LDRD

Quarterly Highlights

Mission Agility | Technical Vitality | Workforce Development

FY22 Q2

IN THIS ISSUE

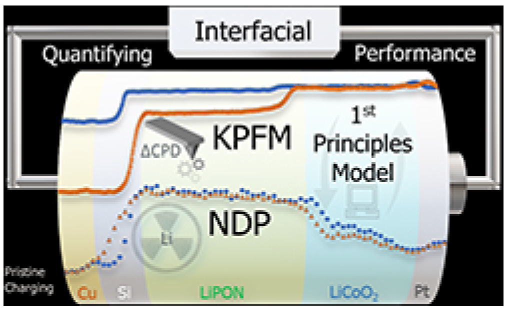
FEATURE STORIES

Sandia testing method yields pathway to better, longer-lasting batteries

Using a microscopic method for measuring electrical potential, a team of scientists at Sandia National Laboratories may have discovered how to make a longer-lasting, more efficient battery.

The team of Elliot Fuller, Josh Sugar and Alec Talin detailed their findings in an article published Oct. 19 in American Chemical Society Energy Letters.

“One of the challenges with solid-state batteries is that at the boundaries between different parts of the battery — a cathode and a layer of ion-conducting electrolyte, let’s say — something interferes with the flow of electrons,” Talin said.



This illustration shows how a team at Sandia National Laboratories used Kelvin probe force microscopy to locate places where electron flows get stuck, potentially leading to engineering longer-lasting, more efficient batteries. (Illustration courtesy of S. Kelley/National Institute of Standards and Technology.)

Solid-state batteries employ solid electrolytes instead of electrochemical gels and liquids and generally power small electronics. Most researchers suspected that there was a loss of voltage or electrical potential at interfaces within the battery, but not which interface was responsible for most of the impedance in the battery. The team started work five years ago to get some clarity.

“There were two main motivations for this. The first was fundamental: we want to have good models for batteries that we can use to develop better materials,” Talin explained. “The second thing was to figure out how we can engineer the interfaces to make them less impeding. In our case, it really has to do a lot with how fast lithium ions can move in the Si anode used in the study.”

They turned to Kelvin probe force microscopy, which measures electrical potential on a surface, and while using instruments in new ways is certainly not something Sandia is unaccustomed to, what the team did next no one had ever done, Talin said.

“The voltage between battery electrodes is relatively straightforward for researchers to calculate and measure,” Fuller said. “However, where that voltage drops within the battery layers has remained a mystery. It’s critical to understand where the voltage drops, as it is intimately tied to the performance-limiting resistances. Kelvin probe force microscopy is a technique that finally enabled us to measure where these drops are occurring.”

“This technique has been used for many years to measure local voltage, with people using it on parts of a battery. It was difficult to interpret because it was not a full functioning battery,” Talin continued. “We cut the battery in half longitudinally, with the elements stacked like a layer cake. You can still charge it and discharge it, so we did this measurement over the entire battery.”

The team found that a large part of the electrical potential of the battery was getting lost at the boundary between the electrolyte and the anode (negative) terminal.

“Most people thought the biggest change was going to happen at the interface between the cathode (positive) and electrolyte,” he added. “Understanding the measurements took a lot of time. We wanted to validate the data by measuring where the lithium ions were at different states during charging.”

To accomplish this, the team worked with researchers at the National Institute of Standards and Technology Center for Neutron Research using a technique called neutron depth profiling that can measure where lithium ions are at a particular moment. Now that NDP has confirmed the Kelvin probe force microscopy data, the team is looking to apply this methodology to a host of technologies that will benefit the nation.

“We’re going to use this technique to look at other batteries as well as other solid-state electrical systems, like the electrochemical random-access memory invented at Sandia,” Talin said. “This will allow us to develop devices that operate like we would like them to operate.”

The work was done in collaboration with NIST, Naval Research Labs, University of Maryland College Park and Brown University. It was sponsored through Sandia’s Laboratory Directed Research and Development Lithium Battery Grand Challenge and the Nanostructures for Electrical Energy Storage Energy Frontiers Research Center as well as the Platforms core program, both led by the University of Maryland and sponsored by the DOE Office of Basic Energy Sciences. *(SAND2021-15439L)*

- Technical Vitality, Workforce Development

Common ‘Core’: Sandia uses molecular fragments to detect deadly opioids

Researchers at Sandia National Laboratories have developed a method to detect trace amounts of synthetic opioids. They plan to combine their approach with miniaturized sensors to create a hand-portable instrument easily used by law enforcement agents for efficient detection in the field.

Fentanyl is a fast-acting, opioid-based pain reliever that is 80 to 100 times more potent than morphine. Illegally produced fentanyl often is mixed with other drugs such as cocaine or heroin and minuscule amounts can cause death by overdose. Drug overdose deaths, predominantly due to synthetic opioids such as illicitly manufactured fentanyl and fentanyl analogs, have accelerated during the COVID-19 pandemic, according to the Centers for Disease Control and Prevention.

A photo illustrating 2 milligrams of fentanyl, a lethal dose for most people, compared to a penny. Matthew Moorman, a Sandia National Laboratories researcher, has developed a new method to detect tiny amounts of fentanyl analogs based on their common molecular structures. (Photo courtesy of the Drug Enforcement Administration)

The chemical structure of fentanyl can be modified to create molecular analogs. These analogs can have different potencies, and it can be difficult for law enforcement agencies to keep up with emerging analogs.

Matthew Moorman, a Sandia researcher, wanted to develop a method to detect fentanyl analogs based on their common molecular structures, or “cores,” rather than by identifying the individual chemical decorations found on each one.

"A lower false-alarm rate with this detection method could lead to more efficient screening of trace amounts of opioids at the border or in mail-sorting stations," he said.

There are thousands of possible analogs of fentanyl, according to the Department of Homeland Security. Lab-based chemical analysis using sensitive techniques, such as infrared spectroscopy or mass spectrometry, can identify new analogs of fentanyl by their molecular "fingerprints."

But the large number of possible fingerprints increases the chance of false alarms. By focusing on the common opioid core, rather than the changeable fingerprints, Moorman's work will streamline the process of detecting synthetic opioids.

Detecting brand-new analogs

In order to detect opioids based on their common cores, Moorman and his colleagues used a technique that decomposed the molecular structure of several fentanyl analogs. They noticed this process frequently produced the same molecular fragments. Using a miniaturized ion-mobility spectrometer developed at Sandia for field-based explosives sensing, they could detect the synthetic opioid-based fragment in a less than a billionth of a gram of sample, even when mixed with cutting agents that drug manufacturers commonly use to dilute the compounds.

Detecting a fragment common to an opioid's molecular core means this approach can identify brand-new analogs, Moorman said. The small set of signatures also means the researchers could fine tune their chemical detection to create reliable, sensitive sensors.

The work to demonstrate the proof-of-concept fragment detection was funded by Sandia's Laboratory Directed Research and Development program. The researchers now want to combine this detection method with their miniaturized chemical sensors to develop an instrument that law enforcement agents could use in the field to detect the presence of synthetic opioids. They expect to have a functional, field-tested prototype within three years.

They also hope to apply the same fragment-based detection approach to other classes of illegal drugs, such as synthetic cannabinoids, cocaines and ketamines, Moorman said. *(SAND2021-3361L)*

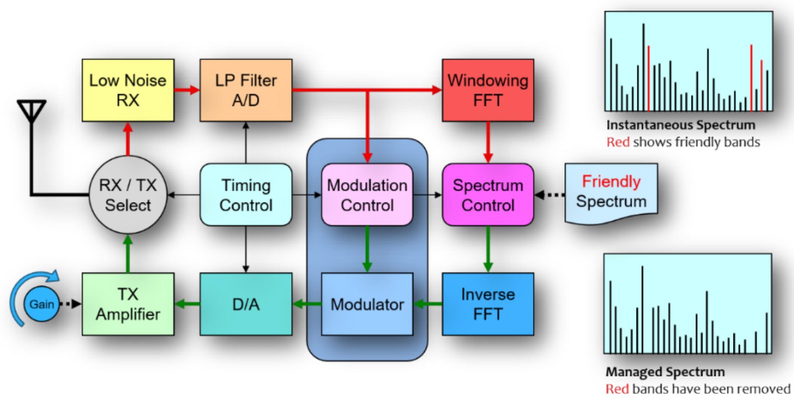
- Mission Agility, Workforce Development

Site-Directed Research and Development long-term project success: patent to commercial startup

During the last decade, Nevada National Security Site (NNSS) Sr. Principal Engineer Douglas Seastrand and an NNSS team have successfully leveraged project funding from the NNSS Site-Directed Research and Development (SDRD) Program to develop patented electromagnetic spectrum management technology. Seastrand worked with Rudolpha "Dolly" Jorgensen, Eric Schmidthuber, Ryan Martin, and Sean Sheehan on the Electromagnetic Spectrum Management System (ESMS) project, which developed into two patents for technologies to prevent unwanted radio frequency (RF) communications that are useful to the national security and law enforcement mission spaces. This SDRD project, initially developed in 2015 and patented in 2017, opens the way for possible follow-on work, such as exploring modulation control, inserting new or modified modulation, or providing real-time situational awareness of the RF environment.

The team's 2015 one-year SDRD project was titled "Concurrent Transceiver with Ultra-high-speed Fourier Transforms for Unrealized SIGINT Applications" (aka ESMS) and was created to control the RF radio waves propagating through an area. The ESMS provides a revolutionary approach to controlling RF signals, removing all modulation from every RF signal that is not designated as "friendly," and optionally replacing it with new modulation—thus preventing (or jamming) and controlling all RF communications. The ESMS selectively allows friendly RF signals to pass without being jammed—including frequency hopping and spread spectrum communication systems. The ESMS technology can near-simultaneously RX [receive] and TX [transmit] to let friendly communications through while blocking all other/unknown communications. ESMS is able to selectively pass or jam any RF signal within its bandwidth, currently up to 8 GHz.

Conventional jamming techniques have high power requirements. In contrast, the ESMS efficiently tailors each RF carrier output amplitude relative to the signal strength of its received carrier, and the user can determine the hemispherical area of influence to further limit power. ESMS inherently works will all modulation techniques and requires no foreknowledge of the unwanted carrier frequencies.



ESMS block diagram. The ESMS rapidly alternates between receive (RX) and transmit (TX) in order to digitize the received RF to produce an Instantaneous Spectrum of all RF carriers. This list of carriers is compared with the Friendly Spectrum to remove them from the Managed Spectrum list. The remaining carriers are considered unfriendly, so they are converted back into RF and retransmitted without their original modulation or with new modulation. The area of jamming influence is dependent upon the RF gain of the TX Amplifier.

It was so promising that in 2021, Seastrand was nominated and accepted as a FedTech Startup Studio Finalist. FedTech connects scientific work done at the government level with public sector, first-time startup entrepreneurs who plan to grow and monetize inventions for the commercial market using government-generated intellectual property. The vetted entrepreneurs gain access to intellectual property information and federal funding and grants, while the NNSS gains recognition for its groundbreaking work that can be used to improve technology on a large scale. Although other NNSS cohorts were invited to compete for FedTech, Seastrand's invention was the first and only one successfully paired with the correct entrepreneurs, who have since worked with the NNSS to begin the engineering and commercialization of the ESMS product, forming the company Enfluxx Tech. Seastrand was involved in helping the newly founded company to understand the technology and identify potential customers. Enfluxx Tech worked with the management and operating contractor's (Mission Support and Test Services, LLC [MSTS]) legal department for licenses to advance the technology from TRL 3 to TRL 6. Enfluxx Tech currently has an MSTS legal agreement for an R&D license to use the technology, and they are in the process of refining the engineering for commercial use.

Patents:

Seastrand, Douglas R. Electromagnetic spectrum management system. US Patent 9,559,803, filed April 4, 2016, and issued January 31, 2017.

Seastrand, Douglas R. Electromagnetic spectrum management system. US Patent 9,794,021, filed January 24, 2017, and issued October 17, 2017.

(DOE/NV/03624--1312)

- Technical Vitality

NNSS researcher wins 2022 Sidney D. Drell Science and Technology Award

Dr. Marylesa Howard, a scientist and mathematician in the Physical Sciences group at the NNSS, has won the 2022 Sidney D. Drell Science and Technology Award from the Intelligence and National Security Alliance (INSA) Achievement Awards Committee. The annual award recognizes one individual who exemplifies excellence in the intelligence, homeland security, and national security communities.

The Sidney D. Drell Science and Technology Award is named in memory of Dr. Sidney D. Drell, a groundbreaking theoretical physicist, advocate for nuclear arms control, and expert advisor to presidents of both parties on satellite reconnaissance and other advanced intelligence programs. It was established in 2010 to recognize early achievers and mentors who inspire future leaders. It also recognizes the accomplishments of early- and mid-career professionals and graduate students for innovative scientific or technological research and development whose applications have made, or have the potential to make, significant impacts in intelligence, defense, or national security.

Dr. Marylesa Howard holding the 2022 Sidney D. Drell Science and Technology Award at the ceremony held in Arlington, VA, on February 16, 2022. (Photo courtesy of Marylesa Howard)

Responding to the award, Howard said, "If I've learned one thing on my journey, it's to apply yourself and dare to dream, even if your dreams lead you to underground tunnels with hard hats and steel-toed boots. Maybe even especially then! My colleagues are a joy, the work is challenging, and I enjoy knowing I'm contributing to our national security. I love my job, and I'm honored to be recognized with this award."

"I heartily congratulate Marylesa on this well-deserved recognition," said Mark W. Martinez, NNSS President. "She is an outstanding scientist and a leader in her field, and has made great contributions to the incredible, cutting-edge work happening at the NNSS. We are proud to have her on our team."

Over the eight years at the NNSS, Howard has contributed significantly to applied mathematics and physics within the Stockpile Stewardship program. She currently leads the Signal Processing and Applied Mathematics team while maintaining a large scientific role in research and development. Her innovative approach to image segmentation has enabled the National Weapons Laboratories to achieve deliverables not previously achieved with image processing.

Quantitative image analysis goes beyond the more common qualitative approach and enables a new class of information to be extracted. In dynamic experiments, images can be used for recovering information, such as material location, density, and/or velocity, which can then be used in simulation for comparision with current physics models of such processes. The challenge lies within extracting this information from images.

To this end, Howard led an SDRD project over the course of three years to develop an image segmentation technique for material location identification, assuming that a given material may have different statistical image properties at different spatial locations within an image. She leveraged her machine learning techniques to develop a spatially aware method for computer-detected material location. Her work has resulted in publications in peer-reviewed journals. The tool developed within this project also has been successfully deployed within the Nuclear Security Enterprise, and the NNSS has licensed it to several National Laboratories and to the Massachusetts Institute of Technology for use in their image analysis endeavors.

The 2022 INSA Achievement Awards Ceremony took place on February 16, 2022, in Arlington, VA, and included keynote speaker Lt. Gen. Scott D. Berrier, Director of the Defense Intelligence Agency. See a video of Howard's award acceptance speech. The INSA Achievement Awards annually welcomes nearly 250 senior intelligence community leaders from across government, industry, and academia.

(Per NNSS classification, this article is confirmed to be unclassified and approved for public release.)

➢ Technical Vitality, Workforce Development

SDRD researchers are working with next-generation talent to lay the groundwork for machine learning in stockpile science at NNSS

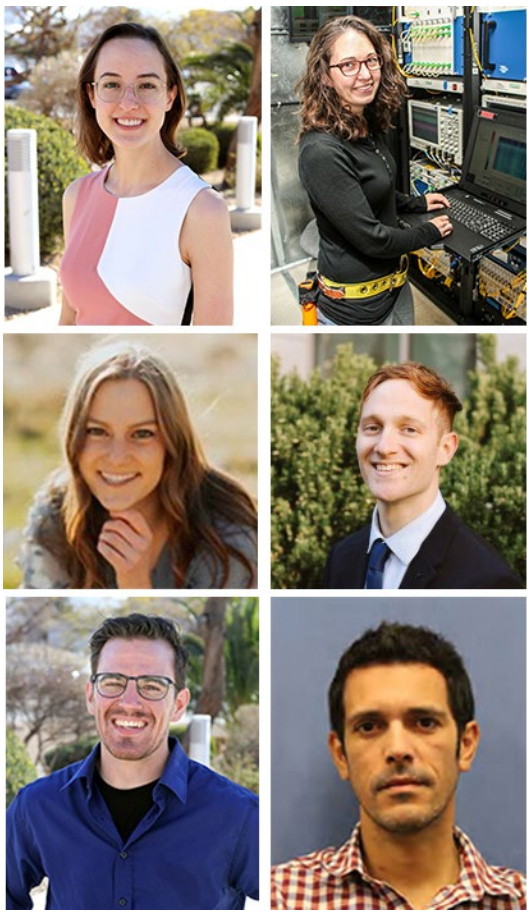
Margaret Lund, senior scientist and mathematician in the NNSS Computing and Data Science group, is leading a dynamic team investigating and developing deep learning methods for applications in stockpile science, specifically in the area of radiographic systems imaging and analysis. Deep learning is a branch of machine learning that uses neural networks to process information in layers. A deep neural network has multiple hidden layers between input and output layers, and as such, has a greater capacity to learn and generalize more complex datasets. Deep learning techniques are especially useful for analyzing complex data such as images. The primary goal of Lund's two-year R&D project is to lay the groundwork for deep learning capabilities within the radiography analysis team at the NNSS. The project is currently in the second year, building on the work accomplished in FY 2021.

Year 1 of the project focused on improving training efficiency and network accuracy, which resulted in the development of a new pooling technique, the implementation of a new unsupervised method for improving training sets, and the exploratation of a new technique for identifying the scope of a trained network. Lund said that every member of her team played an active role in achieveing these results. In particular, she pointed out how important it was for her to have two talented and driven summer student interns on her team. Through the 2021 NNSS student internship program, she hired two recent graduates from Brigham Young University. Chelsey Noorda, with her primary research interest in novel pooling methods, and Jared Slone, with his research focus on uncertainty quantification methods, brought different but complementary skill sets to the team. They contributed independently to the project, but they also worked well as a team, brainstorming ideas and formulating creative solutions to difficult problems. "This model of independent research combined with team problem-solving worked so well that I've decided to hire two interns again this summer," said Lund.

The project team also hosted a group of undergraduate students from the Mathematics Department of Embry-Riddle Aeronautical University (ERAU) last spring. In partnership with ERAU faculty member Mihhail Berezovski, four students from Berezovski's Research Projects in Industrial Mathematics class spent the semester working on developing neural networks for this SDRD project. This partnership was so successful last year that this year, six students from Berezovski's class have chosen to participate in the project during the spring semester. Additionally, the team hosted three Research Experience for Undergraduates program students, two students from ERAU and one student from the University of Toledo, last summer. The students spent the summer months testing the capabilities of the new pooling method the team developed and wrote a research paper to submit to *The Beyond: Undergraduate Research Journal*, ERAU's peer-reviewed research publication.

"I will say one thing about these collaborations," said Lund, "there are times when these students are even better suited to doing this work than I am. When I was an undergrad, my university had zero classes in machine learning. When I was in my master's program, there was one class in machine learning…. Students now are learning things far more advanced than I ever learned. This SDRD project is so well suited to capitalizing on these students' skill sets." This project illustrates the important role the SDRD program plays in maintaining the scientific and technical vitablity of the NNSS through investing in and promoting workforce development. As noted in the 2019 Strategic Framework document for the NNSA LDRD and SDRD programs, "Cutting-edge research and development across the technical spectrum attracts cutting-edge talent." This SDRD project is an example of how the SDRD program helps recruit, train, and retain tomorrow's technical workforce in essential areas of expertise critical to national security.

Find more information about this work on the OSTI.gov website.



Pictured from above left to below right: Dr. Margaret Lund (principal investigator, NNSS Computing and Data Science); Dr. Marylesa Howard (co-investigator, NNSS Physical Sciences); Chelsey Noorda and Jared Slone (2021 NNSS summer student interns); Dr. Jesse Adams and Dr. Arnulfo Gonzalez (co-investigators, NNSS Computing and Data Science). (Photos courtesy of the project team members)

(Per NNSS classification, this article is confirmed to be unclassified and approved for public release.)

➢ Technical Vitality, Workforce Development

Lawrence Livermore scientists closely determine the Earth's source of water

The source of Earth's water has been a long-standing debate, and at Lawrence Livermore National Laboratory (LLNL), scientists think they have the answer — and they found it by looking at rocks from the moon.

Since the Earth-moon system formed together from the impact of two large bodies very early in solar system history, their histories are very much linked. Additionally, since the moon lacks plate tectonics and weathering, processes that tend to erase or obscure evidence on Earth, the moon is actually a great place to look for clues to the history of Earth's water.

Evidence from lunar samples suggests that although the Earth and moon formed from a giant impact, they mostly retained their primordial abundances of volatile elements, including water. (Image Credit: Adam Connell, LLNL)

Even though close to 70 percent of Earth's surface is covered with water, overall, the planet is a relatively dry place compared to many other objects in the solar system. And the moon is even drier. Conventional wisdom was that the lack of volatile species (such as water) on the Earth — and particularly the moon — was due to this violent impact that caused depletions in volatile elements.

But by looking at the isotopic makeup of lunar rocks, the team found that bodies involved in the impact that formed the Earth-moon system had very low levels of volatile elements prior to the impact, not because of it. Specifically, the team used the relative amount of the volatile and radioactive isotope rubidium-87 (^{87}Rb), which is calculated from its daughter isotope strontium-87 (^{87}Sr), to determine the budget of Rb in the Earth-moon system when it formed. The team found that because ^{87}Sr, a proxy for the moon's long-term volatile budget, was so low the bodies that collided must have both been dry to start with, and not much could have been added since.

"Earth was either born with the water we have, or we were hit by something that was basically pure H_20, with not much else in it. This work eliminates meteorites or asteroids as possible sources of water on Earth and points strongly toward the "born with it" option, said cosmochemist Greg Brennecka, co-author of the paper.

In addition to greatly narrowing the potential source of Earth's water, this work additionally reveals that the large bodies that collided must have both come from the inner Solar System, and the event could not have happened prior to 4.45 billion years ago, greatly reducing the formation window of the moon.

According to Lars Borg, the lead author of the study: "There were only a few types of materials that could have combined to make the Earth and moon, and they were not exotic — they were likely both just large bodies that formed in approximately the same area that happened to run into one another a little more than 100 million years after the solar system formed…but lucky for us, they did just that."

The research appears in the *Proceedings of the National Academy of Sciences*. LLNL scientist Thomas Kruijer also contributed to the research. The work was funded by NASA and the Laboratory Directed Research and Development program.

This study was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. This work was supported by Laboratory Directed Research and Development Grant 20-ERD-001 and NASA Emerging Worlds Program Grant NNH19ZDA001N (L.E.B.). *(LLNL-JRNL-827054) (LLNL-WEB-458451)*

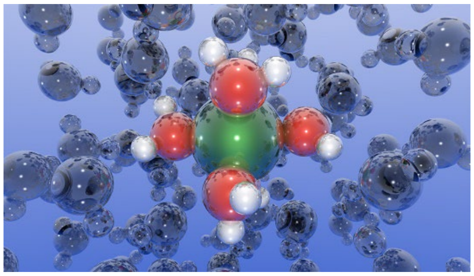
Lawrence Livermore team puts pedal to the metal crossing the solid-liquid interface

Most metal alloys are prone to corrosion, which costs hundreds of billions of dollars of damage annually in the U.S. alone. Accurately predicting corrosion rates is a long-standing goal of corrosion science, but these rates depend strongly on the specific operating environment. At the atomic scale, these environmental factors are associated with how quickly and easily metal ions dissove and transport across solid-liquid interfaces.

Lawrence Livermore National Laboratory (LLNL) scientists have used molecular dynamics simulations to unveil and describe the dynamical behavior of dissolved metal ions and water — a key component of this corrosion puzzle. They introduced a new methodology to describe the strength and nature of chemical bonding between rapidly moving ions in solution. These ions are surrounded by closely held water molecules in the so-called hydration shell, which fluctuates dynamically in ways that can be analyzed computationally. The authors presented a recipe for how these fluctuations could be quantified to ultimately develop computational "descriptors" for the propensity of metals to dissolve in harsh environments. The research appears in *The Journal of Physical Chemistry Letters*.

Beyond corrosion, fluctuations in the hydration shell dictate critical processes in interfacial phenomena relevant to a broad array of applications, including water desalination and crystallization, as well as electrochemical energy storage and conversion.

The team came up with three metrics to represent the dynamical softness of ion hydration shells in terms of their rigidity, deformability, and fluidity.



Water molecules (shown with red oxygen atoms and white hydrogen atoms) form complex dynamic structures around dissolved metal ions (green). How easily these structures can form or break apart often controls the rate at which metals corrode. (Photo credit: Stephan Weitzer/LLNL)

"Directly simulating ion transport across heterogenous interfaces remains technically challenging," said LLNL materials scientist Stephen W Weitzner, lead author of the paper. "In many instances, we need to rapidly and accurately compare the effects of different environmental conditions on ion transport processes, but current simulation strategies can be too resource-intensive for high-throughput studies. So, we developed a set of dynamic metrics that provide a fast and intuitive way to compare the relevant chemical features.

"Our analysis showed that the new set of dynamic metrics not only correctly encoded key physical behavior, but also could explain trends in ion behavior that were challenging to classify using conventional static descriptors."

Weitzner added that beyond aiding the description and discussion of ion transport kinetics, the metrics provide useful targets for the development of machine learning-based force fields that could dramatically accelerate future simulations of metal ion dissolution and transport rates without loss of accuracy.

Other Livermore researchers include Tuan Anh Pham, Christine Orme, S. Roger Qiu, and Brandon Wood. The work is funded by LLNL's Laboratory Directed Research and Development program.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported with Laboratory Directed Research and Development funding under Project 20-SI-004. *(LLNL-WEB-458451)*

➢ Technical Vitality, Mission Agility

Los Alamos NATIONAL LABORATORY

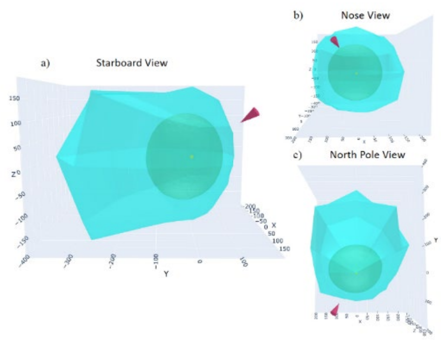
The solar wind bubble that protects Earth has been mapped for the first time

In 2009, using NASA's Intersteller Boundary Explorer, also known as IBEX, astronomers spied a strange ribbon-like structure dancing between our solar system and the rest of interstellar space.

The discovery of the IBEX Ribbon, which is invisible to both telescopes and the human eye, was one of scientists' first forays into understanding more about our heliosphere—a bubble-like shield made up of solar winds.

A new study published in the Astrophysical Journal maps the entire boundary of this shield, and the data collected may be used to usher in a new era of heliophysics exploration.

"Most instruments that detect particles in space are detecting charged particles," says Daniel Reisenfeld, a senior scientist at Los Alamos National Laboratory in New Mexico and lead author of the study. But IBEX is unique.



Orthogonal views of the 3D shape of the heliosphere using the 100 au TS model. The HP is represented in cyan, the embedded TS is green, and the Sun is represented by the yellow dot at the center of the coordinate axes. Axis units are in astronomical units. The positive y-axis points in the upwind direction, and the positive z-axis points toward the north ecliptic pole. The red cone represents the direction of the far interstellar magnetic field at ∼1000 au as determined by Zirnstein et al. (2016).

It detects energetic neutral atoms, or ENAs—ions that originally come off the sun but collide with interstellar electrons, neutralizing them. These atoms can be found everywhere in space, and observing ENA fluxes across time can be a powerful imaging tool.

So what exactly was that mysterious ribbon? Scientists have since determined that what they were seeing was a giant swath of ENAs lighting up the night sky. Using data IBEX collected on ENAs as it charted just one 11-year solar cycle, the time between hifts in the sun's magnetic field, researchers built a three-dimensional map of the entire heliosphere, which Reisenfeld says shields Earth and other planets from harmful radiation.
"Our Earth gets bombarded by cosmic rays, galactic cosmic rays all the time," he says. These rays can subtly affect airplanes that fly near the poles, often on trips between Europe or Asia and the US. *(LA-UR-21-23228)*

Read the original article written by Tatyana Woodall and published in the *MIT Technology Review.*

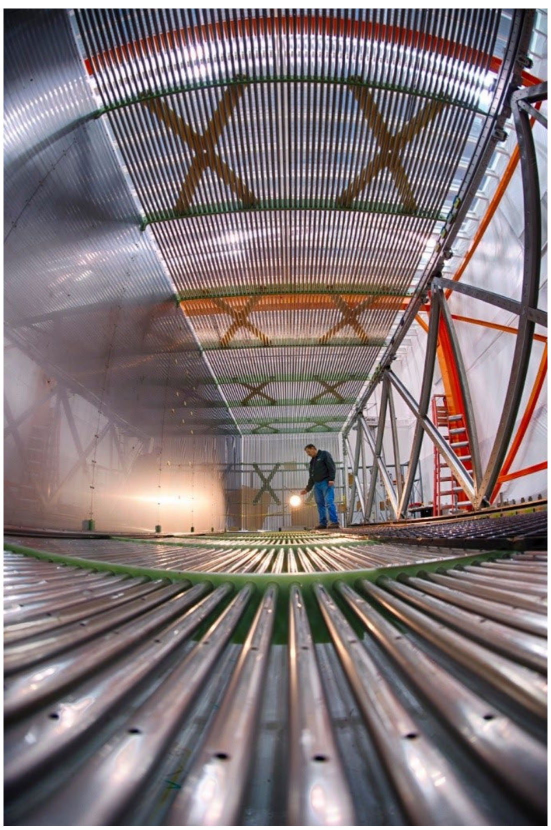
New results from MicroBoone provide clues to particle physics mystery

New results from a more-than-decade long physics experiment offer insight into unexplained electron-like events found in previous experiments. Results of the MicroBooNE experiment, while not confirming the existence of a proposed new particle, the sterile neutrino, provide a path forward to explore physics beyond the Standard Model, the theory of the fundamental forces of nature and elementary particles.

"The results so far from MicroBooNE make the explanation for the MiniBooNE experiment's anomalous electron-like events more likely to be physics beyond the Standard Model," said William Louis, physicist at Los Alamos National Laboratory and a member of the MicroBooNE collaboration. "What exactly the new physics is – that remains to be seen."

The MicroBooNE experiment at the U.S. Department of Energy's Fermi National Accelerator Laboratory explores a striking anomaly in particle beam experimentation first uncovered by researchers at Los Alamos National Laboratory. In the 1990s, the Liquid Scintillator Neutrino Detector experiment at the Laboratory saw more electron-like events than expected, compared to Standard Model-based calculations.

The MicroBooNE experiment seeks to explore the source of the anomaly of the extra events. The MicroBooNE detector is built on state-of-the-art techniques and technology, using special light sensors and more than 8,000 painstakingly attached wires to capture particle tracks. It's housed in a 40-foot-long cylindrical container filled with 170 tons of pure liquid argon. Neutrinos bump into the dense, transparent liquid, releasing additional particles that the electronics can record. The resulting pictures show detailed particle paths and, crucially, distinguish electrons from photons.



Inside of MicroBooNE Time Projection Chamber detector. Credit: Fermilab

“Liquid argon technology is a relative newcomer to neutrino physics, and MicroBooNE has been a trailblazer for this technology, demonstrating what incredible physics one can do with it,” said Sowjanya Gollapinni, Laboratory physicist and a co-leader in the analysis. “We had to develop all the tools and techniques from scratch, including how to process the signal, how to reconstruct it, and how to conduct calibration, among others.”

MicroBooNE included a series of measurements: a photon measurement, and three electron measurements. In early October, results from the photon measurement, which specifically looked for Delta radiative decay, provided the first direct evidence disfavoring an excess of neutrino interactions due to this anomalous single-photon production as the explanation for the MiniBooNE energy excess. Delta radiative decay was the only background the MiniBooNE experiment couldn’t directly constrain.

With only half the data from MicroBooNE yet assessed, possible explanations still to be considered (or tested in future experiments) include the possibility that still-unproven sterile neutrinos might be decaying into gamma rays. Axion decay – the axion is another hypothetical elementary particle – into gamma or an electron-positron pair might also be responsible. Sterile neutrinos and axions could be linked to the dark sector, the hypothetical realm of different yet-unobserved physics and particles.

“The possibilities are endless,” Gollapinni said, “and MicroBooNE will be on a mission to explore each of these with the full dataset. The results provide a pathway for further experimental physics, but a full understanding of the results will also depend on our theoretical physics colleagues, who are very intrigued by these results.” *Read the full article here*. *(LA-UR-21-30697)*

➢ Mission Agility, Technical Vitality

BREAKING NEWS: AMAZING LDRD HIGHLIGHTS

Neutralizing antibodies for emerging viruses: Sandia research defends against COVID-19, prepares for future pandemics

Researchers at Sandia National Laboratories have created a platform for discovering, designing and engineering novel antibody countermeasures for emerging viruses. This new process of screening for nanobodies that “neutralize” or disable the virus represents a faster, more effective approach to developing nanobody therapies that prevent or treat viral infection.

Traditionally used to treat a variety of conditions, including cancer, autoimmune and inflammatory diseases, nanobodies are smaller components of conventional antibodies — a vital element of the body’s immune system that defends against disease-causing viruses or bacteria.

After screening a large, diverse library of synthetic nanobodies, Sandia researchers identified and evaluated several potent nanobodies that can protect against COVID-19. The scientists now aim to replicate this method to defend against current and future biological threats.

“The coronavirus pandemic has made evident the need for a broad range of preventive and therapeutic strategies to control diseases associated with novel viruses,” said Craig Tewell, director of Sandia’s Chemical, Biological, Radiological, and Nuclear Defense and Energy Technologies Center.

With a rich history of biodefense research, Sandia helps protect the nation and the world from threats presented by bioterrorism and naturally occurring diseases, Tewell said.

Sandia National Laboratories researchers create a platform for discovering, designing and engineering novel antibody countermeasures for emerging viruses, including SARS-CoV-2. (Image courtesy of Sandia National Laboratories)

"With a deep understanding of how infectious disease develops and spreads, as well as how the immune system defends from infection," Tewell said, "our researchers are in a unique position to advance the creation of a wide array of disease-fighting tools, including nanobodies."

Virologist Brooke Harmon leads Sandia's nanobody research, a new and growing area of bioscience.

"Vaccines are very good at preventing infection, but they can take a long time to be developed and move through the regulatory process," Harmon said. "We saw a critical need to create effective therapies that can be rapidly developed and deployed."

Once the protein sequence, or genetic coding, of a virus has been identified, Sandia researchers have shown they can produce a nanobody-based countermeasure within 90 days. The method has not yet been tested on humans. Speeding up the discovery of neutralizing antibodies could reduce the impact of future viral outbreaks.

Brooke Harmon, a virologist at Sandia National Laboratories, leads research to discover, design and engineer novel antibody countermeasures for emerging viruses. (Photo by Randy Wong)

"Under current practice, virologists rely upon patients' blood samples to build an antibody library that we can then screen for potential treatments. This means we have to wait, either for people to become infected or for those who are vaccinated to build an immune response," Harmon said. "Sandia's new method is more forward-thinking. Because we have already built a highly diverse, proprietary library, we can begin to screen for extremely potent neutralizing nanobodies as soon as the genetic coding of a virus has been identified."

Nanobodies' diverse attributes

Neutralizing nanobodies represent an attractive strategy, Harmon said, due to their ability to work effectively against an entire family of viruses or variants.

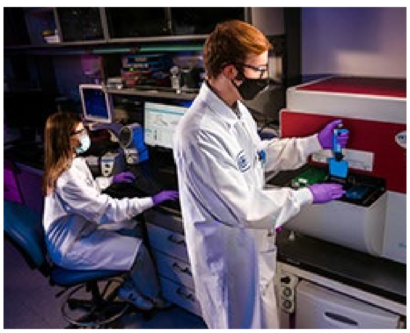
“We can take advantage of the fact that virus families tend to interact with immune response in the same way,” Harmon said. “This makes our treatments rapidly adaptable to all variants of a virus.”

Nanobodies are modular, meaning they can be combined with other nanobodies to increase their ability to bind to the virus or target specific tissues. Nanobodies can also be produced as smaller versions of conventional antibodies with the ability to engage the immune response.

Additionally, due to the small size of the nanobodies, they can be released into the blood and penetrate tissues more thoroughly than conventional antibodies. Nanobody therapies can also target an infection site directly, decreasing the dose needed and increasing efficacy.

Nanobodies can also be administered via aerosol, so they can be given to a patient orally or in an inhalable form. Conventional antibody treatments are less versatile and must be received through injection only.

“All of these qualities and features of nanobodies make nanobody therapies more effective than current solutions. These treatments are also easier and cheaper to manufacture,” Harmon said, “making Sandia’s method for developing and characterizing novel neutralizing antibodies an invaluable addition to the toolset for combatting the COVID-19 pandemic and future health crises.”



Christine Thatcher, left, and Peter McIlroy are members of the nanobody research team at Sandia National Laboratories. With a rich history of biodefense research, Sandia helps protect the nation and the world from threats presented by bioterrorism and naturally occurring diseases. (Photo by Randy Wong)

National recognition

Sandia’s research on nanobodies for emerging viruses received national recognition in October as a recipient of a 2021 R&D 100 Award, which honors the 100 most technologically significant products and advancements in the past year.

This research also received acclamation at the 2021 National Lab Accelerator Pitch Event, where scientists present seasoned investors with business model ideas based on innovations at Department of Energy laboratories. A video of Sandia’s presentation at the event can be viewed here.

One role of the national laboratories is to develop innovative technologies and commercialize the underlying intellectual property through licensing agreements with companies. The labs also engage the expertise of industry and academia to further develop technology using cooperative research and development agreements. Sandia is currently exploring multiple opportunities for licensing this research and partnering with others in the bio and chemical defense, diagnostics and medical research fields.

The research on nanobodies receiving a 2021 R&D 100 Award was funded by Laboratory Directed Research and Development. *(SAND2021-14775E)*

➢ Mission Agility, Workforce Development

Seeing through the fog: Computational imaging research at Sandia focuses on detecting, locating, and sensing images in fog

A team of Sandia researchers recently published a paper in Optics Express describing current results from a three-year project to use computational imaging and the science behind how light propagates and scatters in fog to create algorithms that enable sensors to detect, locate and image objects in fog.

Members of Sandia National Laboratories' fog chamber research team inside the facility after setting up for an experiment. This photo was taken prior to the COVID-19 pandemic. (Photo by Randy Montoya)

"Current methods to see through fog and with scattered light are costly and can be limited," said Brian Bentz, electrical engineer and project lead. "We are using what we know about how light propagates and scatters in fog to improve sensing and situational awareness capabilities."

Bentz said the team has modeled how light propagates through fog to an object and to a detector – usually a pixel in a camera – and then inverted that model to estimate where the light came from and characteristics of the object. By changing the model, this approach can be used with either visible or thermal light.

Bentz says the team has used the model to detect, locate and characterize objects in fog and will be working on imaging objects during the project's final year. The team has been using Sandia's fog facility for experimental validations.

Parallel to this research, the Sandia team created two bench-top fog chambers to support a project at academic alliance partner, West Lafayette, Indiana-based Purdue University.

Sandia is studying and characterizing the fog generated by its new bench-top fog chamber, while Purdue is using its twin system to perform experiments.

Purdue professor Kevin Webb is leading research to develop an imaging technology based on how light interferes with itself when it scatters and using those effects to detect objects.

The Sandia team has recently presented its work at SPIE and CLEO. The computational imaging and academic alliance research was funded by Laboratory Directed Research and Development. *(SAND2021-14052E)*

➢ Technical Vitality

Wildfire and carbon storage: Lawrence Livermore scientist with international team examines effects of wildfire on the global carbon cycle to promote soil carbon stability

Controlled burns to clear flammable brush to reduce the risk of wildfires may help increase long-term carbon storage. (Image courtesy of National Park Service)

Wildfires and prescribed burns may be an important nature-based climate solution to increase long-term carbon storage.

That is the conclusion of an international team of researchers, including a scientist from Lawrence Livermore National Laboratory (LLNL), who looked at the effect of wildfires and prescribed burns on the global carbon cycle. The research appears in *Nature Geosciences*.

Soils are the largest pool of organic carbon (C) on land, and they offer both an opportunity and a risk to climate-C feedbacks in the Earth system because of their role in the global C cycle as well as their vulnerability to disturbance.

Disturbance by fire may lead to carbon losses because fires combust plant biomass and organic soil layers and promote erosion and leaching. This subsequently reduces inputs to and stimulates losses from soils that can persist for several years after the fire.

"What we found, however, is that fires can cause several transformations within an ecosystem that can offset the immediate carbon losses and may ultimately stabilize the ecosystem," said Katerina Georgiou, Lawrence LLNL scientist and Fellow of Lawrence Livermore National Laboratory (LLNL), a co-author of the paper with an international team.

Nearly 70 percent of global topsoil carbon is in fire-prone regions. The team found that fire-driven changes to the persistence of soil organic matter (SOM) are potentially important for offsetting combustion-based C losses by reducing decomposition.

Despite extensive research into how fire alters the properties of SOM, there has been only a limited connection between changes in the SOM properties and the response of soil C fluxes to long-term shifts in fire frequencies and intensities. Most studies that connect fire effects on soil C fluxes with changes in SOM properties focus on the formation of pyrogenic C, which is considered one of the most stable components in soil and can represent more than 30 percent of total soil organic carbon in some soils.

However, pyrogenic C formation can be minimal in ecosystems with a low woody biomass and is just one of the many fire-driven changes relevant to SOM stability. Burning can change the soil porosity, aggregate formation, soil hydrophobicity, potential sorption of organic matter to minerals, microbial biomass and composition and the soil pH — all of which alter the decomposition of the SOM.

In the new research, the team reviewed the evidence for how fire affects the factors that determine the SOM stability — and not just the SOM content alone — to better understand how changes in decomposition dynamics influence the response of soil C storage to shifting fire regimes.

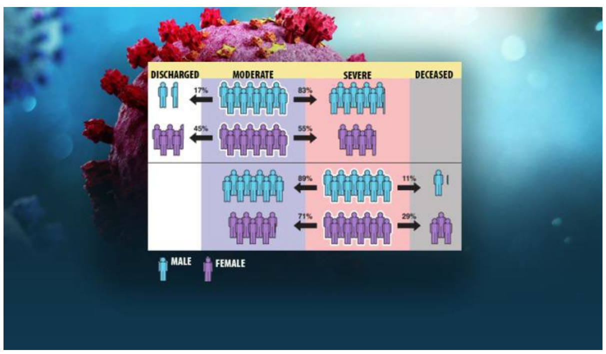
“We examined how fire impacts soil carbon storage and stability across different biomes and explored ways that fire can be used as a natural climate solution in select biomes to promote soil carbon stability,” Georgiou said.

Researchers from the University of Cambridge and Stanford University also contributed to the study. The LLNL portion of the work was funded by the Lawrence Fellow and the Laboratory Directed Research and Development programs.

K.G. was supported as a Lawrence Fellow at Lawrence Livermore National Laboratory (LLNL) by the LLNL-LDRD Program under Project No. 21-ERD-045. Work at LLNL was conducted under the auspices of the US DOE Contract DE-AC52-07NA27344. R.B.J. *(LLNL Release No. LLNL-WEB-458451)*

➢ Mission Agility, Technical Vitality

Covid-19 and risk factors: Lawrence Livermore team models Covid-19 disease progression and identifies risk factors



Being male is a known risk factor for adverse outcomes in hospitalized COVID-19 patients. However, new analysis reveals that when modeling the entire disease trajectory, the degree to which being male is a risk factor depends on the underlying disease severity of the patient. The results are published in the *Journal of the American Medical Informatics Association*. (Photo Credit: Foreground image credit: LLNL Principal Investigator Priyadip Ray; Background image credit: Adobe Stock images.)

A Lawrence Livermore National Laboratory (LLNL) team has developed a comprehensive dynamic model of COVID-19 disease progression in hospitalized patients, finding that risk factors for complications from the disease are dependent on the patient’s disease state.

Using a machine learning algorithm on a dataset of electronic health records (EHRs) from more than 1,300 hospitalized COVID-19 patients with ProMedica — the largest health care system in northwestern Ohio and southeastern Michigan — the team classified patients into “moderate” or “severe” states and tracked disease trajectory as patients moved through different risk states during hospitalization.

Accounting for disease severity — in contrast to previous scientific literature examining only static risk factors — the method allowed the team to identify, as the disease progressed, when certain variables such as age and race, and comorbidities including diabetes and hypertension, led to more severe outcomes.

The model allowed the team, which included co-authors from the University of Toledo, to demonstrate for the first time that links between some factors and more adverse outcomes from COVID-19 can depend on the patient's "current" condition. Most significantly, while male patients were found to be more likely than female patients to have serious complications or die from COVID-19, when starting from the "severe" disease state, women were more likely than men to die of the disease. The results were published Feb. 7 in the *Journal of the American Medical Informatics Association*.

"It's well known in the community that men are at a higher risk than women for eventual death from COVID, and that's true — but certain counterintuitive behavior emerges once you break up the patient trajectory into disease states," said LLNL principal investigator Priyadip Ray. "From the moderate disease state, men are more likely to transition to a more severe disease state. However, if you are in the severe disease state, surprisingly, women are more likely to die than men. This disease-state perspective has not been shown before and indicates that where you are in your disease also determines your risk factors."

By modeling the entire trajectory of hospitalized COVID-19 patients, the team showed "statistically significant differences" in the relative risk of disease progression, which they concluded should be taken into consideration when performing risk assessment among patients in hospitals.

"The vast majority of studies on COVID-19 risk factors ignore the temporal progression of the disease in their analysis," said LLNL co-author Braden Soper. "Our study provides a unique modeling-based approach to understanding how patient demographics and medical comorbidities can present different risk profiles depending on the underlying disease state. Such information is potentially more actionable throughout the course of care, possibly leading to better patient outcomes."

Soper added that disease state-dependent risk assessment also can apply to many other acute and chronic diseases beyond COVID-19, which have thus far largely been assessed only with static data and modeling techniques.

Since EHRs typically suffer from irregularly sampled and/or missing data, the team used a statistical model known as a covariate-dependent, continuous-time hidden Markov model (HMM), known to handle such data well.

The models showed that, while being male, Black or having a medical comorbidity were all associated with an increased risk of progressing from moderate to severe disease states, the same factors resulted in a decreased risk of transitioning from a severe state to death. Researchers attributed the counterintuitive results to the existing prevalence of static models for risk stratification.

"A fixed-time (static) model is susceptible to immortal time bias, as periods of follow-up may be incorrectly assigned to a particular disease state," Ray said. "An HMM is less susceptible to such biases, as it can infer the disease state throughout the patient trajectory."

Among the other findings: body mass index (BMI) alone was not linked to an increased risk of disease progression, while old age was associated with an increased risk in progressing from moderate to severe and from severe to deceased states, the researchers reported.

The team validated the inferred latent disease states with National Institutes of Health-established guidelines and the Epic Deterioration Index risk metric.

Tests on a budget

The LLNL/University of Toledo/ProMedica team's work on dynamic models follows an earlier paper the team published in *Scientific Reports*, where they examined static risk factors for patients who go on to develop severe complications after testing positive for COVID-19.

The team used an interpretability tool to find out which lab tests were most predictive for hospitalization or poor outcomes, identifying which tests should be collected in the case of budget constraints that could give clinicians nearly the same predictions for adverse outcomes as collecting all possible data.

"We tried to look at this problem in a different way," Ray said. "We asked, 'what if you have a budget constraint? What are the biomarkers that you can collect that will give you a good indication of how likely it is that this patient will need to be ventilated or likely to die due to the disease?'

"The interesting thing is that beyond a certain point, collecting more labs will not necessarily give better predictive performance. Can you select a small set of labs and markers that is indicative of risk?" Ray continued. "The answer we found was yes."

To make that determination, the team created a cost structure, grouping types of lab tests and biomarkers with associated costs, from free information (demographics and comorbidities) and low-cost tests such as blood pressure and pulse oximetry, to more expensive lab results — such as liver function and inflammation.

The team then used a machine learning method known to work well for healthcare datasets with missing and/or skewed data to find correlations between patient's features and their risks for death or ventilation from COVID-19 and determine the most predictive set of features. Using the method, they found it was possible to achieve a 43 percent reduction in lab costs with only a 3 percent reduction in performance in predicting the likely need for ventilation from the disease.

"We found that it is possible to achieve a significant reduction in cost at the expense of a small reduction in predictive performance," said co-author Sam Nguyen, who led the data extraction and modeling effort from the LLNL side. "In responding to the pandemic, if one is limited by their testing (vitals, labs, etc.) resources, one could actually do quite well at COVID-19 risk prediction with a limited number of inputs, if one knows the most cost-efficient tests to carry out."

The findings could be useful where certain lab work is unavailable or prohibitively expensive — of particular importance during the COVID-19 pandemic, where many patients and clinicians need to make quick decisions, researchers said.

Co-authors on both papers included LLNL scientists Jose Cadena and Ryan Chan; Paul Kiszka, Lucas Womack and Mark Work of ProMedica; and Joan Duggan, Steven Haller, Jennifer Hanrahan, David Kennedy and Deepa Mukundan of the University of Toledo.

LLNL's Laboratory Directed Research and Development program funded both efforts.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344 and was supported by the LLNL LDRD Program under Project No.19-ERD-009. *(LLNL-JRNL-823909) (LLNL Release No. LLNL-WEB-458451)*

➢ Technical Vitality, Mission Agility

LANL's framework provides a modern approach to protecting crucial infrastructure from storm damage

The deadliest natural disaster in U.S. history was a hurricane in the year 1900 that decimated the island of Galveston, Texas. An estimated 6000–12,000 people were killed. Afterward, in a feat of engineering and a spirit of defiance, the shoreline was elevated by 17 feet, the city was rebuilt, and a 10-mile seawall was erected to protect Galveston's inhabitants and infrastructure against future storms. This brute-force approach to fortification was extreme yet largely effective. More recent storms—Katrina, Sandy, Harvey, Maria—wrought similar devastation to coastal cities and cost hundreds of billions of dollars, hammering home the message that the storms are relentless and it's up to humanity to prepare for them.

Modern human society relies heavily on infrastructure—buildings, roads, power, and water supplies—that is susceptible to damage from extreme weather. More extreme weather threatens to bring more damage, so Los Alamos scientists are helping determine the best approaches to weather the coming storms.

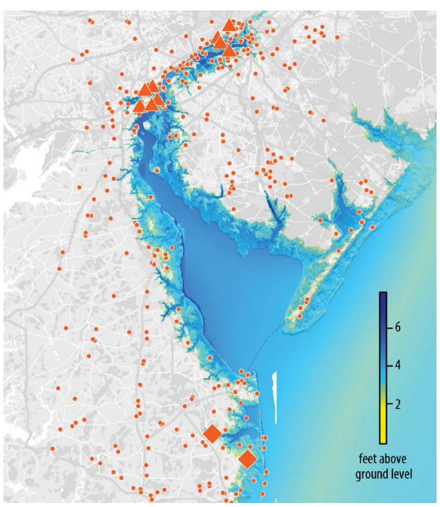
“We are already seeing the effects of climate change,” explains LANL Laboratory physicist Donatella Pasqualini. “Hurricanes, sea-level rise, winter storms, tornados—these are all increasing in frequency and intensity. How can Los Alamos, as a national security laboratory, help local and regional decision makers adapt?”

In two ways, actually: through future planning with investment in new systems and through real-time analysis for situational awareness.

Natural systems and engineered systems coevolve. For example, the beach in Galveston—wide and inviting before the storm—quickly eroded once the seawall was built, taking with it much of the island’s beach-based tourism and compounding its post-storm financial woes. Pasqualini includes the physics of this coevolution in the computer models she builds. She and her team are looking at how coastlines evolve—how the vegetation and geomorphology might change tomorrow, next year, ten years from now—in order to determine where and when to invest money in hardening complex networked infrastructure.

The model can help direct fortification dollars to where they’ll be most effective.
“If I have an idea how a particular coastal region will be 30 years from now, and how the climate will change in that time, that can tell me how to invest today,” says Pasqualini. “It will help me decide where and how to build new power-system assets so they’ll be physically resilient, and whether or not to harden existing assets.”

Pasqualini’s physics-based computer model, the New Science for Multisectors Adaptation (NeSMA) framework, mimics the coevolution between natural and engineered systems by integrating models of the coastal environment with models of energy infrastructure. NeSMA estimates future climate and weather threats, including their statistical uncertainty, to assess the risk to the infrastructure and to inform an optimal adaptation plan. For example, if an existing power plant is determined likely to flood under a set of conditions that might arise every ten years, might the plant be reconfigured to avoid damage? Or can its buildings be reinforced to resist the rising water? Or should the power plant be replaced entirely, by a new one located somewhere safer?



The NeSMA framework can help guide investment decisions by comparing different scenarios. Here, electrical power substations around the Delaware Bay (dots) are at risk of flooding from hurricane storm surge. Though many stations are predicted to flood with or without erosion considerations, certain substations (triangles) are more likely to flood when erosion is included in the model, while others (diamonds) are more likely to flood when erosion is

omitted from the model. This information can help guide asset-hardening investment decisions better than whether or not a certain asset was damaged in the past. (Data for water depth above ground level is included for coastal areas only, not open water areas.) CREDIT: Donatella Pasqualini/LANL, map data © Google

Asset fortification isn't just about threats to physical buildings and brick-and-mortar solutions, though buildings can be costly to repair. Asset fortification is also about adjusting the power-generation capacity within the power plant, or changing distribution routes between substations, or altering the network connections that control operations, so as to either maintain a certain level of functionality or at the very least to avoid complete destruction.

Billions of dollars are spent on infrastructure rebuilding and hardening after every weather-related disaster. But the beauty of NeSMA is that it can help direct those dollars to where they'll be most effective. Rather than automatically hardening the critical assets that were damaged in past events, would it perhaps be more effective, bang-for-the-buck-wise, to harden different assets? Every circumstance is unique, so NeSMA allows the exploration of various *a la carte* solutions, so decision makers can make the best decisions, not just knee-jerk ones.

A pound of cure

Pasqualini developed an automated workflow that takes data from the National Oceanic and Atmospheric Administration (NOAA) and forecasts the intensity and location, by county, of possible power outages as well as the number of people affected. The ability to forecast outages before they occur is a powerful situational-awareness tool for local authorities facing imminent extreme weather who need to decide what to do right now.

While coastal areas are ground zero for a lot of the consequences of climate change, the principals of Pasqualini's models are more broadly applicable. Plunging temperatures, rising rivers, and screaming winds threaten inland infrastructure just as much as hurricanes threaten the coasts. Pasqualini believes her work will help fortify all of these communities against what's coming.

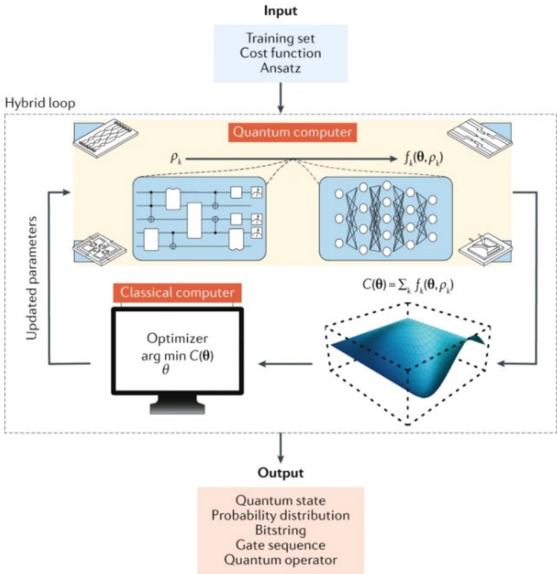
Storms and storm damage are inevitable, so too are the impacts of Earth's changing climate. Long-term climate change and episodic extreme-weather events present critical national security challenges. Helping the nation prepare for the future while being nimble in the present is just one way that Los Alamos scientists are rising to meet those challenges head on. *Read the full article here.* *(LA-UR-21-32363)*

➢ Mission Agility, Technical Vitality

LANL's progress in algorithms makes small, noisy quantum computers viable

As reported in a **new article in Nature Reviews Physics**, instead of waiting for fully mature quantum computers to emerge, Los Alamos National Laboratory and other leading institutions have developed hybrid classical/quantum algorithms to extract the most performance—and potentially quantum advantage—from today's noisy, error-prone hardware. Known as variational quantum algorithms, they use the quantum boxes to manipulate quantum systems while shifting much of the work load to classical computers to let them do what they currently do best: solve optimization problems.

"Quantum computers have the promise to outperform classical computers for certain tasks, but on currently available quantum hardware they can't run long algorithms. They have too much noise as they interact with environment, which corrupts the information being processed," said Marco Cerezo, a physicist specializing in quantum computing, quantum machine learning, and quantum information at Los Alamos and a lead author of the paper. "With variational quantum algorithms, we get the best of both worlds. We can harness the power of quantum computers for tasks that classical computers can't do easily, then use classical computers to compliment the computational power of quantum devices."



Schematic diagram of a variational quantum algorithm. Image Credit: Nature Reviews Physics (Nat Rev Phys)/ ISSN 2522-5820. Cerezo, M., Arrasmith, A., Babbush, R. et al. Variational quantum algorithms. Nat Rev Phys 3, 625–644 (2021). https://doi.org/10.1038/s42254-021-00348-9

Current noisy, intermediate scale quantum computers have between 50 and 100 qubits, lose their "quantumness" quickly, and lack error correction, which requires more qubits. Since the late 1990s, however, theoreticians have been developing algorithms designed to run on an idealized large, error-correcting, fault tolerant quantum computer.

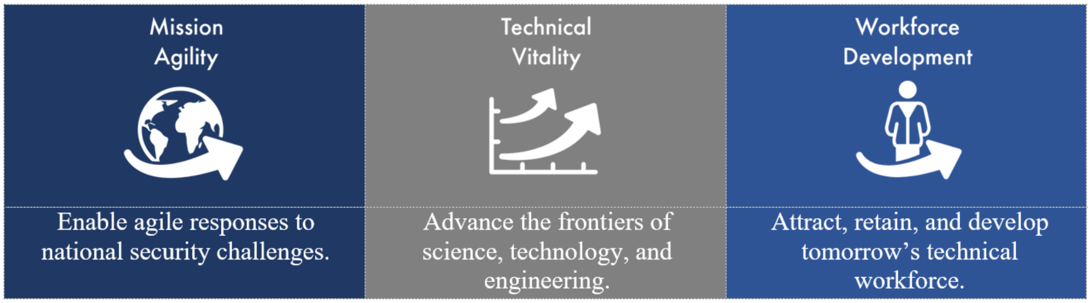
"We can't implement these algorithms yet because they give nonsense results or they require too many qubits. So people realized we needed an approach that adapts to the constraints of the hardware we have—an optimization problem," said Patrick Coles, a theoretical physicist developing algorithms at Los Alamos and the senior lead author of the paper.

"We found we could turn all the problems of interest into optimization problems, potentially with quantum advantage, meaning the quantum computer beats a classical computer at the task," Coles said. Those problems include simulations for material science and quantum chemistry, factoring numbers, big-data analysis, and virtually every application that has been proposed for quantum computers.

The algorithms are called variational because the optimization process varies the algorithm on the fly, as a kind of machine learning. It changes parameters and logic gates to minimize a cost function, which is a mathematical expression that measures how well the algorithm has performed the task. The problem is solved when the cost function reaches its lowest possible value.

In an iterative function in the variational quantum algorithm, the quantum computer estimates the cost function, then passes that result back to the classical computer. The classical computer then adjusts the input parameters and sends them to the quantum computer, which runs the optimization again. *Read the full article here.* *(LA-UR-21-28052)*

➢ Mission Agility, Technical Vitality



This newsletter, published quarterly, features LDRD and SDRD work done by Lawrence Livermore, Los Alamos, Nevada National Security Site and Sandia. For additional issues, visit NNSA-LDRD.lanl.gov. *(Complete Newsletter Review & Release: SAND2022-3917)*

For more information:

NNSA LDRD	LANL LDRD	LLNL LDRD	Sandia LDRD	NNSS SDRD
Anthony Lewis	Laura Stonehill	Doug Rotman	Wahid Hermina	Paul P. Guss
anthony.lewis@nnsa.doe.gov	mailto:lauracs@lanl.gov	rotman1@llnl.gov	wlhermi@sandia.gov	gussPP@nv.doe.gov