B61-12 production begins

5,000 Sandia employees worked to qualify bomb

By **Kristen Meub**

Sandia marked a major milestone when the nuclear security enterprise successfully produced the first completely refurbished bomb for the B61-12 Life Extension Program in November 2021.

"This is the first complete unit built with nuclear and non-nuclear components that has been fully qualified from the ground up," said David Wiegandt, a Sandia senior manager on the B61-12 program. "The first production unit is the first war reserve B61-12 built at Pantex that meets all customer requirements and is acceptable for use by the U.S. Air Force."

More than 5,000 employees have worked on the B61-12 program at Sandia during the last decade.

"Sandia's role within the complex is unique," said Jim Handrock, Sandia Weapons Systems Engineering director. "We have the design engineering responsibility for the non-nuclear components, and also the key systems integration role to put all the individual parts together to make sure that everything does what needs to be done to provide the full system to the customer."

As part of the program, Sandia worked to refurbish, replace or reuse about 50 different components and subsystems that make up the B61-12.

"In addition to design development, we completed the highly rigorous qualification, verification and validation testing to demonstrate that the B61-12 will always work with high reliability when authorized and never function under any other conditions," David said.

TEST PREPARATION — Sandia technologists Curt Tenorio, left, and Jessie Fowler install instrumentation on a B61-12 test unit for a vibration and shaker-shock test in a photo from 2014.
Photo by Randy Montoya from the archives

Improved nuclear accident code helps policymakers assess risks from small reactors

Sandia expands software to support regulators' evaluation of next-generation reactors

By **Mollie Rappe**

BEYOND THE FENCE — Sandia nuclear engineers Jenn Leute, left, and Dan Clayton stroll outside the Annular Core Research Reactor. Recently they updated a consequence assessment code so that it can model the health and economic impacts of an unlikely accident practically to a facility's fence.
Photo by Randy Montoya

Sandia recently updated the Maccs code to better aid the Nuclear Regulatory Commission and the global nuclear industry in assessing the consequences of nuclear accidents. The Maccs code can also evaluate the potential health and environmental risks posed by advanced nuclear reactors and small modular nuclear reactors.

Small modular reactors range from scaled-down conventional nuclear reactors with modern safety features to completely

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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: Please send your comments and suggestions for stories or for improving the paper. If you have a column (500-800 words) or an idea to submit, contact Lab News editor Katherine Beherec at kgbeher@sandia.gov.

Algorithm could shorten quality testing, research in many industries by months

Machine learning used to predict direction-dependent mechanical properties of metals

MAD SCIENTISTS — Sandia researchers David Montes de Oca Zapiain, left, and Hojun Lim examine data generated by the machine-learning algorithm Material Data Driven Design.   **Photo by Bret Latter**

By **Troy Rummler**

A machine-learning algorithm developed at Sandia could provide auto manufacturing, aerospace and other industries a faster and more cost-efficient way to test bulk materials.

The technique was published recently in the scientific journal **Materials Science and Engineering: A**.

Production stoppages are costly. So, manufacturers screen materials like sheet metal for formability before using them to make sure the material will not crack when it is stamped, stretched and

B61-12 milestone

The B61, a nuclear gravity bomb deployed from Air Force and North Atlantic Treaty Organization bases, has been in service since 1968. The B61-12 will replace most older modifications of the B61 and have an extended service life of at least 20 years. The life extension program addresses all known age-related concerns found within the nation's stockpile of B61 weapons, upgrades encryption algorithms, modernizes the safety and use-control features of the weapon and supports compatibility with future aircraft designs.

Sandia, Los Alamos National Laboratory and Boeing are the design agencies responsible for the design and engineering of the B61-12, with Sandia also producing custom electronics. Additional production activities are performed at Kansas City National Security Campus, Y-12 National Security Complex, the Savannah River Site and the Pantex Plant.

The refurbished B61-12 is set to begin full-scale production in May, with completion expected in 2026.

Design, testing and aircraft compatibility

The program began with a concept phase in which the team developed various weapon architectures that would meet NNSA and Air Force requirements. After the design was stabilized, the team started to develop and produce the individual components that go into the weapon, then spent several years integrating those components into systems, and then tested them and made modifications and refinements as necessary. After about three design cycles, the team reached the final design, Matt Kerschen, a Sandia manager on the B61-12, said.

Matt described a couple firsts for the program, including integrating an Air Force supplied tailkit assembly that guides the bomb to its target location and implementing a new digital interface between the bomb and the aircraft flying it.

Another key part of the program was the development and qualification testing

of the bomb. Sandia completed a series of tests determining how the refurbished B61-12 would handle temperature, shock, vibration, radiation, humidity and more throughout its extended lifetime.

"We spent multiple years qualifying the design by running a series of laboratory and ground tests where we built up full-scale mock bombs and subjected them to a lifetime of environments and then subsequently functioned in them," Matt said.

Sandia also coordinated with the Air Force Nuclear Weapons Center to test compatibility between the B61-12 and the different aircrafts that will be capable of deploying it, Rich Otten, a Sandia senior manager on the B61-12, said.

"It starts with on-the-ground evaluations of the electrical system to ensure the B61-12 communicates with the aircraft and usually concludes with a flight test at Tonopah Test Range," Rich said. "We learn a lot from both flight and ground tests. We want to make sure we understand everything before we fly, and a flight test is a final proof that in the combined environments the B61-12 operates as expected."

Exceptional service in the national interest

Jim, who has led the B61-12 program at Sandia for 11 years, said the scope of the program presented challenges and opportunities that helped the Labs rejuvenate its weapons modernization capabilities.

"Sandia hadn't had this level of work in a modernization program for two decades, so there was a lot of work to relearn and reconstitute this capability," Jim said. "We instituted earned-value management at a level that had never been done before on a nuclear weapons system, we built up an assembly operation the lab hadn't seen in decades and set up environmental testing facilities important for the success of the program."

Jim said participation in successful flight and lab tests were great growth opportunities for staff in terms of learning how to realize weapons systems, and that the commitment of the staff was critical to the success of the program.

"For a lot of people, it's been a significant commitment, both professionally and personally, to be able to get this work

UNDER PRESSURE — In a photo from 2014, Sandia's Ryan Schultz adjusts a microphone for an acoustic test on a B61-12 system. The unit is surrounded by banks of speakers that expose it to an acoustic field. The sound pressure reaches 131 decibels, similar to a jet engine.
Photo by Randy Montoya from the archives

done in the timeframe and manner that the nation needs. Everybody who has worked on this program is to be commended for the efforts, contributions and sacrifices they've made to make it successful."

Matt has worked on the B61-12 at Sandia since the program began. He said he has stayed on the program because he believes the work is important for the security of the nation and the engineering challenges have been exciting to solve.

"It's been a once-in-a-career type of experience," Matt said. "When you can take a concept for a weapon that you developed on paper and presentation slides, and then be able to turn that into

actual hardware that functions as designed, that's really rewarding."

Matt recalled the first end-to-end laboratory test and the first flight during the program as being big accomplishments on the way to the first production unit milestone.

"We worked together for years wringing out all of the bugs in the system in the lab before we got to that first flight test off of an F-15E," Matt said. "There was a huge sense of accomplishment for the entire team to see everything we've worked on finally come together and function as designed. There's been a lot of examples like that on the program, where the team is working to accomplish a major milestone for a long period of time and then that tremendous sense of accomplishment when you finally get there."

For David, working on the B61 runs in the family. His father, Karl Wiegandt, started working at Sandia in 1968 and supported B61 modifications — believed to be B61-1 — as his first program out of school. He performed mechanical drafting for flight test sensing and the handling equipment, or H-Gear, before moving to another weapon system.

"There's something really special about this program, the people, the morale and the legacy," David said. "It has really solid team members who believe in how to do sound engineering and really bring the future of safety and security into modern nuclear weapons. That culture is infectious and has drawn a lot of people to it."

Rich said he's proud of the work the team, current and past members, has done to achieve this milestone and modernize the B61 for the nation.

"This is a critical element of the nation's nuclear deterrent, and I'm proud to be part of the team delivering on the common goal of completing the first production unit," Rich said. "This is not an end; it's the beginning of production. We've designed, tested and proved this completely refurbished B61, and now it's ready for the transition to full-scale production."

DAVIS GUN — In a photo from 2015, Tyler Keil, Sandia lead engineer for an impact test series using Sandia's Davis gun, performs a final diagnostics check on a data recorder for an impact test on the nose assembly of a mock B61-12, mounted on an aluminum tube to replicate the body of the bomb. Data gathered from the test is helping analysts calibrate computer models.

Photo by Randy Montoya from the archives

Improved nuclear

innovative designs that use different cooling methods and fuel designs. Some could even be constructed at a central facility and transported to wherever reliable carbon-neutral electricity is needed.

Previously, Maccs was not recommended for modeling consequences closer than five football fields from the reactor. The improved Maccs can now model consequences starting much closer to the reactor building as well as provide options to improve the model's results out to 1,000 miles.

"Advanced reactors and small modular reactors are expected to be smaller, therefore leading to an expectation of lower radioactive releases in the case of an accident," said Jenn Leute, a Sandia nuclear engineer who is working on the Maccs updates. "With this expectation that releases will be lower, we want to ensure we can model much closer to the point of release, as understanding consequences closer in will become more important. This will allow for decision-makers to make the most informed decisions about new plants and mitigate these very unlikely consequences."

Smaller reactors require refined code

Maccs is used by the Nuclear Regulatory Commission and the nuclear industry worldwide to assess the environmental impact for new and existing nuclear power plants, Jenn said. The system is also used for assessing the risks of licensing new reactors, especially next-generation nuclear reactors, and informing the industry and regulators about decisions on upgrading existing power plants.

"We, essentially, look at what happens outside the building in the case of an accident at a nuclear power plant, and we model how any radioactive material released moves through the atmosphere and environment," Jenn said. "We look at where the radioactive material goes and any type of radiological health effects and economic effects."

Small modular reactors are expected to take up to one-tenth or less of the area of current nuclear power plant, while producing about one-quarter to one-eighth of the carbon-neutral electricity of a current nuclear power plant, said Dan Clayton, another Sandia nuclear engineer

involved in updating Maccs. Additionally, advanced reactors will be even safer than previous generations of nuclear reactors, taking 60 years' worth of experience and technological improvement into account.

Many of these new advanced reactors are fundamentally different than existing light-water reactor designs. The Nuclear Regulatory Commission understands it would be inefficient to review these reactors against existing criteria for light-water reactors. The agency is developing new regulations to support a risk-informed, technology-inclusive regulatory framework for advanced reactor licensing, said John Fulton, manager for Sandia's department that supports the commission's Maccs modeling efforts. The commission is investigating how Maccs and other tools can help set risk-informed safety criteria that are based on specific consequences, such as the radioactive dose a person is projected to receive being within a certain area during and after an accident.

To help the commission with these more targeted assessments, the Sandia team has been improving Maccs' atmospheric models, economic models and the ability to model close-in since 2016.

New atmospheric model aids health impact assessments

One way Maccs can aid members of the nuclear industry is by determining the health effects of a potential accident on the public. These effects include the radioactive dose a population within a certain area of the proposed or existing reactor would receive, the risk of acute radiation poisoning and what the dose would mean for the population's lifetime risk of cancer.

Maccs can do these assessments based on an assumed population density and average weather conditions, if, say, the location for a proposed reactor isn't finalized, Jenn said. Or Maccs can also do these consequence assessments for a very specific location — using actual weather and population data for that location, she added.

One significant improvement from the Sandia team's five-year effort involves modeling the health effects of an accident.

Maccs can now utilize a new model of how particles move in the air, said Dan, who has been heavily involved in these improvements.

"HYSPLIT is the gold-standard model for 4D atmospheric transport — so up-down, left-right, forward-back and through time," John said. "It's highly detailed and provides the ability to accurately model larger distances. It also allows us to look at fine meteorological details like sea breezes or the valley flow effect. With small modular and advanced reactors, those localized effects are expected to have greater influence on accident impacts. Having HYSPLIT as part of Maccs is a massive step forward in being able to capture these fine-resolution atmospheric flows which will be critical to addressing environmental impacts."

This atmospheric model allows researchers and regulators to look at how radioactive material would move after an accident under very specific weather conditions, or a random representative collection of weather conditions, Dan said. This is just one example of how Maccs can provide answers, even if there is uncertainty in weather conditions.

Adding GDP to refine economic impacts

Another way Maccs can aid decision-making at the Nuclear Regulatory Commission and other regulators is by determining the economic impacts of a potential accident.

Prior to last year, Maccs would add up the costs for evacuating and relocating the people within a certain area, as well as the cost to get rid of affected crops and clean up the affected land and water, Jenn said.

Now, Maccs can also estimate the Gross Domestic Product-based losses caused by a potential accident — again for either a general area in the contiguous U.S. or for a specific location — and include that in the assessment. This improvement was led by Sasha Outkin, a Sandia systems analyst.

Maccs can also use the atmospheric transport results and a food chain model to aid regulators in determining the impacts of farmland contamination after an accident.

Over the past few years, the team also added a tool to turn Maccs' simulations into movies or images to better visualize and share the results, Dan said.

These visualization tools ensure decision-makers have a full picture of the economic and environmental consequences of a highly unlikely accident at a nuclear power plant. This should allow a more complete comparison of potential new plants' benefits from reliable carbon-neutral electricity and their potential risks, and for refined planning and mitigation strategies for existing plants.

"Maccs models what could happen in an accident," Dan said. "This helps the Nuclear Regulatory Commission determine whether the reactor design meets current regulations. By using Maccs for these analyses, the commission can assess what could happen so that they can make an informed decision if the reactor will meet regulatory safety requirements. These improvements will help existing analyses and assessments for new reactors."

Recent Patents

October–December 2021

- **Andrea Ambrosini and Eric Nicholas Coker:** Redox-active oxide materials for thermal energy storage. Patent #10800665

- **David W. Raymond:** Systems and methods that use harmonic drives for converting reciprocating axial motion to continuous rotary motion, helical drives for converting reciprocating rotary motion to reciprocating axial motion. Patent #11143275

- **Timothy Briggs, Stacy Michelle Nelson and Brian T. Werner:** Enhanced composites via selective interfacial modification. Patent #11148392

- **Adam Cook:** Self-assembly assisted additive manufacturing of thermosets. Patent #11149108

- **Christopher Todd DeRose, Michael Gehl, Randolph R. Kay and Daniel Lynn Stick:** Trapped ion platform with optical input and output. Patent #11150609

- **Gabriel Carlisle Birch, Amber Lynn Dagel, John Clark Griffin, Christian Turner and Bryana Lynn Woo:** Computational optical physical unclonable function. Patent #11151263

- **Bryan James Kaehr:** Polarization-based coding/encryption using organic charge-transfer materials. Patent #11151345

- **Jeffrey P. Koplow:** Low modulation index 3-phase solid state transformer. Patent #11152918

- **Jiann-CherngSu:** Multilayer solid lubricant architecture for use in drilling tool applications. Patent #11156033

- **Avery Ted Cashion IV, William Corbin and Ryan Falcone Hess:** Systems, methods and tools for subterranean electrochemical characterization and enthalpy measurement in geothermal reservoirs. Patent #11156583

- **Michael Gehl:** Optical coupler for heterogeneous integration, Patent #11163115

- **Laura Butler Biedermann, Michael Hibbs, David R. Wheeler and Kevin R. Zavadil:** Filtration membranes. Patent #11167250

- **Darren W. Branch, DeAnna Marie Campbell and Bryan Carson:** Active shunt capacitance cancelling oscillator for resonators. Patent #11171604

- **Matt Eichenfield and Daniel Beom Soo Soh:** Remote quantum state transfer for qubits with different frequencies. Patent #11177890

- **Ryan Wesley Davis and Sungwhan Kim:** Algal harvesting and water filtration. Patent #11186507

- **Gregory O'Bryan:** Surface treatment of ultra-high molecular weight polymers. Patent #11186945

- **Robert J. Anderson and Tian J. Ma:** Multi-frame moving object detection system. Patent #11188750

- **John Monson and Irfan Nadiadi:** Locking side pull hoist ring assembly. Patent #11192760

- **Leonard E. Klebanoff and Vitalie Stavila:** Ternary borides and borohydrides for hydrogen storage and method of synthesis. Patent #11192783

- **Ryan Wesley Davis:** Fatty acid derived alkyl ether fuels for compression ignition. Patent #11193075

- **Harlan James Brown-Shaklee, Christopher Hammetter and Timothy Walsh:** Additively manufactured locally resonant interpenetrating lattice structure. Patent #11195504

- **Peter A. Knee:** Systems and methods for electronic communication with a device using an unknown communications protocol. Patent #11196611

- **John Curry, Michael T. Dugger and Brendan L. Nation:** Friction testing and torque sensing systems. Patent #11199485

- **Leah Appelhans, Douglas Read, David R. Wheeler and Joshua J. Whiting:** Functionalized coating polymers and uses thereof. Patent #11203702

- **Nelson S. Bell, Jessica Nicole Kruichak, Edward N. Matteo, Melissa Marie Mills, Amanda Christine Sanchez and Yifeng Wang:** Sorption agent, method of making a sorption agent and barrier system. Patent #11207658

Note: Patents listed here include the names of active Sandians only; former Sandians and non-Sandia inventors are not included.

Following the listing for each patent is a patent number, searchable at the U.S. Patent and Trademark Office website (uspto.gov).

Truman and Hruby 2022 postdocs advance to their positions

Prestigious awards allow unusual freedom in research investigations

By **Neal Singer**

Postdoctoral students who are designated Truman and Hruby fellows tend to experience Sandia differently from other postdocs.

Appointees to the prestigious fellowships are given the latitude to pursue their own ideas, rather than being trained by fitting into the research plans of more experienced researchers. To give wings to this process, the four annual winners — two for each category – are 100 percent prefunded for three years. This enables them, like bishops or knights in chess, to cut across financial barriers, walk into any group and participate in work by others that might help illuminate the research each has chosen to pursue.

This year's Truman postdocs are Alicia Magann, who is working to create a quantum information science toolkit, and Gabriel Shipley, who is working to mitigate instabilities at Sandia's Z machine. The 2022 Hruby fellows are Sommer Johansen, who will be experimenting at Sandia/California's Combustion Research Facility, and Alex Downs, who wants to create wearable biosensors.

The extraordinary appointments are named for former President Harry Truman and former Sandia president Jill Hruby, now the DOE undersecretary for nuclear security and administrator of the NNSA.

Truman, who wrote to the president of Bell Labs that he had an opportunity, in managing Sandia in its very earliest days, to perform "exceptional service in the national interest," wrote words the Labs have repurposed over the following seven decades to in effect apply to each member of the workforce. The **Truman Fellowship program** could be said to assert Sandia's intention to continually fulfill Truman's hope.

The **Hruby Fellowship**, which offers the same pay, benefits and privileges as the Truman, honors Hruby, the first woman to direct a national laboratory. While "all qualified applicants will be considered for this fellowship," and its purpose is to pursue independent research to "develop advanced technologies to ensure global peace," reads the program's description, another aim is to develop a cadre of women in the engineering and science fields who are interested in technical leadership careers in national security.

Alicia Magann: The quantum information science toolkit

To help speed the emergence of quantum computers as important research tools, Alicia is working to create a quantum information science toolkit. These modeling and simulation algorithms should enable quantum researchers to "hit the ground running with meaningful science" as quantum computing hardware improves, she said.

Her focus will extend aspects of her doctoral research at Princeton University to help explore the possibilities of quantum control in the era of quantum computing.

At Sandia, she will be working with the quantum computer science department to develop algorithms for quantum computers that can be used to study the control of molecular systems.

"I'm most interested in probing how interactions between light and matter can be harnessed towards new science and technology," she said. "How well can we control the behavior of complicated quantum systems by shining laser light on them? What kinds of interesting dynamics can we create, and what laser resources do we need?"

A big problem, she said, is that "it's so difficult to explore these questions in much detail on conventional computers. But quantum computers would give us a much more natural setting for doing this computational exploration."

Her mentor at Sandia, Mohan Sarovar, is "an ideal mentor because he's knowledgeable about quantum control and quantum computing — the two fields I'm connecting with my project."

During her doctorate, she was a DOE Computational Science Graduate Fellow and also served as a graduate intern in Sandia's

TRUMAN FELLOWS — During her fellowship, Alicia Magann, left, will explore the possibilities of quantum control in the era of quantum computing. Gabriel Shipley, who broadened the use of Mykonos, a small pulsed power machine, in a past internship, plans to investigate the origins and evolution of 3D instabilities in pulsed-power-driven implosions at Sandia's powerful Z machine.

Photos courtesy of Alicia Magann and Gabriel Shipley

extreme-scale data science and analytics department, where she heard by word of mouth about the Truman and Hruby fellowships. She applied for both, was "thrilled to be interviewed and thrilled to be awarded the Truman."

Technical journals in which her work has been published include Quantum, Physical Review A, Physical Review Research, PRX Quantum and IEEE Transactions on Control Systems Technology. One of her most recent 2021 publications is "Digital Quantum Simulation of Molecular Dynamics & Control" in Physical Review Research.

Gabriel Shipley: Mitigating instabilities at Sandia's Z machine

When people mentioned the idea to Gabe about applying for a Truman fellowship, he scoffed. He hadn't gone to an Ivy League school. He hadn't studied with Nobel laureates. What he had done, by the time he received his doctorate in electrical engineering from the University of New Mexico in 2021, was work at Sandia for eight years as an undergraduate student intern from 2013 and a graduate student intern since 2015. He didn't feel that service would measure up against projects with more obvious appeal.

"The candidates for the Truman are rock stars," Gabe told Sandia colleague Paul Schmit. "When they graduate, they're offered tenure track positions at universities."

Paul, himself a former Truman selectee and in this case a walking embodiment of positive reinforcement, advised, "Don't sell yourself short."

That was good advice. Gabe needed to keep in mind that as a student, he led 75 shots on Mykonos, a relatively small Sandia pulsed-power machine, significantly broadening its use. "I was the first person to execute targeted physics experiments on Mykonos," he said. He measured magnetic field production using miniature magnetic field probes and optically diagnosed dielectric breakdown in the target.

He used the results to convince management to let him lead seven shots on Sandia's premier Z machine, an expression of confidence rarely bestowed upon a student. "I got amazing support from colleagues," he said. "These are the best people in the world."
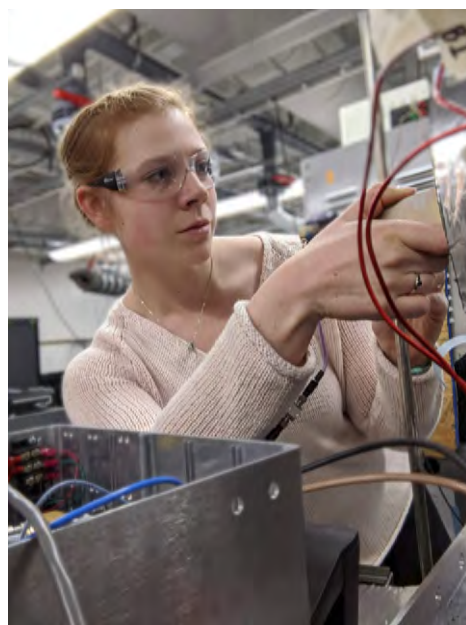
Among them is theoretical physicist Steve Slutz, who theorized that a magnetized target, preheated by a laser beam, would intensify the effect of Z's electrical pulse to produce record numbers of fusion reactions. Gabe has worked to come up with physical solutions that would best embody that theory.

With Sandia physicist Thomas Awe, Gabe developed methods that may allow researchers to scrap external structures called Helmholtz coils to provide magnetic fields and instead create them using only an invented architecture that takes advantage of Z's own electrical current.

His Truman focus — investigating the origins and evolution of 3D instabilities in pulsed-power-driven implosions — would ameliorate a major problem with Z pinches if what he finds proves useful. Instabilities have been recognized since at least the 1950s as weakening pinch effectiveness. They currently limit the extent of compression and confinement achievable in the fusion fuel. Clearly, mitigating their effect would positively affect Z-pinch research worldwide.

Gabe has authored articles in the journal Physics of Plasmas and provided invited talks at the Annual Meeting of the APS Division of Plasma Physics and the ninth Fundamental Science with Pulsed Power: Research Opportunities and User Meeting. His most recent publication in Physics of Plasmas — "Design of Dynamic Screw Pinch Experiments for Magnetized Liner Inertial Fusion" — represents another attempt to increase Z machine output.

Sommer Johansen: Where's the nitrogen?

Sommer Johansen received her doctorate in physical chemistry from the University of California, Davis, where her thesis involved going backward in time to explore the evolution of prebiotic molecules in the form of cyclic nitrogen compounds; her time machine consisted of combining laboratory spectroscopy and computational chemistry to learn how these molecules formed during the earliest stages of our solar system.

"Cyclic nitrogen-containing organic molecules are found on meteorites, but we have not directly detected them in space. So how were they formed and why haven't we found where that happens?" she asked.

That work, funded by a NASA Earth and Space Science Fellowship, formed the basis of publications in The Journal of Physical Chemistry and resulted in the inaugural Lewis E. Snyder Astrochemistry Award at the International Symposium on Molecular Spectroscopy. The work also was the subject of an invited talk she gave at the Harvard-Smithsonian Center for Astrophysics Stars & Planets Seminar in 2020.

At Sandia, she intends to come down to Earth by experimenting at Sandia's Combustion Research Facility in Livermore on projects of her own design.

She hopes to help improve comprehensive

HRUBY FELLOWS — Sommer Johansen, left, aims to improve models that demonstrate how burning bioderived fuels affect the Earth's planetary ecology and severe forest fires caused by climate change. Alex Downs hopes to create wearable biosensors that gather real-time molecular measurements from health markers and would lessen the need to visit doctors' offices and labs for evaluations.

Photos courtesy of Sommer Johansen and Alex Downs

chemical kinetics models of the aftereffects on Earth's planetary ecology of burning bioderived fuels and the increasingly severe forest fires caused by climate change.

"Every time you burn something that was alive, nitrogen-containing species are released," she said. However, the chemical pathways of organic nitrogen-containing species are vastly underrepresented in models of combustion and atmospheric chemistry. "We need highly accurate models to make accurate predictions. For example, right now it isn't clear how varying concentrations of different nitrogenated compounds within biofuels could affect efficiency and the emission of pollutants," she said.

Sommer will be working with the gas-phase chemical physics department, studying gas-phase nitrogen chemistry at Sandia/California under the mentorship of Lenny Sheps and Judit Zádor. "UC Davis is close to Livermore, and the Combustion Research Facility there was always in the back of my mind. I wanted to go there, use the best equipment in the world and work with some our field's smartest people."

She found particularly attractive that the Hruby fellowship not only encouraged winners to work on their own projects but also had a leadership and professional development component to help scientists become well-rounded. Sommer had already budgeted time outside lab work at UC Davis, where for five years she taught or helped assistants teach a workshop for incoming graduate students on the computer program Python.

"We had 30 people a year participating, until last year, when we went virtual, and had 150."

The program she initiated, she said, "became a permanent fixture at my university."

Alex Downs: Long-lived wearable biosensors

As Alex completed her doctorate at the University of California, Santa Barbara in August, she "liked" Sandia on LinkedIn. The Hruby postdoc listing "happened to show up," she said, and it interested her. She wanted to create wearable biosensors for long duration, real-time molecular measurements of health markers that would be an ongoing measurement of a person's well-being. This would lessen the need to visit doctors' offices and labs for evaluations that were not only expensive but might not register the full range of a person's illness.

Her doctorate thesis title was "Electrochemical Methods for Improving Spatial Resolution, Temporal Resolution, and Signal Accuracy of Aptamer Biosensors."

She thought, "There's a huge opportunity here for freedom to explore my research interests. I can bring my expertise in electrochemistry and device fabrication and develop new skills working with microneedles and possibly other sensing platforms."

That expertise is needed because a key problem with wearable biosensors is that on the body, they degrade, she said. To address this, Alex wants to study the stability of different parts of the sensor interface when it's exposed to bodily fluids, like blood.

"I plan not only to make the sensors longer lasting by improved understanding of how the sensors are impacted by biofouling in media, I will also investigate replacing the monolayers used in the present sensor design with new, more fouling resistant monolayers," she said.

The recognition element for this type of biosensor are aptamers — strands of DNA that bind specifically to a given target, such as a small molecule or protein. "When you add a reporter to an aptamer sequence and put it down on a conductive surface, you can measure target binding to the sensor as a change in electrochemical signal," she said.

The work fits well with Sandia's biological and chemical sensors team, and when Alex came to Sandia in October, she was welcomed with coffee and donuts from her mentor Ronen Polsky, an internationally recognized expert in wearable microneedle sensors. Ronen introduced her to other scientists, told her of related projects and discussed research ideas.

"Right now, meeting with people all across the Labs has been helpful," she said. "Later, I look forward to learning more about the Laboratory Directed Research and Development review process, going to Washington, D.C. and learning more about how science policy works. But right now, I'm mainly focused on setting up a lab to do the initial experiments for developing microneedle aptamer-based sensors," Alex said.
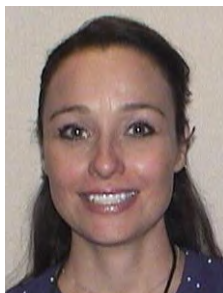
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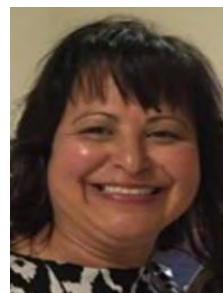
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Mathematician proud to help climate security studies

By **Michael Ellis Langley**

Sandia applied mathematician Khachik Sargsyan has brought his mind to bear on problems involving combustion, fusion and chemical kinetics — specifically from the viewpoint of probability modeling and quantifying uncertainties in physical systems.

Khachik is now turning his expertise to climate security.

"I am developing algorithms to improve model predictions in light of observational data," he said. "These are not the weather predictions that we see on media every day, but rather climate trends on decadal scales. The exploding field of machine learning, fueled by traditional statistical methods, helps us tune climate models and provide quantifiable estimates of risks and uncertainties under various scenarios."

And in climate change, there can be a lot of uncertainty. When considering just the nation, the many climates, carbon absorption of different species of plant life and the climate change impact of different industries are just some of the sources of data climatologists must take into account.

"Simulating complex climate models under multiple scenarios helps draw conclusions augmented with confidence estimates," Khachik said.

DATA MINER — Applied mathematician Khachik Sargsyan is helping climate scientists analyze climate models. **Photo courtesy of Khachik Sargsyan**

Khachik is doing uncertainty quantification for the Energy Exascale Earth System Model, DOE's flagship climate model, assisting climate scientists from Oak Ridge, Lawrence Berkeley, Pacific Northwest and Argonne national laboratories in their efforts to improve predictability of the land model.

"The algorithm helps them optimally create parameter settings and scenarios so they can run multiple simulations that inform the data in the most efficient way," Khachik explained.

Data from observational campaigns and accurate model simulations can help decision-making and potentially inform national policy.

"We are far from comprehensive understanding of all of these models — land model, for example, looks at CO_2 uptake, vegetation impact and biogeochemistry on climate systems, involving a variety of complex physical phenomena and modeling assumptions," he added.

Khachik describes himself as a "math person" who derives personal satisfaction when things on paper are justified by numerical simulations, leading to results that benefit his colleagues. He is happy to do his part to help not just a Sandia priority but the threat of climate change.

"Part of me thinks this is leading to improvements in some small corners of the climate modeling community, improving the models, steering toward better data which can potentially lead to better decisions," Khachik said. "It makes you proud that you are part of that."

Scientists and engineers inspire STEM learning in local high school forums

Speaker series born out of collaboration with Sandia Women's Connection

By **Paul Rhien**

Math and science students at two California high schools are making connections between their classroom learning and future careers in science, technology, engineering and math thanks to volunteers from Sandia's Livermore site.

Each spring, the Sandia Women's Connection recognizes young women from area high schools for their outstanding accomplishments in math and science. After last year's recognition event, teachers from Amador Valley High School in Pleasanton and Mountain House High School near Tracy, California approached the Labs about the possibility of bringing Sandia scientists and engineers to speak to students in their classrooms.

Sandia Women's Connection volunteer Helena Jin responded to their request by organizing the "Multivariable Calculus Forum" at Amador Valley High School. The forum features six Sandia research scientists who will give classroom presentations throughout the school year about how they are applying calculus and advanced math in the various engineering fields. Sandia volunteers participating in the Amador Valley forum include Neil Cole-Filipiak, David Couch, Francesco Di Sabatino, Kimberley MacDonald, Rajavasanth Rajasegar and Maher Salloum.

Through these partnerships, students realize the application of the principles they are learning and get a better understanding of future career interests and how to better prepare for college and post-graduate success, said Gauri Reyes, a math teacher at Amador Valley High School. These are lessons typically not provided by the standard high school math and science curriculum, Reyes said.

"When I tell my students that 'math is everywhere' and 'you will use this stuff in the future,' they dismiss me. After all, that is what all math teachers are supposed to say," Reyes said. "But when a scientist from a national laboratory doing cutting edge research says the same thing, the students listen. After these guest talks, students tend to engage more in the fundamental math lessons we discuss in our day-to-day work in class. It's a winning situation for all involved and furthers the students' education."

In the "STEM Innovator Speaker Series" at Mountain House High School, Sandia experts Christopher Blackstone, Diana Hackenburg, James Siacunco and Elizabeth "Bette" Webster are sharing their professional experience with students, helping them get a glimpse of "a day in the life of a scientist" and explore possible careers. Each session covers a different area of STEM such as chemistry, engineering, biology and environmental science.

The objective of the series is to inspire high school students to reach beyond the classroom and learn about real-world STEM applications by meeting and learning from professionals in fields they might consider for their future careers, explained Donna Earle, science department chair at Mountain House High School.

"As most adults will admit, they had no idea in high school what different career fields might have in store," Earle said. "Giving students a snapshot of life outside of high school is beneficial on a variety of levels."

"It's been awesome to pair speakers who have expertise in the curriculum that I'm currently teaching and for students
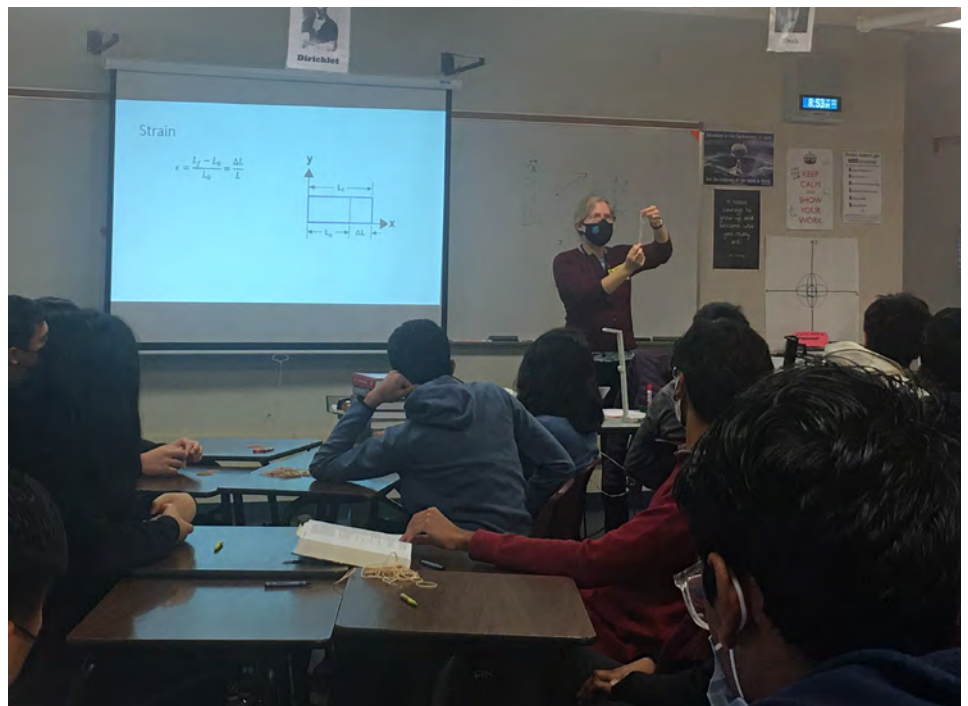
STEM SPEAKER SERIES — Sandia mechanical engineer Kimberley MacDonald gives a guest lecture to multivariable calculus students at Amador Valley High School in Pleasanton.

Photo courtesy of Gauri Reyes

to hear something from a professional in an area they just learned about in the classroom," Earle said.

Students have reacted positively to the guest speaker presentations.

"Scientists are really fun people to interact with. They are really passionate about what they are doing, which is very exciting," said Amador Valley senior Richard Li. "It's important to have local mentors because they provide concrete evidence that the concepts we learn in math class are actually being used."

Mentorship and community outreach are important to many Sandia employees, described Chris Blackstone, a physical chemist participating in the Mountain House STEM forum.

"I see the opportunity to communicate with and educate the public — students in particular — to be an essential component of my job," Chris said. "If students are considering careers in STEM, it's important that they know that people working in STEM are just ordinary people who simply focus their efforts on answering interesting and often complicated questions."

High school students are under a lot of pressure, said mechanical engineer James Siacunco.

"Students are often worried about their ability to succeed, and some guidance and reassurance can go a long way," James said. "I hope the students can feel confident making big life choices and know that there is not just one way to a satisfying career. They are seeing a wide variety of paths that we took to arrive at our careers and hopefully can feel less afraid of making a mistake and more able to enjoy the educational process."

Sandia researchers update software tool for wind turbine blades

By **Kelly Sullivan**

Researchers from Sandia's wind energy program have released a new version of the software tool Numerical Manufacturing and Design, or NuMAD, for the structural design and modeling of wind turbine blades.

NuMAD version 3.0, which was funded by DOE's Wind Energy Technologies Office, is an object-oriented, open-source software program written in the MATLAB programming language that simplifies the process of creating a 3D model of a wind turbine blade. The tool manages all blade information, including aerodynamic properties, material properties and material placement. Blade data can be modified by

a structural optimizer in NuMAD, or it can be used to run other tools in a stand-alone mode.

When used in conjunction with these other tools, NuMAD can provide computation of blade cross-section properties, various structural analyses and estimation of blade aeroelastic instability.

"Automation summarizes the capabilities of the new version," said project lead Ernesto Camarena. "The newly released NuMAD is structured to run from a

scripting environment and can easily be called by computer design procedures that pick the best material layouts, while minimizing blade weight." Ernesto said this process can be done with minimal user intervention, and the trial-and-error approach required by prior versions of NuMAD is no longer an issue.

Users also have the added flexibility to create blade models from data found in the International Energy Agency Wind Task 37 Blade Ontology to efficiently collaborate
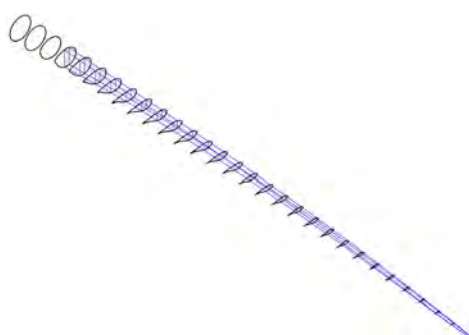
TURBINE SOLUTION — NuMAD produces blade geometry visualizations, like the one pictured here. **Graphic by Ernesto Camarena**
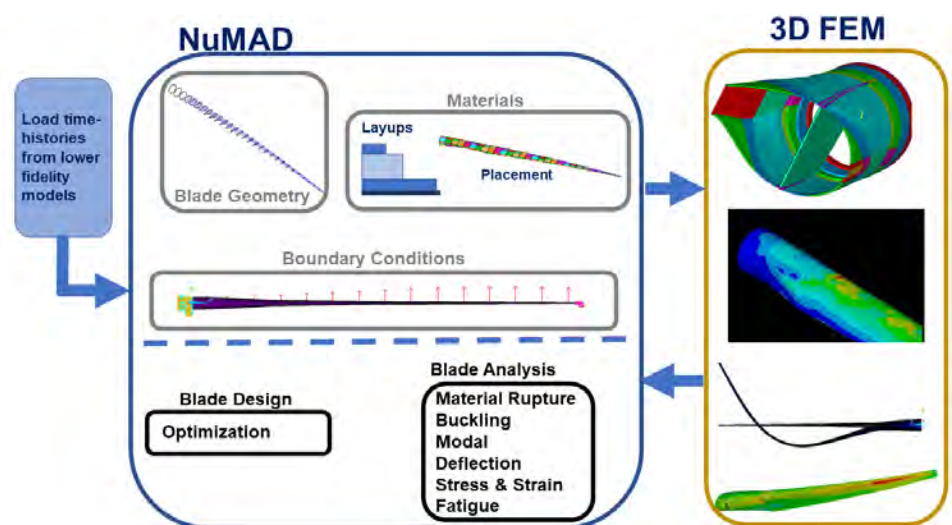
BLADE OPTIMIZATION — NuMAD is an open-source software program that simplifies the process of creating 3D models of wind turbine blades. The program selects the best materials and geometry for a blade, while minimizing its weight. **Graphic by Ernesto Camarena**

with other organizations that use different tools but are modeling the same blade.

"The update still retains the use of a graphical user interface, but also provides flexibility to upload specific file types with blade parameters," Ernesto said.

The latest NuMAD version and the highly flexible blade designs are now available on GitHub, a cloud-based software development host site that can track source code history. The NuMAD team, including Ernesto, principal investigator Josh Paquette and Sandia wind-program researchers Evan Anderson and Ryan Clarke, said their aim is to build a NuMAD community, including national laboratories, university researchers, students, manufacturers and others, such as wind plant owners. 🖼

Wind turbine blade data can be modified by a structural optimizer in NuMAD, which can also run other tools in a stand-alone mode, including the **Ansys Inc**. software company commercial finite element package; the National Renewable Energy Laboratory's National Wind Technology Center codes Pre-Processor for Computing Composite Blade Properties, or PreComp, **Computing Rotating Beam Coupled Modes**, or BModes, and **Fatigue, Aerodynamics, Structures and Turbulence**, or FAST; and PLOT3D file format for CFD mesh building.

Learn more by visiting the **NuMAD version 3.0 GitHub site**, reading the **user documentation** and going to the Sandia **wind energy program** webpage.

COMPUTING CONSTRAINTS — Researchers can input boundary conditions into NuMAD to create structural models of wind turbine blades.

Graphic by Jonathan Berg

Quality testing

strained as it's formed into different parts. Companies often use commercial simulation software calibrated to the results of various mechanical tests, said Sandia scientist David Montes de Oca Zapiain, the lead author on the paper. However, these tests can take months to complete.

And while certain high-fidelity computer simulations can assess formability in only a few weeks, companies need access to a supercomputer and specialized expertise to run them, David said.

Sandia has shown machine learning can dramatically cut time and resources to calibrate commercial software because the algorithm does not need information from mechanical tests, said David. Nor does the method need a supercomputer. Additionally, it opens a new path to perform faster research and development.

"You could efficiently use this algorithm to potentially find lighter materials with minimal resources without sacrificing safety or accuracy," David said.

Algorithm replaces mechanical tests

The machine-learning algorithm named MAD[3], pronounced "mad cubed" and short for Material Data Driven Design, works because metal alloys are made of microscopic, so-called "crystallographic" grains. Collectively, these grains form a texture that makes the metal stronger in some directions than others, a phenomenon that researchers call mechanical anisotropy.

"We've trained the model to understand the relationship between crystallographic texture and anisotropic mechanical response," David said. "You need an electron microscope to get the texture of a metal, but then you can drop that information into the algorithm, and it predicts the data you need for the simulation software without performing any mechanical tests."

Teaming with Ohio State University, Sandia trained the algorithm on the results of 54,000 simulated materials tests using a technique called a feed-forward neural network. The Sandia team then presented the algorithm with 20,000 new microstructures to test its accuracy, comparing the algorithm's calculations with data gathered from experiments and supercomputer-based simulations.

"The developed algorithm is about 1,000 times faster compared to high-fidelity simulations. We are actively working on improving the model by incorporating advanced features to capture the evolution of the anisotropy since that is necessary to accurately predict the fracture limits of the material," said Sandia scientist Hojun Lim, who also contributed to the research.

As a national security laboratory, Sandia is conducting further research to explore whether the algorithm can shorten quality assurance processes for the U.S. nuclear stockpile, where materials must meet rigorous standards before being accepted for production use. NNSA funded the machine-learning research through the **Advanced Simulation and Computing program**.

To enable other institutions to take advantage of the technology, Sandia formed a cross-disciplinary team to develop the user-friendly, graphics-based Material Data Driven Design software. It was developed with input from more than 75 interviews with potential users through the DOE's **Energy I-Corps** program. Individuals and organizations interested in licensing can contact **ip@sandia.gov** for more information. 🖼

Failing successfully

By **Paul Rhien**

The Telemetry Systems Engineering organization at Sandia's California site has introduced a series of seminars highlighting how to overcome failure and embrace lessons learned.

The series, "Fabulous failures and the wonderful successes that followed," includes presentations from individuals in the organization about the technical and professional failures they have encountered over their careers and what those setbacks taught them about their products, relationships, teaming and more.

The goal of the quarterly seminar series is to foster a culture where people understand that at the end of the day what matters isn't the interim setbacks, it's the perseverance, learning and commitment to making the final product better, said Jennifer Clark, senior manager of Telemetry Systems Engineering.

"If we are more open about the challenges we are facing, the easier it will be to resolve them, learn from them and move on to the next iteration where we can make things better," she said. "That is the main intent of this series."

Everyone makes mistakes, Jennifer said, emphasizing that it is important not to blame or make others feel ashamed for these errors, but to create an environment where everyone feels comfortable bringing mistakes out into the open so the person can draw on the team's, and Sandia's, collective expertise to solve them.

"We can't just give up in the face of setback," Jennifer said. "We also don't want people to repeat the same mistakes over and over. We must learn from our mistakes, or we won't succeed as a team. Eventually, if you stick with it, failures can lead to strong personal growth and team success."

Jennifer added she hopes problems can be discovered and worked through during earlier stages of development when the stakes are lower.

"If we're not willing to investigate the little failures upfront, they might become bigger failures later," she said. "It is so much easier to spend a little more time bringing a problem to the light and fixing it in the first place, instead of brushing it off or being too embarrassed to raise the concern."

Sharing personal experiences from his career, mechanical engineer Ryan Layton presented the first talk of the series last fall. Ryan spoke of a trusted mentor who taught him a valuable lesson.

"He taught me that at the end of the day, nobody remembers that a particular issue was your fault, but they absolutely do remember if you and your team worked hard to fully explain and correct the issue after it appeared," Ryan said.

"Digging into failures, even the ones that were the result of my own initial oversights and learning from that process have been the most engaging times of my career at Sandia," he said. "We talk a lot about lessons learned, but I think those are really lessons earned."

A key theme of the talks has been Sandia's culture of creative problem-solving.

"Sandians look for opportunities to solve hard problems," Jennifer said. "Bringing in others to help you think about a problem is key to driving innovation."

The next session in the series will be held in March. Details for the speaker and topic are still being finalized.

FABULOUS FAILURE — Introducing the "Fabulous failures" seminar, Jennifer Clark shared a **blooper video from SpaceX** illustrating the repeated failures the aerospace company encountered in the development of their orbital rocket booster.   **Image courtesy of SpaceX / YouTube**

BLACK HISTORY MONTH
2022 EVENTS

Meals with the Thunderbird

When: **All of February**
Time: Breakfast and lunch
Location: Thunderbird Café
Menu: Afro Inspired dishes
(Soul Food, Caribbean, African…)

FEB 17 THURSDAY

BLC Monthly Meeting: Heritage Quiz Bowl

Time: 12 – 1 p.m. MDT

Location: _Add Event to Outlook_

Meet employees around the Labs and Kirtland Air Force Base while putting your knowledge to the test during this virtual event.

FEB 24 THURSDAY

Soul Food Taster

Time: 11a.m. – 1p.m.

Location: Pick up at Base Chapel

The annual Soul Food Taster is hosted by the Kirtland Air Force Base African American Heritage Committee. Presale and day-of tickets are available.

FEB 16 WEDNESDAY

Black Leadership Committee and Sandia Women's Action Network Lunch and Learn Series: _Removing Bias from the Interview Process_

Time: 11a.m. – 12 p.m. MDT

Location: _Add Event to Outlook_

The joint lunch and learn will be hosted virtually by the Black Leadership Committee and Sandia Women's Action Network. Director Jonathan Huff and Jacquilyn Weeks, editor and writing consultant, will moderate a discussion about bias in interviewing.

FEB 23 WEDNESDAY

Diversity Cinema: Black Health and Wellness, Past and Present

Time: 12 – 1 p.m. MDT

Location: _Add Event to Outlook_

In a virtual presentation, the Black Leadership Committee will discuss the importance of Black Health and Wellness and encourage thoughtful discussion about the relationship between African Americans and the past and present healthcare system.

https://wp.sandia.gov/blc/

BLACK
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