn. When another burn of the rocket is needed, the cowl is reset to its original position.”

This new technology will help solve the increasing problem of space traffic, as more small satellites (CubeSats) are sent into orbit. The restartable motor will enable satellites to maneuver around other orbiting objects on short notice, preventing costly space crashes.

Electrolysis ignition is safe and environmentally sound

The LDRD researchers also designed a safe, reusable ignition system that relies on the electrolysis of water instead of volatile pressurized chemicals. This enhances the safety of material handling as well as the safety of any flight crew and the environment.

The water is separated into hydrogen and oxygen through electrolysis. These are sent to the combustion chamber, where a spark ignites the gas. This can occur over and over for multiple burns. Re-ignition is one of the key features of this technology.

This system is also stable for very long periods (multiple decades), which is ideal for the lifetime of space flight or storage of a missile. (LA-UR-20-22531)
Los Alamos researcher wins first place in IBM quantum challenge

Lukasz Cincio of the Physics of Condensed Matter and Complex Systems Group at Los Alamos won first place in the May 2020 IBM Quantum Challenge. In its fourth year, the IBM Quantum Experience put forth four programming exercises to be solved in four days.

Cincio placed first out of 1,745 participants. For the most challenging of the four exercises, Cincio’s result bested the result discovered by IBM's experts—offering a solution even they didn’t think was possible.

Cincio achieved his top-performing result by using a specific machine learning algorithm that he created as part of a Laboratory Directed Research and Development (LDRD) project. It was a substantial victory for the entire project team because it demonstrated the power and credibility of the software, which removes the burden from a human and automates the problem-solving instead.

IBM Quantum Challenge

“The technique that I created as part of the LDRD came out on top, which I find very reassuring that the work we do is of high quality,” said Cincio. “As typically happens with machine learning, the most optimal solution to the problem was very unintuitive and surprising, even to the organizers, whose solution was slightly less optimal.”

LDRD team members included Scott Pakin, Wojciech Zurek, Nikolai Sinitsyn, Andrew Arrasmith, Patrick Coles, Hristo Djidjiev, Andrew Sornborger, Petr Anisimov, Avadh Saxena, Yigit Subasi, Stephan Eidenbenz, Lukasz Cincio, Rolando Somma, Tyler Volkoff, and Akira Sone.

“I had a lot of fun participating in the IBM Challenge,” Cincio said. “It was a real-time competition—the best score kept changing as the challenge was ongoing and new participants were joining in. We don’t have much of this in our everyday work.”

Cincio is offering unique opportunities for others interested in quantum computing. He (along with two LDRD colleagues) developed and leads the Los Alamos Quantum Computing Summer School, a program intended to address the workforce shortage in this area, which doesn’t exist as a subject in universities. The 10-week immersive program — now in its second year — accepts students from all over the world from a variety of disciplines and offers them the unique opportunity to work directly on quantum computers. Through the school, LANL builds awareness of the advantages of working in the national security enterprise, one being working at the leading edge of this field. (LA-UR-20-23920)
In 2018, Sandia National Laboratories committed $40 million of its LDRD funds to explore autonomy and machine learning technology for hypersonic flight vehicles, and on March 19, 2020, Sandia saw the work culminate in a hypersonic flight test conducted by the U.S. Navy and U.S. Army on March 19 at the Kauai Test Facility in Hawaii.

The Navy and Army executed the launch of a common hypersonic glide body, which flew at hypersonic speed to a designated impact point. Sandia provided design and fabrication of the flight vehicle; pre-flight modeling, simulation and analysis; ground testing of common hypersonic glide body components; and launch support at the test range. Information gathered from this and future experiments will further inform the Department of Defense’s hypersonic technology development.

Hypersonic flight is defined as air travel at least five times the speed of sound. Other vehicles, including ballistic missiles, can reach these speeds, but hypersonic missiles follow less predictable flight paths and are harder to detect by interceptors. This makes hypersonic research essential. A Sandia-led initiative called AutonomyNM leverages academic partnerships with the objective of developing autonomy customized for hypersonic flight. Funding for AutonomyNM research is provided by Sandia’s LDRD and LDRD-funded Academic Alliance program. Sandia is aiming to complete the foundational technologies of new autonomous flight systems by 2024. In addition to hypersonic flight systems, AutonomyNM plans to explore other applications of autonomy in aerospace, emphasizing solutions to national security challenges.

Sandia has been conducting hypersonic flight research for about 40 years, including the first successful flight test of a non-ballistic hypersonic glide vehicle in 1985. In 2018, a memorandum of agreement signed by multiple DOD agencies established a Sandia-developed design as the common hypersonic glide body that is now being further developed and produced by industry contractors. (SAND2020-3521E)

To deter attempts to disable U.S. electrical utilities and to defend U.S. nuclear weapon systems from evolving technological threats, Sandia National Laboratories began two multiyear initiatives to strengthen U.S. responses. One is focused on defending large U.S. electrical utility systems from potential attacks by hostile nations, as well as from damage inflicted by extreme natural disasters like hurricanes and solar flares. The Resilient Energy Systems Campaign, a multi-year research portfolio with up to $40 million in total funding, is supported by Sandia’s LDRD program, which funds exploratory work in science and technology. The original electric grid was not designed with security in mind.
against cyberhacks, or protection from electromagnetic disturbances, or natural disasters such as hurricanes or geomagnetic solar storms. The primary objective of the mission portfolio is to mitigate vulnerabilities caused by antiquated technology in transformers and other components.

The second research campaign is developing enabling technical capabilities to help the U.S. maintain its strategic nuclear deterrent. The Assured Survivability and Agility with Pulsed Power research campaign is a multi-year portfolio with up to $40 million in total funding, again by Sandia’s LDRD program. The mission portfolio is intended to explore technologies that use brief but powerful bursts of electrical energy to simulate nuclear explosions — without resorting to actual nuclear tests — to better understand their impact on electronics and materials.

Additional benefits from both mission portfolios are expected to include more efficient electrical generation, more accurate data for astrophysicists, and a closer approach to break-even and even high-yield fusion, which can generate electrical energy by fusing atoms — a goal of a branch of physics for 70 years. (SAND2020-6173 E)

Sandia robotics experts identify, track, capture

Sandia National Laboratories robotics experts are working on a way to intercept enemy unmanned aircraft systems midflight. They successfully tested their concept indoors with a swarm of four unmanned aircraft systems that flew in unison, each carrying one corner of a net. Acting as a team, they intercepted the flying target, trapped it in air like an insect caught in a web and safely lowered it to the ground.

This test was part of a two-year LDRD project called Aerial Suppression of Airborne Platforms. That demonstration led to external funding for three years to continue research and testing for the Mobile Adaptive/Reactive Counter Unmanned System, or MARCUS, project, which will address current and future national security threats posed by small unmanned aircraft systems. Airborne systems with sensors, used in the MARCUS project, could dramatically enhance the ability to mitigate threats, even as the technology continues to evolve. The idea of MARCUS is that the unmanned aircraft systems could intercept small threats and keep them at a safe distance from protected facilities and people.

Sandia is implementing the LDRD-funded Multi-Mission Radio Frequency Architecture (MMRFA) and associated radio frequency (RF) module on next-generation systems for deployed programs. This architecture will be the backbone of next-generation airborne systems and will be leveraged across the hypersonic, space, and future...
Nuclear Deterrence mission portfolios. The MMRFA architecture enables arbitrary waveform generation/detection needed in current mission spaces. The MMRFA capability was developed through an LDRD project that provides a flexible multi-functional (imaging/non-imaging radar, Electronic Warfare, Signal Intelligence (SIGINT), communications, radiometry, etc.) high-performance, high instantaneous bandwidth RF processing architecture with integrated military utility and tailored responses in complex and hostile environments. A multi-mission software defined radar capability provides tactical and strategic advantages by utilizing a “sense, analyze, and respond” set of capabilities necessary for operations in hostile environments. Leveraging this capability into deployed systems will allow for a modular, interoperable, flexible and extensible architecture across multiple program areas. *(SAND2019-15453 E)*

**LLNL HIGHLIGHTS**

**Livermore second skin protects against chem, bio agent**

Recent events such as the COVID-19 pandemic and the use of chemical weapons in the Syria conflict have provided a stark reminder of the plethora of chemical and biological threats that soldiers, medical personnel and first responders face during routine and emergency operations. Personnel safety relies on protective equipment which, unfortunately, still leaves much to be desired. For example, high breathability (i.e., the transfer of water vapor from the wearer’s body to the outside world) is critical in protective military uniforms to prevent heat-stress and exhaustion when soldiers are engaged in missions in contaminated environments. The same materials (adsorbents or barrier layers) that provide protection in current garments also detrimentally inhibit breathability.

The smart protection mechanism of responsive nanotube membranes against environmental threats. The collapse of actuating polymer chains on the contaminated membrane surface prevents nerve agents like sarin from entering the SWCNT pores. In a safe environment, the responsive polymer chains remain extended and allow rapid transport of water vapor, thus conferring high breathability to the membrane material. *(Image courtesy of Ryan Chen/LLNL)*
To tackle these challenges, a multi-institutional team of researchers led by Lawrence Livermore National Laboratory (LLNL) scientist Francesco Fornasiero has developed a smart, breathable fabric designed to protect the wearer against biological and chemical warfare agents. Material of this type could be used in clinical and medical settings as well. The work was recently published online in Advanced Functional Materials and represents the successful completion of Phase I of the project, which is funded by the Defense Threat Reduction Agency through the Dynamic Multifunctional Materials for a Second Skin “D[MS]2” program.

“We demonstrated a smart material that is both breathable and protective by successfully combining two key elements: a base membrane layer comprising trillions of aligned carbon nanotube pores and a threat-responsive polymer layer grafted onto the membrane surface,” Fornasiero said. These carbon nanotubes (graphitic cylinders with diameters more than 5,000 times smaller than a human hair) could easily transport water molecules through their interiors while also blocking all biological threats, which cannot fit through the tiny pores. This key finding was funded by the Laboratory Directed Research and Development Program and published in Advanced Materials.

The team has shown that the moisture vapor transport rate through carbon nanotubes increases with decreasing tube diameter and, for the smallest pore sizes considered in the study, is so fast that it approaches what one would measure in the bulk gas phase. This trend is surprising and implies that single-walled carbon nanotubes (SWCNTs) as moisture conductive pores overcome a limiting breathability/protection trade-off displayed by conventional porous materials, according to Fornasiero. Thus, size-sieving selectivity and water-vapor permeability can be simultaneously enhanced by decreasing SWCNT diameters.

Contrary to biological agents, chemical threats are smaller and can fit through the nanotube pores. To add protection against chemical hazards, a layer of polymer chains is grown on the material surface, which reversibly collapses in contact with the threat, thus temporarily blocking the pores.

“This dynamic layer allows the material to be ‘smart’ in that it provides protection only when and where
it is needed,” said Timothy Swager, a collaborator at the Massachusetts Institute of Technology who developed the responsive polymer. These polymers were designed to transition from an extended to a collapsed state in contact with organophosphate threats, such as sarin. “We confirmed that both simulants and live agents trigger the desired volume change,” Swager added.

The team showed that the responsive membranes have enough breathability in their open-pore state to meet the sponsor requirements. In the closed state, the threat permeation through the material is dramatically reduced by two orders of magnitude. The demonstrated breathability and smart protection properties of this material are expected to translate in a significantly improved thermal comfort for the user and enable to greatly extend the wear time of protective gears, whether in a hospital or battlefield.

“The safety of warfighters, medical personnel and first responders during prolonged operations in hazardous environments relies on personal protective equipment that not only protects but also can breathe,” said Kendra McCoy, the DTRA program manager overseeing the project. “DTRA Second Skin program is designed to address this need by supporting the development of new materials that adapt autonomously to the environment and maximize both comfort and protection for many hours.”

In the next phase of the project, the team will aim to incorporate on-demand protection against additional chemical threats and make the material stretchable for a better body fit, thus more closely mimicking the human skin. –Soldier Center (Christopher Doona) (LLNL-WEB-458451)

Livermore AI identifies change in microstructure in aging materials

Technological progress in materials science applications spanning electronic, biomedical, alternate energy, electrolyte, catalyst design, and beyond is often hindered by a lack of understanding of complex relationships between the underlying material microstructure and device performance. But artificial intelligence (AI)-driven data analytics provide opportunities that can accelerate materials design and optimization by elucidating processing-performance correlations in a mathematically tractable way.

Recent developments in artificial-neural-network-based “deep learning” methods have revolutionized the process of discovering such intricate relationships using the raw data itself. However, to reliably train large networks, one needs data from tens of thousands of samples, which, unfortunately is often prohibitive in new systems and new applications due to the cost of sample-preparation and data collection. In situations such as these, innovative algorithms are needed to extract the most appropriate “features” or “descriptors” out of the raw experimental characterization data.

As an example, polymer-bonded high explosives constitute an important materials system whose 3D bi-phasic microstructure can: (1) vary greatly depending on processing parameters such as high-energy particle morphology and size distribution, (Image courtesy of LLNL)
binder content, solvents/stir-rates, pressing forces, and temperature; (2) evolve over long-term material aging under varying environmental conditions; and (3) display variation in performance as a function of sample microstructure and age.

While each 3D microstructure can be nondestructively imaged with x-ray computed tomography (CT) scans (at multiple time points), the process of data collection is time consuming and expensive, which limits the number of samples to typically just a few hundred. The challenge is to make the best use of such limited data to uncover any process-microstructure-performance correlations, quantify long-term aging trends, provide micro-scale insights into physics-based simulation codes, and design future materials with improved performance.

In research supported by the Laboratory Directed Research and Development Program, teams of researchers from across disciplines at Lawrence Livermore National Laboratory (LLNL) and the University of Utah used recently developed methods in scalar-field topology and Morse theory to extract useful summary features like “grain count” and “internal boundary surface area” from the raw x-ray CT data. These feature variables were then analyzed using a variety of statistical machine learning techniques, which enabled the team to: (1) objectively distinguish different microstructures resulting from processing differences; (2) systematically track microstructure evolution under aging; and (3) build microstructure-dependent performance models.

“With an increased emphasis on AI-inspired data-centric research, the paradigm of how we approach model building and materials discovery is changing rapidly,” according to lead author Amitesh Maiti (MSD). “The pace and quality of progress hinges critically on such multi-team collaborations that bring together complementary knowledge and skills.”

Livermore researchers see metal interfaces as they transform

The regions separating individual crystals in a material are notorious defects, spoiling the simple arrangement of atoms within the crystals. To improve the understanding of how those defects, called grain boundaries, create stronger and more durable materials, a team of researchers from Lawrence Livermore National Laboratory and Max-Planck-Institut für Eisenforschung, have for the first time observed how they transition from one form to another in an elemental metal. The research appears in the March 19 edition of the journal *Nature.*
Livermore ARC results provide a ‘pleasant surprise’

When researchers saw the results from the first Discovery Science experiment on the National Ignition Facility’s (NIF) Advanced Radiographic Capability (ARC) laser, they were genuinely surprised: The experiment produced much higher energy electrons than predicted based on the laser energy and power used on these shots.

The results, which were not typical of new experiments on new facilities, still required rigorous analysis — including complex computer simulations that only Lawrence Livermore National Laboratory’s world-class supercomputers could accomplish. But, as detailed in a Rapid Communication paper published March 4 in *Physical Review E*, researchers verified ARC can accelerate electrons to relativistic energy levels previously expected only from higher-intensity lasers.

“That means the electrons come out at much higher energy than you would suspect based on previous experiments,” said Bruce Remington, leader of NIF’s Discovery Science program. “It was a very big and a very pleasant surprise.”

The paper identifies a new regime of laser-matter interaction that is critical to all projects using ARC, since the electrons underpin the mechanisms for x-ray, proton, and ion production. The findings open new avenues of using ARC to explore the frontiers of laboratory science on topics such as gamma-ray bursts and black hole accretion disks. (*LLNL-WEB-458451*)

**SDRD HIGHLIGHTS**

**Small UAS radiological survey flights at the NNSS**

A team led by researchers from the Nevada National Security Site (NNSS) Special Technologies Laboratory and Remote Sensing Laboratory-Nellis demonstrated a radiation detection, measurement and mapping mission using a small unmanned aircraft system (sUAS). Using a sUAS equipped with a high-efficiency radiation detector, the team successfully performed radiation scans over two Yucca Flat test locations and successfully demonstrated how UAS technology can be leveraged in support of national security and public health and safety, particularly in the area of emergency response and consequence management. The flyover mission was sponsored by the Site-Directed Research and Development UAS initiative and led by scientists Rusty Trainham, from the NNSS Special Technologies Laboratory, and Paul Guss, from the NNSS Remote Sensing Laboratory-Nellis.
A small UAS in flight with radiation detector mounted below it (Click image for a related video.)

A sUAS can be used in conjunction with existing capabilities from manned aircraft to provide more detailed follow-on surveys of radiation and contamination following a radiological emergency. The team is planning more field work to further explore the ability of a sUAS to fly into and assess difficult areas, such as tunnels and other GPS-denied environments, during national emergency situations. The team is moving closer to achieving their goal of developing hardware, methods and expertise to provide critical information that helps protect emergency responders and the public in the event of a radiological emergency.

Aerial radiological surveys have been conducted at the NNSS since the 1960s; what was unusual about this mission was that the team conducted aerial radiological surveys using a sUAS, commonly known as a drone, and a lightweight yet sturdy radiation detector. UAS can augment existing aerial radiation detection capabilities because they can fly much lower and slower than a manned aircraft, enabling the team to collect more detailed radiation measurements and geographical information; they can maneuver into an area that would be unthinkable for a manned aircraft to collect data.

The gamma imager was attached to the hexacopter and flown over the Sedan and Baneberry nuclear test craters. (The Sedan test was conducted on July 6, 1962, and the Baneberry test took place on December 18, 1970.) The gamma imager weighs about 10 pounds, and it fits into a volume of 18 by 3 by 4 inches. The hexacopter is about the size of a card table, and the gross weight is about 50 pounds with the payload and fuel. At sea level, it can fly for up to two hours at a time, but at the altitude of the NNSS, the time is limited to ~30 to 40 minutes. The sUAS flew over a distance of a few kilometers to complete the surveys. Data collected during the surveys demonstrated that greater sensitivity and geographical resolution can be achieved with UAS technology.

The team revisited the Sedan and Baneberry craters for more measurements. During this visit, they traveled to the Palanquin nuclear test crater (the Palanquin test took place April 14, 1965) to collect additional survey/imaging data. (DOE/NV/03624--0800)