

California & Beyond Edition

Extending nuclear power accident code for advanced reactor designs



ADVANCING NUCLEAR SAFETY — Brad Beeny, left, a Sandia nuclear engineer and code developer, and Larry Humphries, the lead code developer for Sandia's nuclear accident modeling computer code, examine remnants from a series of Lower Head Failure experiments. The results from these experiments, and many others, are used to inform the code. **Photo by Randy Montoya**

Sandia expands accident modeling software to support nuclear safety and regulatory activities

By **Mollie Rappe**

Nuclear power is a significant source of steady carbon-neutral electricity, making the design and construction of new and next-generation nuclear reactors critical for achieving the U.S.'s green energy goals.

A number of new nuclear reactor designs, such as small modular reactors and non-light water reactors, have been developed over the past 10 to 15 years. In order to help the **Nuclear Regulatory Commission** evaluate the safety of the next generation of reactors, fuel cycle facilities and fuel technologies, Sandians have been expanding their **severe accident modeling computer code**, called Melcor, to work with different reactor

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Demonstration of high-speed alloy creation might revolutionize hydrogen's future

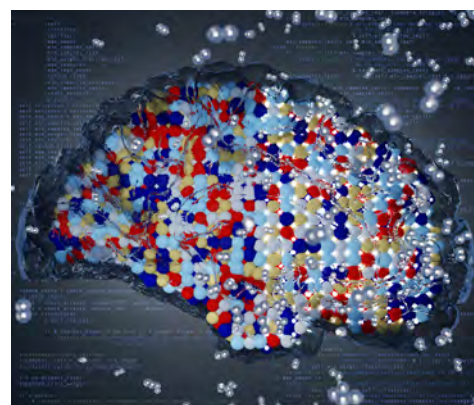
By **Michael Ellis Langley**

A Sandia team of materials scientists and computer scientists, with some international collaborators, have spent more than a year creating 12 new alloys — and modeling hundreds more — that demonstrate how machine learning can help accelerate the future of hydrogen energy.

Vitalie Stavila, Mark Allendorf, Matthew Witman, Jeffery Chames, Sapan Agarwal and Justin Wong — teaming with researchers from Ångström Laboratory in Sweden and Nottingham University in the

United Kingdom — recently published **a paper detailing their approach** as the cover feature of the American Chemical Society's "Chemistry of Materials."

"There is a rich history in hydrogen storage research and a database of thermodynamic values describing hydrogen interactions with different materials," Matt said. "With that existing database, an assortment of machine-learning and other computational tools, and state-of-the-art experimental capabilities, we assembled an international collaboration group to join forces on



HIGH-SPEED CREATION — A group of Sandians and international collaborators used computational approaches, including explainable machine learning models, to elucidate new high-entropy alloys with attractive hydrogen storage properties and direct laboratory synthesis and validation.

Image by Matt Witman

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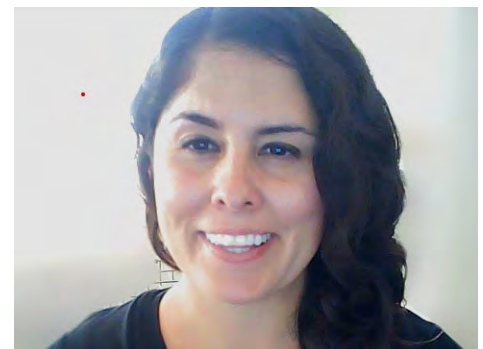
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LABNEWS Notes

Lab News may contain photos shot prior to current COVID-19 policies. Individuals in photos followed all social distancing and masking guidelines that were in place when photos were taken.

EDITOR'S NOTE: We've stopped printing the *Lab News*, but will continue to publish every two weeks. We want you to remain in our community of readers, so please send your comments and suggestions for stories or for improving the paper. *Lab News* welcomes guest columnists who wish to tell their own "Sandia story" or offer their observations on life at the Labs or on science and technology in the news. If you have a column (500-800 words) or an idea to submit, contact *Lab News* editor Katherine Beherec at kgbeher@sandia.gov.



CA & BEYOND LAB NEWS STAFF — The team for this year's CA & Beyond issue and authors of Integrated Security Solutions content throughout the year are, clockwise from top left, Michael Ellis Langley, Paul Rhien, Kayla Norris, Mollie Rappe, Trina West and Tatiana Del Cid.

A study in resilience in a year of pandemic

By **Michael Ellis Langley**

Andy McIlroy, associate labs director of the Integrated Security Solutions division that stretches across Sandia's sites, understands how unsettled many may feel after enduring the past 18 months because he feels the same way. But for Andy, the disorientation that pervaded most of that time was dwarfed by the heart and dedication he saw his fellow Sandians display.

"We have 14,000 people conducting some of the most important work in the nation," he said. "It's easy to lose sight of the incredible positive momentum at the Labs, but I think it's important to step back and remember that Sandia does truly amazing things."

March 2020 — Evolution and revolution

When the pandemic forced Sandia to empty its campuses for a time, Andy and the senior leadership team knew we had to find a way to resume work on vital national security projects. But even he admits that his expectation that the Labs would continue mission activities and meet all major deliverables in the midst of a pandemic might have been greeted with incredulity at that time.

"I think I would have been laughed out of the Laboratories," he said with a wry smile. "And if I had said, 'Oh, and we'll do this next week,' people would have said I was in need of a much longer vacation."

Yet, with some technical issues to overcome, that is exactly what happened.

"It was remarkably successful. That was a bit revolutionary because we took a much bigger leap than we would have under almost any other circumstance," he said. "The ingenuity and dedication of our IT folks to deal with some very real issues were on full display when 14,000 people suddenly began telecommuting. Our staff

overcame those challenges and then successfully brought back the people who needed to be on-site."

But there was also the matter of making the site safe for everyone, which fell to the Facilities team. Andy credited the team for their smooth handling of the tricky situation.

"All of a sudden we had to figure out capacities in conference rooms and how to bring our janitorial staff on-site often enough for cleaning," Andy recalled. "We had to understand the airborne transmission characteristics of COVID-19. We also had to think through the process for increasing airflow in all the buildings."

So Sandia's biomedical experts compiled everything that was known about COVID-19, drew upon early data and developed guidance for creating a safe worksite.

"All of this happened almost invisibly to most people who were working remotely while our on-site staff labored feverishly to apply new knowledge and set up a safe environment," he said. "Put yourself in their shoes. Those folks really stepped up, taking on duties in an extremely stressful environment. Simply put, they were awesome and did an amazing job."

Engineering safety — at work and at home

Sandia is used to thinking about safety and creating safe environments. Andy acknowledged that this mindset was put to the most extreme of tests, in which failure might not just endanger a member of the workforce but their entire family.



EVOLUTION — Associate Labs Director Andy McIlroy, director of Integrated Security Solutions, called the last 18 months part evolution and part revolution. **Photo by Randy Wong**

"We were used to thinking about safety problems as situations we could control very tightly on-site," Andy said. "By engineering safety protocols, we could be extremely confident in the safety of everyone involved. But the safety scenarios typically considered at Sandia essentially ended at the Labs' gates. Our safety considerations didn't extend to people's houses. The pandemic was a completely different challenge because we could theoretically do everything right at work yet still experience infections in our private lives."

This twist led Sandia to talk about safe practices in very different terms, creating guidance as a lifestyle. Today it seems clear to Andy that people took these recommendations to heart.

"When you look at infections within our Sandia population, we are at a tenth or lower of the infection rate in our surrounding communities, both in New Mexico and in California," he said. "It seems clear that folks internalized the safety practices they used at work and practiced them at home to keep their families safe."

Andy says a big part of creating safe spaces at work and peace of mind at home came from the many Sandians in New Mexico and California who created a robust COVID-19 testing program.

“The testing program we stood up at Sandia was based on having in-house expertise. Not only could we safely conduct nasal swabs, but we could perform the analysis of these swabs in a way that met all regulatory requirements,” he said with pride. “We were one of the last DOE national labs to submit a plan to stand up a testing program because we spent a lot of time examining the safety protocols and establishing safe ways to bring people on-site. However, we were the first national lab to have our plan approved and actually begin the testing.”

He called the effort “heroic.”

“We identified early on that testing would be crucial to keep mission activities going,” Andy said. “Sandia has unsung heroes who continued to execute our testing capability for more than a year. These are R&D scientists. They were not hired to run routine samples, but they conducted these tests because it was the right thing to do for the Laboratories during the pandemic.”

Diversity and individuality

As work at Sandia stabilized and settled into a temporary new normal, Andy worried that members of the workforce were stretched thin.

“The workforce writ large just showed incredible resilience,” he said. “The situation was and continues to be quite dynamic and stressful. I was so impressed with how willing people were to make significant adjustments, sometimes on what felt like a daily basis.”

Andy observed that more facets of inclusion and diversity came to light during the pandemic.

“During this past year, we realized that understanding individual circumstances is key when caring for the diversity of people at the Labs and that needs can vary from day to day,” he said. “For example, in the pandemic, parents found themselves burning the candle at both ends — and sometimes in the middle — as they cared for and taught kids who were home all day while simultaneously getting work done. People who were caregivers for other family members found themselves in similar situations.”

Andy said the inclusion and diversity teams also saw participation increase in their programs.

“In the past, maybe 10 people would show up for an event — or perhaps 50 for a really interesting Diversity Cinema — but hundreds of people began attending the virtual inclusion and diversity sessions online,” he recalled. “All in all, it’s important for Sandia to continue to seek to engage and support our workforce members as different needs arise.”

“I’m the executive champion for both the Sandia Parents Group and the Division Diversity & Inclusion Ambassadors Labs-wide, as well as for the African American Outreach Committee at Sandia/California,” he continued. “Together, we are working to realize Sandia’s vision of providing an inclusive and engaging work environment for all. I’m especially glad that we have been highlighting our employee resource groups this year, and I encourage everyone to visit or join a group. They are a great way to expand awareness of other perspectives, build relationships and strengthen our cross-functional teamwork across the Labs.”

Evolution of the Labs

Andy has begun to look forward.

“We’ve seen both evolution and revolution this past year, and I anticipate even more evolution as we shift from the Labs’ maximum telework stance to a new hybrid work environment,” he said. “It won’t be the same Sandia that we left 18 months ago.”

Beyond the new hybrid work environment of people working on- and off-site, Andy said NNSA and Sandia have invested in infrastructure improvements on both the California and New Mexico campuses that enhance and sustain Sandia’s service to the nation.

“President Biden’s budget proposal remains robust in support of national defense,” he said. “With respect to the Energy and Homeland Security Portfolio, which is a major responsibility for our division, we are experiencing a very strong mission pull from the Cybersecurity and Infrastructure Security Agency, within the Department of Homeland Security, as they increasingly recognize Sandia’s very deep expertise in cybersecurity.”

Andy also talked about the important contributions the division’s new Climate Change Security Center is poised to

immediately make.

“The center’s work in renewable energy and geosciences is well-positioned to attack some thorny issues for the nation,” he said. “Sandia has the only concentrating solar power research station in the nation. The combination of renewable power generation and the clean storage that comes with it has the potential to be game-changing. It’s a bit of a moonshot, but we are looking at how our Sandia sites may also be able to transition to renewable energy. We think this is practical enough that we’re willing to eat our own cooking here.”


Andy added that Sandia’s “secret power” is its ability to nucleate the larger community of engineers who know how to take science and turn it into national impact through fully engineered systems ready for end users.

“That is very rare in the national lab complex,” he explained. “There is a lot of great science throughout the DOE national labs. However, taking that science all the way to application is a core competency near and dear to Sandia.”

Looking forward with optimism

Andy knows that so much change in so little time — whether through a worldwide pandemic or natural evolution — can be disorienting for any Sandian. But after looking back at what we have accomplished, he said it is almost impossible not to be optimistic about the Labs’ future outlook.

“We have a workforce that will move heaven and earth to get us where we need to go. The COVID-19 pandemic is a stellar example of the Labs once again stepping up to do something that seemed impossible at the outset. But we made it happen the very next week,” Andy said.

“Our motto is ‘exceptional service in the national interest,’ and we live up to that on a daily basis,” he continued. “So be proud and enjoy riding this freight train of positive momentum at the Labs. If there’s ever a day where you feel a little unsteady, look around you, talk to some of your friends and learn about some of the accomplishments happening across the Labs. You can be confident that Sandia is strong, headed in a great direction and a leader in national security for our country — and that we will continue to be so into the future.” 

COVID-19 diagnostics testing makes clear impact

National security mission continues under safety framework

Story by **Paul Rhien**

Photos by **Lonnie Anderson**

In the early days of the COVID-19 pandemic, it became apparent that Sandia was up against a significant challenge — how would the Laboratories continue their mission-essential work, especially classified and laboratory work, during a stay-at-home order?

Despite pandemic restrictions, the Labs' nuclear deterrence programs continued to be under tremendous pressure to execute modernization programs on schedule, explained Mike Hardwick, director of weapon systems engineering at Sandia's California site.

“Our staff in the nuclear deterrence programs worked on-site through all but the first two weeks of the Laboratories' response to the pandemic,” Mike said.

“And since most of our work is classified, we needed our mission-essential staff to feel safe returning to the site and working around others.”

Meeting a critical need

Proven public health practices during a disease outbreak call for timely testing of those potentially exposed to the contagion, contact tracing to identify other individuals who may have been in close contact with the infected and quarantine or isolation to slow the further spread of the virus.

But the health care infrastructure was overwhelmed by the emerging pandemic, and demand for diagnostic testing from commercial and public health agencies was extremely high. Equipment and supplies were also in short supply. Available diagnostic testing was taking five to 10 days to return results, said Steve Casalnuovo, senior manager of biosciences and chemical defense.

“That was too long to be useful to Sandia,” Steve said.

In early March 2020, a team of bioscientists in the Chemical, Biological,



DIAGNOSTICS LAB TOUR — Labs Director James Peery and Deputy Labs Director Dori Ellis toured the COVID-19 diagnostics laboratory in June 2020.

Radiological, and Nuclear Defense and Energy Technologies Center went to work to set up a federally registered diagnostic lab and develop a diagnostic test

authorized by the U.S. Food and Drug Administration. The goal was to provide a more rapid response and highly reliable diagnostic results for Sandia and

Department of Energy personnel in New Mexico and California.

“This was no small feat,” Steve said. “It took a lot of work to convert existing research laboratories at Sandia into diagnostic laboratories. Research labs are creative; they’re flexible. They’re doing new things all the time. Diagnostics labs do the same thing over and over again. They do it really well and never get it wrong — because people’s lives depend on it.”

With critical support and guidance from the New Mexico Department of Health, Sandia was processing patient samples in their newly converted diagnostic lab three weeks after being directed to establish this capability by Sandia’s executive leadership.

Sandia has great expertise in biotechnology and biological research and development, and we’ve built that capability over more than two decades, Steve explained.

“I don’t know that anyone ever anticipated the need to apply that expertise to a public health crisis like this one, but Sandia had the technological infrastructure for doing molecular biology. That turned out to be critical for us to perform medical diagnostics,” Steve said. “Because we have trained personnel who are experts in the field, when it became apparent that the pandemic response was overwhelming the public health infrastructure, Sandia was able to redirect that expertise to meet a very critical need.”

COVID-19 diagnostic testing capacity was quickly expanded, and Sandia

was able to offer testing not only to those who were displaying symptoms but to the asymptomatic as well. Testing was also available to members of the workforce at the Labs’ Livermore and Carlsbad sites, as well as to household members who had potentially been exposed to the virus.

Keeping Sandia operating

With an on-site diagnostics lab, most test results were processed and returned within 24 hours, enabling Employee Health Services to quarantine and isolate those testing positive for COVID-19 sooner, perform contact tracing and evacuate or decontaminate impacted facilities.

“By performing our own testing, Sandia was able to provide reliable results to members of the workforce very quickly,” Steve said. “Imagine how ineffective it would be to conduct contact tracing or building evacuation and decontamination when you start that process several days after someone is tested, as opposed to one day after.”

“The biggest impact was certainly keeping Sandia operating and our national security mission moving forward,” Mike said. “Diagnostic testing by Employee Health Services and our biosciences group was a vital part of the safety framework that provided the assurance that staff needed.”


As a result, nuclear deterrence programs were able to meet all hardware commitments to their U.S. Air Force partners.

“Our modernization and stockpile stewardship programs have considerable national security work, and a fair portion of this work is classified and deemed mission-essential by our NNSA customer,” added Dan Fonte, director of stockpile systems and component engineering. “Diagnostic testing has allowed our personnel to conduct classified work on-site and meet critical deliverables.”

In total, more than 9,800 COVID-19 samples were analyzed from March 2020 to June 2021, identifying over 840 positive cases.

To ensure a safe and healthy work environment, Sandia’s testing program continues to address cases where there is a higher risk of spread. However, with the expansion of testing capacity at commercial laboratories, Sandia now contracts out all COVID-19 laboratory testing and analysis.

Regardless of vaccination status, those who have COVID-19 symptoms or who are required to work on-site and have come into close contact (within six feet for a total of 15 minutes or more over a 24-hour period) with someone suspected or confirmed as COVID-19 positive should be tested. Sandia Medical testing coordination is also available for those who need to be tested before or after domestic or international [business travel](#).

Members of the workforce should contact Sandia Medical before reporting to work to discuss the needed testing and follow-up. 



COVID-19 LABORATORY ANALYSIS — The COVID-19 Diagnostics team analyzes samples collected from Sandia and Department of Energy personnel in New Mexico and California, providing quick-response and highly reliable diagnostic results.

Nuclear safety

CONTINUED FROM PAGE 1

geometries, fuel types and coolant systems.

These advancements have been demonstrated at several virtual public meetings this summer. The purpose of these meetings is to show U.S. policy-makers, members of the nuclear energy industry, international nuclear energy regulators and members of public interest groups that the NRC has the tools needed to evaluate the safety of new and advanced nuclear reactor designs.

“This computer code really is the Swiss Army knife of nuclear system safety,” said Dave Luxat, manager for Sandia’s nuclear reactor severe accident modeling group. “It is a flexible toolbox of physics and chemistry that allows us to simulate how a nuclear power plant or another nuclear facility reacts during an accident that could potentially lead to the release of radioactive material into the environment. In my view, the code is central to enabling the innovation of nuclear energy in the U.S. and thus mitigating the worst outcomes from climate change.”

Advancing the safety code for the next generation

Sandia and the NRC have worked together for decades to advance the understanding of system performance under accident conditions. This research covered areas such as accident progression, combustible gas generation and transport, molten core concrete interaction, fuel coolant interactions and many others. Starting in the 1980s, the NRC directed Sandia to consolidate these capabilities into one software package.

The Melcor code can model a wide array of phenomena including severe accidents that can occur at a nuclear power plant, then estimate the extent of radioactive material release possible due to the accident. Work on the code began after the **Three Mile Island accident** in 1979.

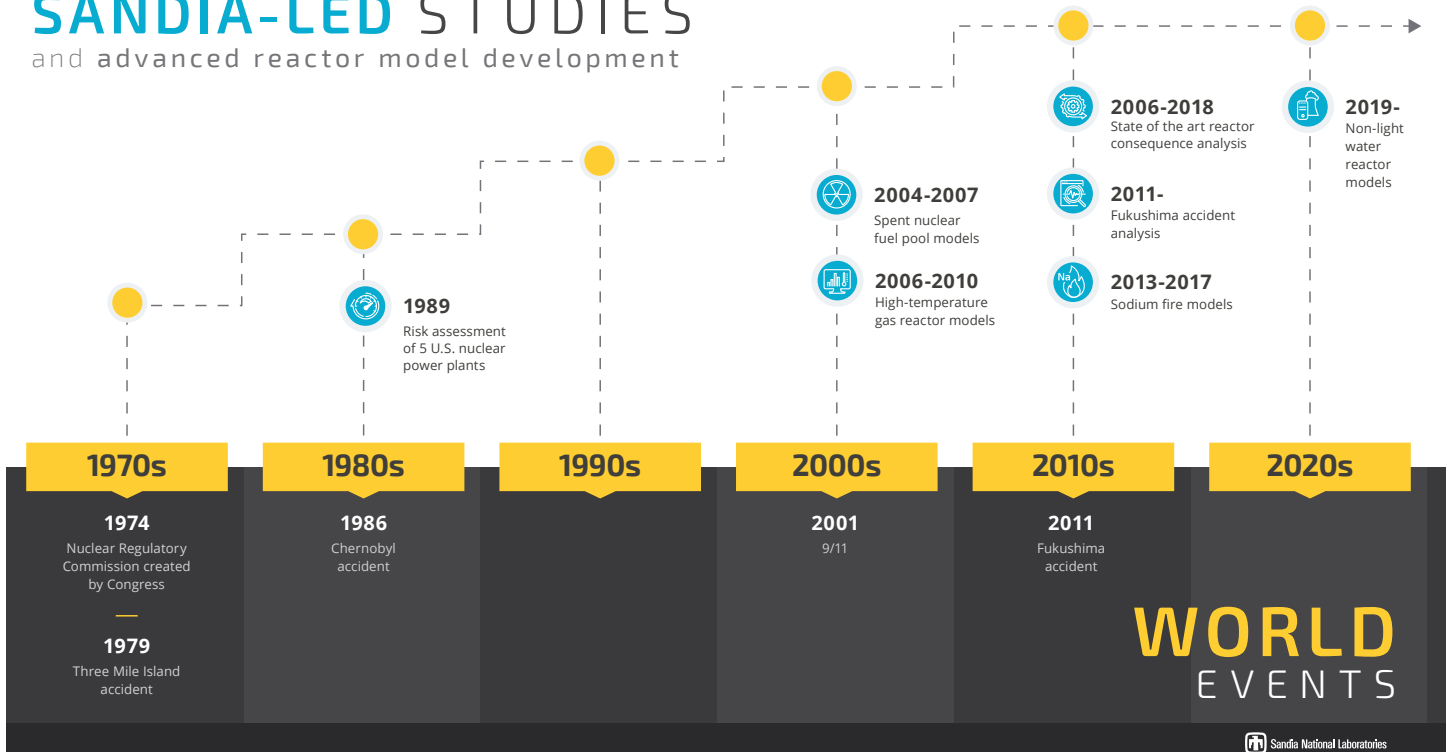
Currently, the computer code is used to inform the NRC’s regulatory decision-making activities, including licensing reviews for new reactors, regarding the risks from very low-likelihood but high-impact accidents during. In fact, Sandia’s code was used to study the **Fukushima accident** and evaluate the

risk-reduction potential of several safety improvements to U.S. nuclear reactors for the NRC, Dave said.

There are many different types of next-generation nuclear reactors, each with their own performance attributes. Small modular reactors take up a tenth of the area or less of current reactors, with lower initial investments, and could possibly be manufactured at one central location and moved to remote locations. As the industry develops new methods and technologies, however, existing capabilities must also advance, based on decades of foundational work. Some advanced designs, such as helium-cooled high-temperature reactors, can use more robust, graphite-pebble-based nuclear fuel. This approach requires adjustments to Melcor for modeling reactor geometry and the physics of the coolant.

Since 2018, Dave’s team has expanded the severe accident code to tackle these differences, and more, to enable the evaluation of the risks of next-generation reactors and impacts to the fuel cycle in general. In order to expand the code capabilities, Larry Humphries, the lead code developer, has

SANDIA-LED STUDIES and advanced reactor model development



POWERFUL, HISTORICAL CODE — A timeline of Sandia-led studies to inform the severe accident code, efforts to expand Melcor to advance reactor designs, as well as world events that led to further Sandia studies.

Image by Laura Hatfield

been working with experts at other DOE labs to determine the critical phenomena for the reactor types. He then works to fit those phenomena into the existing physics-based code, determine what physical parameters are missing and fill in those knowledge gaps.

“We want to leverage the decades of experience and validated models in the code and extend it to new reactor designs and new applications,” said Larry, who has worked on Melcor for two decades, and before that he spent a decade doing experiments to inform and refine the base code. “This code is an ideal tool to apply to new reactor designs where there is a great deal of uncertainty. It has the ability to set sensitivity parameters and determine which variables are critical to produce risk assessment data for regulators.”

Demonstrating risk-assessment readiness

In order to demonstrate that Melcor is ready to assist the NRC in reviewing new reactor designs, the team developed models of three published nuclear reactor designs. The three reactor designs were chosen to represent the diversity of next-generation reactors, including a microreactor originally designed by Los Alamos National Laboratory, a high-temperature helium-cooled reactor, and a high-temperature molten-fluoride-cooled reactor, said K.C. Wagner, a Sandia nuclear engineer who has been leading the demonstration calculations.

The reactor models include everything from the radionuclides expected to be in the reactor vessel and the building that surrounds it to the coolant pipes and the physical properties of the fluid within, K.C. said. Then the team simulated a wide range of potential accidents. They analyzed what happens as time progressed to see how much, if any, fission products are released.

The results of these simulations were presented at the public meetings to highlight the code’s capabilities as the NRC works to establish its readiness to evaluate next-generation reactors.

“If industry is ever going to be able to build anything new and exciting, we need



ACROSS THE WORLD — A map showing all of the countries that use Sandia’s severe accident modeling code to improve the safety of their nuclear power plants. After the U.S., Korea is the country with most licensed users of the code at 120 individuals.

Image by John Reynolds

to be able to do safety and licensing calculations of the next generation designs so that the U.S. regulators can assess them,” said Brad Beeny, a Sandia nuclear engineer and code developer. “We’re mostly concerned with characterizing the radiological hazard that could be posed to the public, should an accident happen. It may not be the most flashy aspect of nuclear energy, but it is one of the most necessary.”

However, it’s not just the U.S. that will benefit from the extension of the nuclear safety code.

“This best-estimate, severe-accident analysis code is used by maybe 1,000 people around the globe in about 30 countries,” K.C. said. “Through the [Cooperative Severe Accident Research Program](#), we are giving these folks access to a tool that they can also use to improve nuclear power plant safety world-wide.”

Since the early 2000s, Melcor has been expanded and updated to support safety assessments for other kinds of nuclear facilities — including research reactors, reactors that produce medical isotopes and DOE facilities that work with radioactive material — and even fusion reactors, Dave and Larry said.

“The code is a repository of decades of knowledge on nuclear accidents, which shows nuclear energy is fundamentally low risk for society,” Dave said. “We have been able to leverage this knowledge to enhance the safety and economics of nuclear power plants in the U.S. Now, Sandia is working to expand on and apply this knowledge to enable the next generation of even safer, more economic nuclear power reactors. This will be critical to combatting climate change and enhancing the energy security of future generations.”

The team is also working to restructure the safety code so that it will be easier to model new reactor designs and answer new safety questions, Larry said. He added, “I have every reason to believe that in the next 10 years the code will continue to be an important tool for the NRC, an important contributor to our understanding of severe accidents, no matter the new type of reactors.”

Melcor is discussed in NRC’s vision and strategy for non-light-water reactors for both [reactor accidents](#) and in the [nuclear fuel cycle](#). The NRC’s independent Advisory Committee on Reactor Safeguards has favorably reviewed the code’s role in the strategy.

Pathways to production

Comprehensive software aids scientists in synthetic biology analysis

By **Paul Rhien**

B iologists at Sandia developed comprehensive software that will help scientists in a variety of industries create engineered chemicals more quickly and easily. Sandia is now looking to **license the software** for commercial use, according to the researchers.

Sandia's stand-alone software RetSynth uses a novel algorithm to sort through large, curated databases of biological and chemical reactions, which could help scientists synthetically engineer compounds used in the production of biofuels, pharmaceuticals, cosmetics, industrial chemicals, dyes, scents and flavors.

The software platform uses retrosynthetic analysis to help scientists identify possible pathways to production — the series of biological and chemical reactions, or steps, needed to engineer and modify the molecules in a cell — to create the desired biological product or compound. By using the software to rapidly analyze all pathways, scientists can determine the production sequence with the fewest steps, the sequences that can be completed with available resources or the most economically viable process.

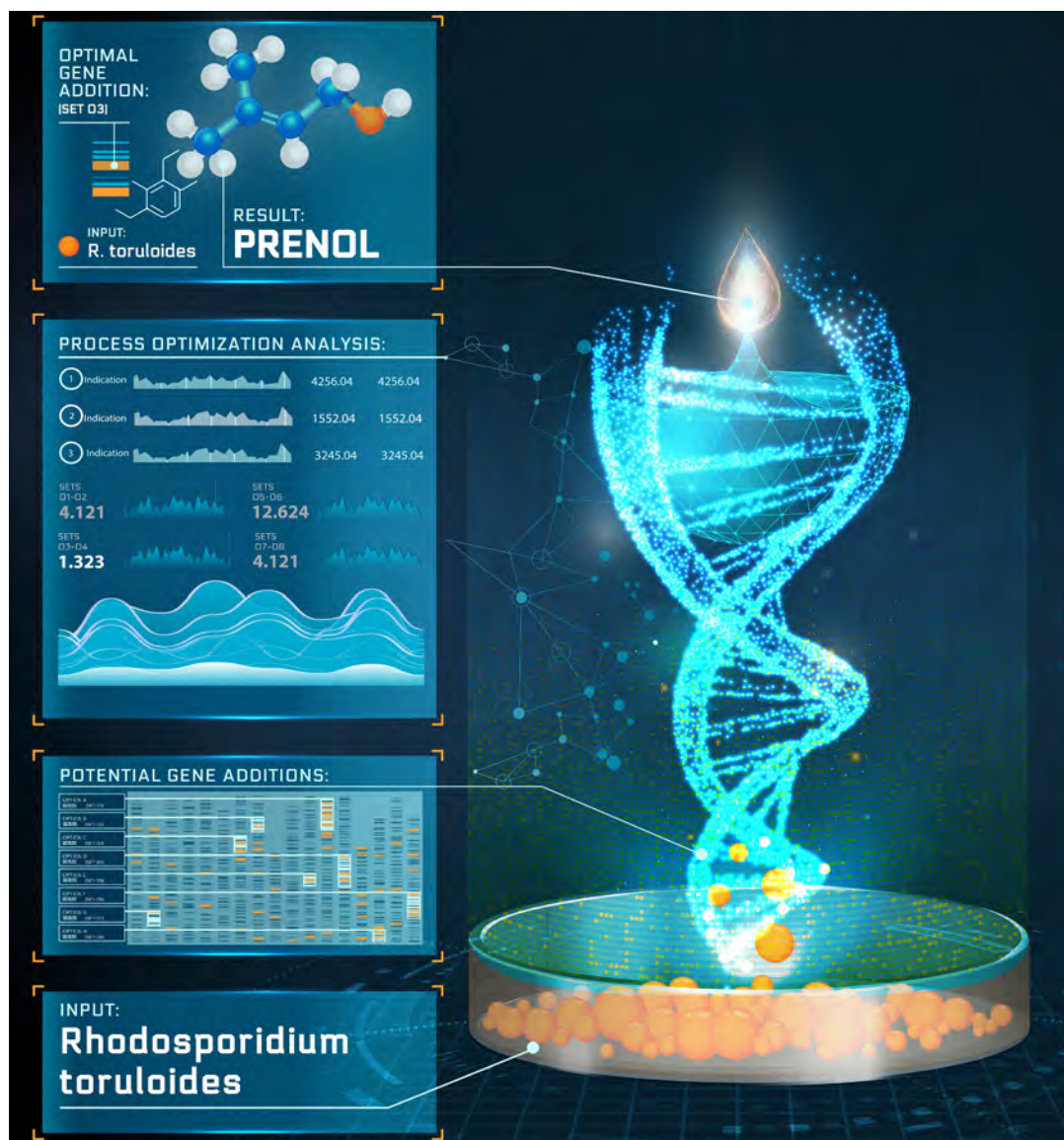
Synthetic biology involves redesigning organisms for useful purposes by engineering them to have new abilities. Researchers and companies around the world are using synthetic biology to harness the power of nature to solve problems in medicine — such as the development of vaccines, antibodies and

therapeutic treatments — as well as in manufacturing and agriculture.

“Synthetic biology is becoming a critical capability for U.S. manufacturing. It has the potential to dramatically reduce waste, eliminate or curtail emissions and create next-generation therapeutics and materials,” said Corey Hudson, a computational biologist at Sandia. “That is where people will see RetSynth have the biggest impact.”

“The diverse functionality of RetSynth opens a lot of opportunities for researchers, giving them multiple options, including biological, chemical or hybrid pathways to production,” Corey said. “All the while, the software is accelerating the research and development process associated with bioproduction. Traditionally, this process has been relatively slow and complex.”

RetSynth is designed to save researchers time and money by suggesting process



SYNTHETIC BIOLOGY SOFTWARE — A graphic illustration of the kind of retrosynthetic analysis conducted by RetSynth software. Using a novel algorithm, the software identifies the biological or chemical reactions needed to create a desired biological product or compound.

Graphic by **Laura Hatfield**

modifications to maximize theoretical yield, or the amount of bioproduct that could be produced, Corey said. All available pathways are rendered using clear visual images, enabling software users to quickly interpret results.

Commercial licensing for broader impact


The RetSynth software was originally developed as part of the DOE’s

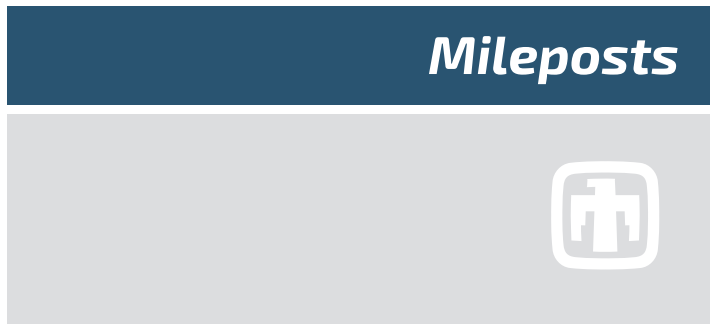
Co-Optimization of Fuels & Engines

initiative, a consortium of national research labs and scientists that have researched how to use synthetic biology to create innovative fuels and high-efficiency engines that reduce emissions.

Today, RetSynth has been expanded to support a variety of diverse applications and is ready to license the software to an industry partner for commercial use, Corey said.

Transfer of Sandia’s innovative technologies to the marketplace through outside technology partners leads to billions in economic impact and supports tens of thousands of high-paying jobs each year, according to a recent report.

To learn more about licensing opportunities, visit Sandia’s Licensing and Technology Transfer webpage. 



Kevin Carbiener 40



Michael Mazarakis 40



Adrian Romero 40



Paul Shoemaker 40



Darrick Jones 30



Mabel Pecos 30



Dave Wheeler 30



Heidi Smartt 25



Steven Wix 25



Adele Doser 20



Jason Gale 20



Steve Garcia 20



David Lord 20



Kyle McDonald 20



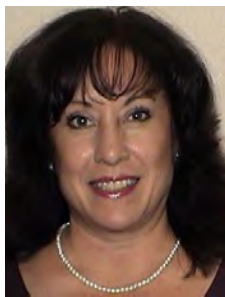
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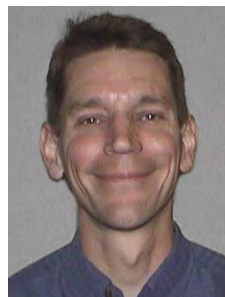
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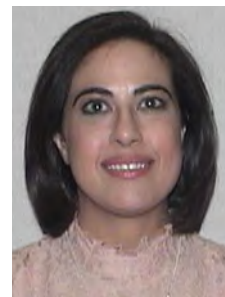
Chad Staiger 20



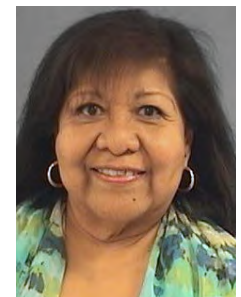
JoAnna Trujillo 20



Douglas Vangoethem 20



Alice Kare 15



Cynthia Torrez 15

High-speed alloy

CONTINUED FROM PAGE 1

this effort. The starting point was demonstrating that machine learning techniques could indeed model the physics and chemistry of complex phenomena which occur when hydrogen interacts with metals.”

Having a data-driven modeling capability to predict thermodynamic properties can rapidly increase the speed of research. In fact, once constructed and trained, such machine learning models only take seconds to execute and can therefore rapidly screen new chemical spaces: in this case 600 materials that show promise for hydrogen storage and transmission.

“Machine learning, coupled with targeted synthesis, lead to a dramatic reduction in the amount of time required to develop a new material,” Mark added. “This was accomplished in only 18 months. Without the machine learning it could have taken several years. That’s big when you consider that historically it takes something like 20 years to take a material from lab discovery to commercialization.”

The team also found something else in their work — results that have dramatic implications for small-scale hydrogen generation at hydrogen fuel-cell filling stations.

“These high-entropy alloy hydrides could enable a natural cascade compression of hydrogen as it moves through the different materials,” Vitalie said, adding that compressing hydrogen is traditionally done through a mechanical process.

He describes building a storage tank with multiple layers of these different alloys. As hydrogen is pumped into the tank, the first layer compresses the gas as it moves through the material. The second layer compresses it even further and so on through all of the layers of differing alloys, naturally making the hydrogen usable in motors that generate electricity.


Hydrogen produced under atmospheric conditions at sea level has a pressure of approximately 1 bar — the metric unit of

pressure. For hydrogen to power a vehicle or some other engine from a fuel cell, it must be pressurized — compressed — to much higher pressure. For example, hydrogen at a fuel-cell charging station must have a pressure of 800 bars or higher so that it can be dispensed as 700-bar hydrogen into fuel-cell hydrogen vehicles.

“If hydrogen at 1 bar is pushed through a sequence of metal hydrides with varying thermodynamics, it automatically compresses as part of the migration from one material to another,” Vitalie explained. “As hydrogen moves through those layers, it gets more and more pressurized with no mechanical effort. You could theoretically pump in 1 bar of hydrogen and get 800 bars out — the pressure needed for hydrogen charging stations.”

Vitalie said that some American industries have already expressed interest. The team is still refining the model. However, since the database is already public through the DOE, the potential of the method could be limitless once it is better understood. In fact, Sapan said that using machine learning can lead to breakthroughs in a

myriad of fields — including even more advances in materials science.

“The next step,” Vitalie suggested, “is to investigate whether the machine can tell us which order we should synthesize these materials to extract the best data, improve the model and increase the accuracy of the predictions? That’s really the future. Without all these pieces, this discovery would not have been possible.” 



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Sandia uncovers hidden factors that affect solar farms during severe weather

Machine learning found farm age, cloud cover impact performance during a storm



WEATHERPROOF — Sandia researchers Thushara Gunda, front, and Nicole Jackson examine Sandia solar panels as summer monsoon clouds roll by. Using machine learning they uncovered the age of a solar farm, and well as the amount of cloud cover, have pronounced effects on farm performance during severe weather.

Photo by Randy Montoya

By **Mollie Rappe**

Sandia researchers combined large sets of real-world solar data and advanced machine learning to study the impacts of severe weather on solar farms, and sort out what factors affect energy generation. Their results were published earlier this month in the scientific journal [Applied Energy](#).

Hurricanes, blizzards, hailstorms and wildfires all pose risks to solar farms both directly in the form of costly damage and indirectly in the form of blocked sunlight and reduced electricity output. Two Sandia researchers scoured maintenance tickets from more than 800 solar farms in 24 states and combined that information with electricity generation data and weather

records to assess the effects of severe weather on the facilities. By identifying the factors that contribute to low performance, they hope to increase the resiliency of solar farms to extreme weather.

“Trying to understand how future climate conditions could impact our national energy infrastructure, is exactly what we need to be doing if we want our renewable energy sector to be resilient under a changing climate,” said Thushara Gunda, the senior researcher on the project. “Right now, we’re focused on extreme weather events, but eventually we’ll extend into chronic exposure events like consistent extreme heat.”

Hurricanes and snow and storms, oh my!

The Sandia research team first used natural-language processing, a type of

machine learning used by smart assistants, to analyze six years of solar maintenance records for key weather-related words. The [analysis methods they used](#) for this study has since been published and is freely available for other photovoltaic researchers and operators.

“Our first step was to look at the maintenance records to decide which weather events we should even look at,” said Thushara. “The photovoltaic community talks about hail a lot, but the data in the maintenance records tell a different story.”

While hailstorms tend to be very costly, they did not appear in solar farm maintenance records, likely because operators tend to document hail damage in the form of insurance claims, Thushara said. Instead, she found that hurricanes were mentioned in almost 15% of

weather-related maintenance records, followed by the other weather terms, such as snow, storm, lightning and wind.

“Some hurricanes damage racking — the structure that holds up the panels — due to the high winds,” said Nicole Jackson, the lead author on the paper. “The other major issue we’ve seen from the maintenance records and talking with our industry partners is flooding blocking access to the site, which delays the process of turning the plant back on.”

Using machine learning to find the most important factors

Next, they combined more than two years of real-world electricity production data from more than 100 solar farms in 16 states with historical weather data to assess the effects of severe weather on solar farms. They used statistics to find that snowstorms had the highest effect on electricity production, followed by hurricanes and a general group of other storms.

Then they used a machine learning algorithm to uncover the hidden factors that contributed to low performance from these severe weather events.

“Statistics gives you part of the picture, but machine learning was really helpful in clarifying what are those most important variables,” said Nicole, who primarily conducted statistical analysis and the machine learning portion of the project. “Is it where the site is located? Is it how old the site is? Is it how many maintenance tickets were submitted on the day of the weather event? We ended up with a suite of variables and machine learning was used to hone in on the most important ones.”

She found that across the board, older solar farms were affected the most by severe weather. One possibility for this is that older solar farms had more wear-and-tear from being exposed to the elements longer, Nicole said.

Thushara agreed, adding, “This work highlights the importance of ongoing maintenance and further research to ensure photovoltaic plants continue to operate as intended.”

For snowstorms, which unexpectedly were the type of storm with the highest effect on electricity production, the next most important variables were low sunlight levels at the location due to cloud cover

and the amount of snow, followed by several geographical features of the farm.

For hurricanes — principally hurricanes Florence and Michael — the amount of rainfall and the timing of the nearest hurricane had the next highest effect on production after age. Surprisingly low wind speeds were significant. This is likely because when high wind speeds are predicted, solar farms are preemptively shut down so that the employees can evacuate leading to no production, Thushara said.

Expanding the approach to wildfires, the grid

As an impartial research institution in this space, Sandia was able to collaborate with multiple industry partners to make this work feasible. “We would not have been able to do this project without those partnerships,” Thushara said.

The research team is working to extend the project to study the effect of wildfires on solar farms. Since wildfires aren’t mentioned in maintenance logs, they were not

able to study them for this paper. Operators don’t stop to write a maintenance report when their solar farm is being threatened by a wildfire, Thushara said. “This work highlights the reality of some of the data limitations we have to grapple with when studying extreme weather events.”

“The cool thing about this work is that we were able to develop a comprehensive approach of integrating and analyzing performance data, operations data and weather data,” Nicole said. “We’re extending the approach into wildfires to examine their performance impacts on solar energy generation in greater detail.”

The researchers are currently expanding this work to look at the effects of severe weather on the entire electrical grid, add in more production data, and answer even more questions to help the grid adapt to the changing climate and evolving technologies.

This research was supported by DOE’s [Solar Energy Technologies Office](#) and was conducted in partnership with the [National Renewable Energy Laboratory](#). 



MISSION FORWARD

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Videoconferencing growth fuels collaboration

Digital tools prove to be a necessity during pandemic

By **Paul Rhien**

The COVID-19 pandemic and resulting stay-at-home orders have led to significant changes to the way people work. Expanding the use of videoconferencing and other digital collaboration tools was critical for Sandia to continue to meet mission deliverables — and that has meant explosive growth for the Integrated Video Solutions team.

With a rise in telecommuting and virtual work for much of the Labs' workforce, the videoconferencing team worked tirelessly to ensure everyone had an effective way to communicate while working remotely, as well as to provide new options so that workforce members could maintain social distancing when returning to work.

"It's not widely known, but Division 8000 is responsible for videoconferencing throughout all of Sandia," said Andy McIlroy, associate labs director for Integrated Security Solutions. "Last March we went from 'Videoconferencing is nice to have' to 'I can't live my day without it.'"

Andy called the overnight change in demand for video communications tools "daunting."

Rise in demand

Marc Campanozzi, a member of the Integrated Video Solutions team, quantified the increase in demand for videoconferencing services.

"Before COVID, our team was focused on installing and maintaining conference rooms," Marc said. "We supported a large-group meeting here or there, but it wasn't our primary concentration."

In March 2020, the team quickly shifted to providing online videoconferencing support and today helps stream and record more than 50 large-group meetings on Skype and Microsoft Teams each month — meetings such as health education seminars, division town halls,



STREAM TEAM — Dave Nagel, with the Integrated Video Solutions team, stands in with equipment he helped design and install in a Sandia conference room that enabled classified and unclassified meetings to occur even under COVID-19 quarantine.

Photo by Michael Ellis Langley

Labs-wide all-hands meetings, intern events and more.

In addition to large-group meetings, the use of Skype conferences and Microsoft Teams for smaller one-on-one collaborations, department meetings, hiring interviews or external presentations has also grown substantially, rising to an average of 138,000 virtual meetings each month.

"We quip that Skype was a savior during COVID. But the fact is that without it, we would have been at a standstill," Marc said. "Our team was proud to be able to do our part to keep the mission moving forward in the face of adversity."

"We had some issues early on, but it is remarkable how fast the team was able to respond — really within just a few days," Andy said. "Our videoconferencing team, as well as the networking team across the Laboratories, really stepped up to make sure that we had the capacity to deal with this. That was huge."

Innovative teaming

Throughout the transition to remote work, the videoconferencing team worked closely with many partnering organizations from across the Labs.

Central to the operating strategy for Integrated Security Solutions is the **Integrated Service Delivery** model, which emphasizes being proactive, thinking critically, taking personal accountability and teaming for mission success. Embracing this mindset, the Integrated Video Solutions team collaborated with Enterprise Collaboration Services, Creative Services, Digital Media Operations and other partners to create innovative solutions.

"We were all teaming to provide new and innovative ways for large meetings and other communication to happen online," Marc said, explaining how the partners resolved urgent issues by pooling resources, cross-training staff and combining the functionality of video-streaming platforms with existing equipment in on-site auditoriums. This allowed them to increase participant capacity, more efficiently record meetings and archive videos for later viewing.


"While the pandemic caused a lot of teams to be more separated and even isolated from one another, in a way it brought our team closer, encouraging us to work with other organizations to solve new problems together," Marc said.

The future of videoconferencing

The Integrated Video Solutions team has also been preparing for an eventual return to increased on-site work. Because of the Labs' maximum telework posture, many of the 300 on-site conference rooms have been unoccupied. The team took advantage of

the opportunity to transition these collaboration spaces: adding more modern video-conference tools for improved user experience, updating software and hardware and expanding on-site classified options.

"We don't know entirely what the future will look like or what role videoconferencing will play moving forward," Marc said, noting that supporting a hybrid workforce

will present new challenges. "Things keep on changing, and we're learning more about the virtual meeting space, trying to make it better. But we certainly don't expect to see an end to video calls. If anything, videoconferencing is going to be a substantial component of meetings, if not a complete necessity." 

Sandia poised to help lead national energy, homeland security efforts for coming decades

By **Michael Ellis Langley**

Arise in attention to the threats posed to national security is already proving the value of Sandia's Energy & Homeland Security portfolio.

The portfolio, which is managed by the Integrated Security Solutions Division based in Sandia's Livermore site, includes members from throughout the laboratories. One of five mission portfolios, Energy & Homeland Security focuses on securing "the nation's critical infrastructures and environment against attacks, threats, and climate change by performing world-class research and development."

"The E/HS portfolio is in great shape right now," said Associate Labs Director and Program Manager Andy McLlroy. "We are seeing strong demand for our work."

Andy added that as a DOE lab, and with our vital relationship with Department of Homeland Security, Sandia is the ideal partner to assist in national security.

"Both of these departments have a deep interest in the nation's critical infrastructures and the security of those systems," he said. "This really aligns well with our core capability of system engineering. We want to ensure resiliency and security and reduce the vulnerabilities of critical infrastructure. The portfolio is particularly well aligned with our country's future direction and is positioned to take on big challenges such as cybersecurity and climate change."

Making America's energy systems more resilient

Andy said that the formation of the Climate Change Security Center in January

was a crucial step in helping the nation understand climate change as well as the resilience and reliability of America's energy infrastructure. Sandia is exploring ways to protect vital systems from human interference and severe weather events, which are increasing in frequency and intensity because of climate change.

"We are looking at making energy systems more resilient from human threats and natural disasters," he said. "You can't talk about energy without also discussing the economics of the industry because the largest users are private citizens. So we are trying to figure out how to bake economic issues into our analysis."

Finding ways to safeguard the energy supply for the nation is just one part of the portfolio's transformational and emerging initiatives.

Demand for Sandia's cybersecurity expertise

Andy added that DHS in particular is asking Sandia to step up in a big way following a dramatic uptick in attacks upon the nation's systems — including holding cities and utilities like Colonial Pipeline for ransom.

"Cyber threats to the nation have accelerated and in the last year reached critical levels," said Cindy Veitch, program manager for cyber and critical infrastructure security. "Non-nation-state actors can now have nation-state-level impact in their attacks. We need to have a national understanding of critical digital-infrastructure connections and vulnerabilities."

Cindy said Sandia is working with DHS's Cybersecurity and Infrastructure Security Agency.

"Because of our relationships with the

Department of Defense and other sponsors, we bring threat-informed expertise to our cybersecurity R&D," she added. "This is a differentiating capability that enables us to help CISA, which is responsible for civilian cybersecurity and critical infrastructure. They trust Sandia as a partner and thought leader."

Cindy said hundreds of Sandians are working on more than 40 cybersecurity projects for CISA and that there is potential to significantly expand this set of projects over the next few years for an even greater impact on our nation's cybersecurity.


Detection of toxic drugs

Sandia is also helping the nation confront toxic synthetic opioids. Mechanical engineer Matt Moorman said some opioid analogs have the same level of toxicity as chemical warfare agents.

"The way to think about synthetic opioids is not as a drug of abuse but a toxic chemical compound. This is a national challenge," he said.

The drugs are being produced by chemical cartels that constantly modify and introduce new variations. Matt said Sandia is in the process of creating technologies — coupled with a library of cataloged drugs — that can analyze residue quickly to identify entire groups of synthetic opioids.

"Instead of trying to categorize all these different compounds, what if we could get a molecular fingerprint to categorize whole classes of synthetic opioids?" Matt said. "We can now detect the entire class with a few key molecular fingerprints."

In all of these ways and more the Sandians who work as part of the E/HS portfolio are helping America confront a host of threats to national security. 

Virtual volunteer events a silver lining in a year of uncertainty

By **Tatiana Del Cid**

Sandia is committed to serving our nation and supporting communities by promoting family stability and educational success, annually contributing \$1.4 million in corporate grants via impactful partnerships with local nonprofits in California and New Mexico.

In California alone, \$175,000 was awarded in fiscal year 2021 to nonprofit organizations working to ensure that all students and families have equitable opportunities and access so they can thrive. In addition to grant money, Sandia contributed passion and ingenuity through its many volunteers, magnifying the impact in the lives of the families and future STEM leaders served.

“Although this past year brought challenges and uncertainty, virtual functions were a silver lining,” said Kayla Norris, community relations specialist at Sandia’s California site. “We saw community volunteer opportunities move beyond geographical borders, resulting in an expanded impact of Sandia’s community outreach.”

“It was gratifying to see virtual interactions and collaborations between hundreds of students and families in California, New Mexico and across the country,” Kayla said, expressing appreciation for the generous contributions volunteers across the Labs made through their time, passion and talent.

Mentoring future leaders of innovation

Sandia showed support for future leaders of innovation through a wide variety of educational outreach opportunities.

In March 2021, eight volunteers from the Labs navigated a new online platform to participate in the virtual Alameda County Science and Engineering Fair. Sandians mentored more than 200 young scientists and future professionals as they presented their STEM projects.



EXPLORING STEM — The daughter of Debbie Senesky, associate professor of aeronautics and astronautics at Stanford University, enjoys a hands-on STEM activity during a March 2021 virtual Women’s History Month celebration organized by Sandia, Scientific Adventures for Girls and Stanford University.

Photo by Debbie Senesky

Volunteers also led virtual Women's History Month celebrations in March 2021. These energizing online gatherings kicked off with the Building the Future: Women in STEM event organized by Sandia, Scientific Adventures for Girls and Stanford University. More than 80 California and New Mexico families of elementary school students enjoyed virtual dance parties and STEM demonstrations about climate change. They also performed at-home experiments, constructing marshmallow geodesic dome crafts and exploring chemistry by making flubber soap.

Another March 2021 event brought together more than 300 high school and college students across America as they tuned in for Finding Your Path: Climate Action Careers. This inspiring online event featured Sandia and Department of Energy women panelists who shared about their careers in climate action impact.

In April 2021, Sandia volunteers led virtual innovation stations at the STEM Day for Girls PREP Activity. More than 30 middle school problem-solvers from California and New Mexico teamed together online while collaborating with seven Sandia and three Dublin High volunteers to solve a hypothetical bubonic plague scenario.

Promoting family stability by feeding those in need

Sandia has also consistently partnered with nonprofit organizations to support the nutritional needs of local communities.

Fertile Ground-Works in Livermore, Calif., hosted four Sandia Serves events at their community garden between October 2020 and January 2021. In total, almost 40 Sandia volunteers — including interns, staff and managers — barreled compost, prepared plant beds, cultivated seedlings and planted many types of vegetables. Their actions are helping Fertile GroundWorks grow 20,000 pounds of fresh produce yearly to feed families in need throughout the Bay Area.

Families in the California Central Valley have also been assisted by Sandia's community outreach efforts. In April 2021, ten Sandia volunteers helped the Second Harvest Food Bank in Manteca pack and

ship an estimated 1,083 meals to local families throughout the region.

Continuing to serve our local communities

“Looking back on a fruitful year of generous volunteering, Sandia is both proud and grateful for the heart and dedication

Sandians consistently bring to local community outreach events,” Kayla said.

Since nonprofits rely on the generosity of passionate volunteers to carry out many vital community functions, the Sandia Community Outreach team will continue to plan Sandia Serves and community outreach events in the future. [📷](#)



HARVESTING KINDNESS — Volunteers at Fertile GroundWorks in Livermore, Calif., help harvest fresh vegetables for families in need in the Bay Area. **Photo by Tatiana Del Cid**



PROVIDERS — Sandians and their families volunteered to help Second Harvest Food Bank in Manteca, Calif., provide food for people in need in San Joaquin County. **Photo by Tatiana Del Cid**

Protected raptors build nest at Livermore campus



KEEPING WATCH — A male Swainson's hawk guards his chick in their nest along East Street at the western parking lot. **Photo by Craig Taylor**

By **Trina West**

Sitting atop the trees and defending his nest from predators, the male hawk holds a fiercely protective gaze over his newborn chick.

The latest addition to Sandia/California's wildlife is the Swainson's hawk (*Buteo swainsoni*). A breeding pair of the raptors built their nest in a pine grove along the west parking lot this past April, and their chick subsequently hatched around May 26. The medium-sized birds are recognizable by their white bellies and brown bodies, which typically blend into their surroundings. To the untrained eye, the hawks look like large pinecones.

These feathered masters of disguise are living proof that nature is the ultimate magician — most people are unaware that a protected species is lodging just fifty feet above them.

Federally protected under the [Migratory Bird Treaty Act](#), the Swainson's hawk is listed by the [California Department of Fish and Wildlife](#) as a threatened species. While both California and the U.S. government prohibit the illegal taking of a hawk, additional protections regarding the hawk's nest and habitat are enforced solely by the Department of Fish and Wildlife.

Biologists from Lawrence Livermore National Laboratory first reported the presence of the hawks, and a biologist from Condor Country Consulting is under contract with Sandia to monitor the birds' stress levels. Nearby construction on-site has been halted occasionally to prevent disturbing the hawks as their chick develops its wing feathers. After the chick is fully fledged and ready for flight, a process that takes approximately 44 days, the hawks are expected to remain in the area for several weeks before migrating south.

According to the consulting biologist, the hawks will migrate in late August, after which Sandia's Environment, Safety and Health department will develop a monitoring plan to survey future activity at the site of the nest. It is unlikely that the California Department of Fish and Wildlife will grant the removal of the nest if any of the birds return, noting that the young hawk may come back if the nest is still accessible.

The family of Swainson's hawks has been drawing interest from local bird-watchers. Stephanie Klein, a member of the Talon Ecological Research Group, stated during a July 1 visit, "This is the first [Swainson's hawk] nest we've ever recorded in Alameda County."

Move over, Thunderbird; there's a new chick in town. [📷](#)



LOOKOUT — A Swainson's hawk rests at the top of a tree on the Livermore campus, keeping an eye on everyone below.

Photo courtesy of Condor Country Consulting



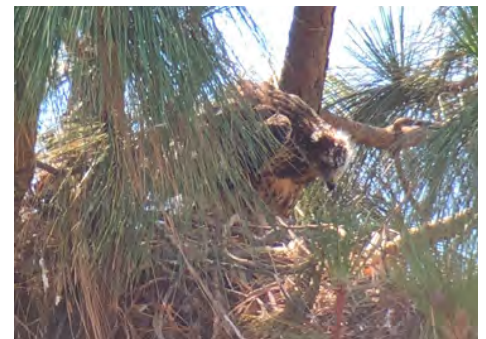
EYE ON THE SKY — Condor Country Consulting, contracted by Sandia to observe the nesting Swainson's hawks and make sure they were not disturbed, set up an observation post on East Street.

Photo courtesy of Condor Country Consulting



FRESH OUT OF THE EGG — The recently hatched Swainson's hawk chick in its nest on June 25.

Photo by Craig Taylor



READY TO FLY — The Swainson's hawk chick, with more developed plumage, on July 6.

Photo by Craig Taylor