

Measuring a quantum computer's power now faster and more accurate



SCALING UP — Sandia has designed a faster, more accurate style of test for quantum computers, such as the one pictured here. Photo by Bret Latter

Scientists at Sandia invent new yardstick for benchmarking performance

By Troy Rummler

hat does a quantum computer have in common with a top draft pick in sports? Both have attracted lots of attention from talent scouts.

Quantum computers, experimental machines that can perform some tasks faster than supercomputers, are constantly evaluated, much like young athletes, for their potential to someday become game-changing technology.

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Economic impact: Sandia spends \$3.9B, exceeds small-business goals

Labs' payments benefit nation, state economies

By Manette Newbold Fisher

upporting a growing workforce and a wide range of businesses, Sandia contributed an all-time high of \$3.9 billion into the economy during fiscal year 2021. This is about \$139 million more than the previous fiscal year. The spending includes labor, subcontracts, purchases and other expenditures.

"We are proud of the story these numbers tell," said Associate Labs Director Scott Aeilts, referencing the newly released



LARGEST-EVER SUBCONTRACT — An employee completes a walk-through of the Thunderbird computer. Sandia awarded its largest subcontract to New Mexico small business Encantado Technical Solutions LLC during fiscal year 2021. Photo by Randy Montoya

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Sandia National Laboratories

Albuquerque, New Mexico 87185-1468 Livermore, California 94550-0969 Tonopah, Nevada | Nevada National Security Site Amarillo, Texas | Carlsbad, New Mexico | Washington, D.C.

Katherine Beherec, Editor	kgbeher@sandia.go
Alicia Bustillos, Production	abustil@sandia.go
Paul Rhien, California Site Contact	prhien@sandia.go

CONTRIBUTORS

Michelle Fleming (milepost photos, 505-844-4902), Neal Singer (505-846-7078), Stephanie Holinka (505-284-9227), Kristen Meub (505-845-7215), Michael Baker (505-284-1085), Troy Rummler (505-284-1056), Manette Fisher (505-844-1742), Valerie Alba (505-284-7879), Luke Frank (505-844-2020), Michael Langley (925-294-1482), Meagan Brace (505-844-0499), Mollie Rappe (505-288-6123), Darrick Hurst (505-844-8009) Jim Danneskiold (jddanne@sandia.gov), Heather Clark, manager (505-844-3511)

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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: 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.

Opening architecture to make air travel safer and easier

Faster algorithm development may keep shoes on

By J.C. Ross

ir travelers may see faster, safer security checkpoints — no need to open bags or remove liquids or shoes — thanks to the award-winning work of Sandia and their partners who have developed an open architecture for airport screening systems.

The Open Threat Assessment Platform, developed with Pacific Northwest National Laboratory, NASA and industry partners for the Department of Homeland Security's Science and Technology Directorate and the Transportation Security Administration, will allow officials to respond more quickly and easily to rapidly changing threats to air travel safety.



FASTER TRAVEL AHEAD — With Sandia's work on the Open Threat Assessment Platform and Pacific Northwest National Laboratory's new shoe scanner, TSA won't have to add steps for travelers like removing shoes. It will be able to capitalize on advances in machine learning and tap third-party vendors to develop algorithms to detect emerging threats. **Photo by Andrea Starr, Pacific Northwest National Laboratory**

The TSA's current screening systems, such as X-ray machines and body scanners, are proprietary systems that scan, annotate and report in different ways, without communicating with each other. "Only existing vendors can develop ways to address new threats, which have limited the TSA's flexibility to innovate," said project lead Andrew Cox, a Sandia research and development systems analyst previously at the TSA.

"When we wanted to change how we screen in response to new threats, the technology was too rigid. The TSA compensated by adding procedures. There's a shoe bomber and you have to take your shoes off; liquid explosives arrived, and the TSA had to limit liquids and gels," Andrew said.

Sandia partnered with Pacific Northwest National Laboratory, which developed a new high-definition body scanner, and industry partners like Stratovan to create the Open Platform Software Library, which will allow the TSA to work with any vendor for a needed algorithm.

Austin Silva, a Sandia cognitive scientist who oversees development of the library, said the open architecture will provide a common set of interfaces to develop against.

A wider variety of vendors will more quickly and reliably be able to create security upgrades with new algorithms that integrate into existing screening — seamlessly for travelers. "Like LEGOs, you'll be able to rapidly introduce new pieces," Austin said. The system may also be able to use different algorithms at different times based on threat level.

Better data collection means safer, more seamless travel

Faster innovation in detection will make air travel safer, said Ed Jimenez, an optical engineer at Sandia. The TSA will be able to collect data continuously and improve algorithms every few months. Standardizing and modularizing design with an open architecture should benefit industry. Once the TSA approves them for access, companies will be able to collaborate.

Improved scanners will also improve



NEXT STEP, BODY SCANNER UPGRADES — Researchers, including Pacific Northwest National Laboratory's R. Trevor Clark, left, and Stratovan President and CTO David Wiley, far right, work on next phases of OTAP. The team's testing focus has moved beyond carry-on bags. "We're branching out into helping not just computed tomography – X-ray – algorithm developers but body scanner development," Ed Jimenez said. Photo by Eric Francavilla, Pacific Northwest National Laboratory

passenger experience. "When you put an object in your bag that's mistakenly flagged as a threat, the enhanced algorithm has the potential to not ring as a false positive alarm," Ed said. "You won't have to open the bag and slow down the line."

Now in its seventh year, the Open Threat Assessment Platform project has involved almost a dozen industry partners, including algorithm developers, X-ray vendors and software specialists. It's part of a worldwide push to open software architecture. Once deployed in the field, the platform will "change the safety profile of airports rapidly," Austin said. "We'll be able to say, we've seen this emerging threat; can anyone in the community develop this algorithm? From there, we'll be able to manage updates across the aviation security infrastructure."

While the Open Threat Assessment Platform is likely to save the TSA money and provide revenue to industry, Sandia's involvement benefits the project because, Andrew said, "if you're going to develop a standard for one open architecture, you want it to be market-neutral. We're not going to be playing favorites with any vendor. Everything we or our subcontractors develop would be government owned. We were one of few with the technical expertise to oversee it, and we could implement contracts and partnerships to test out these ideas quickly and effectively."

The Open Platform Software Library's main code was primarily developed by Stratovan; Sandia continues to contribute cybersecurity expertise for analysis. "We can be the neutral party to evaluate code, then share our results in ways that are actively changing some of their design principles," Austin said. "We have been able to build cybersecurity into the design process."

Sandia also built a prototype TSA checkpoint at Kirtland Air Force Base to rapidly gather data on detection of live explosives in bags. "These systems are locked down in an airport," Ed said, "but we were able to procure an X-ray machine, stand up a checkpoint at an explosive range and collect data from real explosives scanned in suitcases. It increased our data acquisition; something that would take a full day took only hours."

Award-winning work to make real-world impact

In October, Andrew, Austin and Ed received an Interagency Partnership



RESPONDING TO EMERGING NEEDS — A Pacific Northwest National Laboratory staffer stands in a traditional millimeter wave body scanner. "Screening has largely been unchanged for the last 20 years, and this project provides an opportunity to really transform how this technology is leveraged for national security and safety," Sandia optical engineer Ed Jimenez said. Photo by Andrea Starr, Pacific Northwest National Laboratory

Award, Mid-Atlantic Region, from the Federal Laboratory Consortium for their work with Pacific Northwest National Laboratory, NASA, TSA and the Department of Homeland Security's Science & Technology Directorate (Screening at Speed Program and Transportation Security Laboratory), for their work to develop and transition high-definition advanced imaging technology with Pacific Northwest National Laboratory's new shoe scanner, which will allow travelers to keep their shoes on. The Federal Laboratory Consortium National Awards recognize federal labs and their partners for outstanding technology transfer achievements.

The Open Platform Software Library

has been approved for international distribution; partners in the United Kingdom are already using it, Andrew said. The project aligns with DOE's Office of Science priorities on artificial intelligence and machine learning and the Department of Homeland Security's focus on proactive responses to identify, detect and prevent attacks. The team is using real automated threat recognition software to look at proving sensors — CT and advanced imaging technology systems — by testing with real bags, toiletries, laptops and simulated explosives to demonstrate system accuracy. They hope to be in select airports by late 2022.

The project has been personally

rewarding for Sandians. "In the research world, sometimes you wait decades for your work to make a difference," Ed said. "This is already impacting the way next-generation systems should be designed."

"It's very exciting," Austin added. "Most of my work is very research focused. This is fully proving out a concept to have a technology that affects millions of people traveling every day. Other airports and agencies across the world are saying this could be a gamechanger. When we're walking through the airport, we'll be able to directly see how our work has changed aviation security."

Quantum

CONTINUED FROM PAGE 1

Scientist-scouts now have their first tool to rank a prospective technology's ability to run realistic tasks, revealing its true potential and limitations.

A new kind of benchmark test, designed at Sandia, predicts how likely it is that a quantum processor will run a specific program without errors.

The so-called mirror-circuit method, published recently in **Nature Physics**, is faster and more accurate than conventional tests, helping scientists develop the technologies that are most likely to lead to the world's first practical quantum computer, which could greatly accelerate research for medicine, chemistry, physics, agriculture and national security.

Until now, scientists have been measuring performance on obstacle courses of random operations.

But according to the new research, conventional benchmark tests underestimate many quantum computing errors. This can lead to unrealistic expectations of how powerful or useful a quantum machine is. Mirror-circuits offer a more accurate testing method, according to the paper.

A mirror circuit is a computer routine that performs a set of calculations and then reverses it.

"It is standard practice in the quantum computing community to use only random, disordered programs to measure performance, and our results show that this is not a good thing to do," said computer scientist Timothy Proctor, a member of Sandia's **Quantum Performance Laboratory** who participated in the research.

The new testing method also saves time, which will help researchers evaluate increasingly sophisticated machines. Most benchmark tests check for errors by running the same set of instructions on a quantum machine and a conventional computer. If there are no errors, the results should match.

However, because quantum computers perform certain calculations much faster than conventional computers, researchers can spend a long time waiting for the regular computers to finish. With a mirror circuit, however, the output should always be the same as the input or some intentional modification. So instead of waiting, scientists can immediately check the quantum computer's result.

The research was funded by DOE's Office of Science and Sandia's Laboratory Directed Research and Development program. Sandia is a leading member of the Quantum Systems Accelerator, a DOE national quantum research center.

New method reveals flaws in conventional performance ratings

Tim and his colleagues found that randomized tests miss or underestimate the compound effects of errors. When an error is compounded it grows worse as the program runs, like a wide receiver who runs the wrong route, straying farther and farther from where they are supposed to be as the play progresses.

By mimicking functional programs, Sandia found results often had larger dis-

crepancies than randomized tests showed.

"Our benchmarking experiments revealed that the performance of current quantum computers is much more variable on structured programs" than was previously known, Tim said.

The mirror-circuit method also gives scientists greater insight into how to improve current quantum computers.

"By applying our method to current quantum computers, we were able to learn a lot about the errors that these particular devices suffer — because different types of errors affect different programs a



QUANTUM PERFORMANCE — Sandia computer scientist Timothy Proctor is the first author on the Nature Physics paper describing a new way to benchmark quantum computers. Photo courtesy of Tim Proctor

different amount," Tim said. "This is the first time these effects have been observed in many-qubit processors. Our method is the first tool for probing these error effects at scale."



Four researchers recognized by Society of Women Engineers

By Mollie Rappe

his fall, four Sandia researchers were recognized by the Society of Women Engineers. Laura Biedermann, Annie Dallman, Erica Douglas and Chris LaFleur were recognized for their professional excellence, leadership and support of women in science, technology, engineering and mathematics.

The society has empowered women to achieve their full potential in careers as engineers and leaders for more than 70 years. In October, SWE held an in-person reception in honor of the award winners as part of their annual conference, held in a hybrid format. Annie attended the gathering in person, as part of Sandia's recruiting team.

"I've recruited at other events, but it was nice to be at the event for women in engineering," Annie said. "Many of the collegiate attendees asked for career advice, not just about Sandia, so it felt more impactful."

Spark Award — Laura Biedermann



CLICK HERE TO READ LAURA'S PROFILE IN SWE MAGAZINE

A PHYSICIST WITH SPARK — Sandia physicist Laura Biedermann received a SWE 2021 Spark Award for her work co-founding the PI Workshop in 2013 and co-creating Sandia's Peer Mentoring Steering Committee in 2016. Both efforts support the career development and retention of Sandia employees.

Photo by Lonnie Anderson

Investigator Workshop Series in 2013 and co-creating Sandia's Peer Mentoring Steering Committee in 2016. Both efforts support the career development and retention of Sandia employees, whether they are female or not. "I'm a physicist who mentors both men and women, so I was flabbergasted to be nominated for the award, and to win," Laura said. "It just made me think of all the amazing folks I've worked with, and how the mentoring initiatives have grown and evolved. My advice for new employees is to reach out and get involved in activities professional activities, networking organizations, volunteering opportunities — it's very important to not only have a strong technical depth in your field, but also to be exposed to the breadth of research and mission work at Sandia."

Distinguished New Engineer Award — Annie Dallman

Annie was one of 10 women who received a SWE 2021 Distinguished New Engineer Award. This award recognizes women with outstanding technical performance and leadership in SWE who are in the first 10 years of their career.

Laura was one

of five women who received a SWE

2021 Spark Award,

those who have con-

tributed significantly

to the advancement

of women in STEM

through mentoring

those around them.

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Annie received her doctorate in engineering from the University of Notre Dame in 2013. She joined Sandia as a postdoctoral researcher in renewable energy and has since applied her



CLICK HERE TO READ ANNIE'S PROFILE IN SWE MAGAZINE

A DISTINGUISHED ENGINEER — Annie Dallman, a Sandia mechanical engineer, received a SWE 2021 Distinguished New Engineer Award for her outstanding technical performance and contributions to several fields, and her leadership in SWE. Photo by Lonnie Anderson

expertise in modeling and simulation, fluid dynamics and data analysis to other mission areas, such as nuclear nonproliferation. Her leadership in SWE began in graduate school where she focused on organizing programs of interest for female engineering graduate students. These later grew into a more widespread GradSWE program. After graduate school, Annie joined the Central New Mexico Section of SWE and is the scholarship co-chair for the section.

"I'm grateful to be formally recognized by SWE for my technical achievements and community impact," Annie said. "I've been fortunate to work in a variety of research areas at Sandia, and I enjoy taking on new challenges. Of course, I'm very appreciative of my manager and mentors for their support."

Emerging Leader Award — Erica Douglas

Erica was one of 10 women nationwide who received a SWE 2021 Emerging Leader Award, which recognizes women

who have been

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had been a part of,

groups as mission

actively engaged



CLICK HERE

AN EMERGING LEADER — Erica Douglas, a Sandia manager, received a SWE 2021 Emerging Leader Award for her engineering work and outstanding leadership. Even before she became a manager, she found mentoring postdoctoral researchers very rewarding.

Photo by Lonnie Anderson

needs arose. Even before she became a manager, she found mentoring technologists, engineering staff and postdoctoral researchers very rewarding, especially when the postdocs transitioned to independent staff members.

"It's an honor to represent Sandia and the teams I've worked with," Erica said. "I think it speaks to the exemplary nature, and quality of work, of the individuals I've had the pleasure to lead. My advice for women considering the management track is to not be afraid of making the jump. It's very rewarding to see folks realize the potential they may not have seen in themselves."

Advocating for Women in Engineering Award - Chris LaFleur

Chris was one of five women who received a SWE 2021 Advocating for Women in Engineering Award. This award recognizes women with professional excellence and advocacy for women in STEM. Chris evaluates fire risks for emerging energy technologies, such as hydrogen-powered cars and natural gas-powered trains.

She has mentored postdocs and junior staff and is the chair of the Sandia Pride Alliance Network. She is especially proud of her advocacy work through the employee resource group to make Sandia a more supportive workplace for transgender individuals over the past five years or so. This includes planning educational seminars and developing a resource guide for transitioning Sandians and their managers and co-workers.

The guide includes everything from advice on how to come out as transgender to your co-workers to the in engineering and process of changdemonstrated outing your name and standing leadership gender legally and in the first 15 years within the human resources system.

> "If trans women aren't comfortable working at Sandia, they'll go work somewhere else," Chris said. "And these are highly educated engineers who are among the best and the brightest. This work helps everyone at Sandia."



AN ADVOCATE FOR ALL - Chris LaFleur, a Sandia fire protection engineer, received a SWE 2021 Advocating for Women in Engineering Award for her service as chair of the Sandia Pride Alliance Network, especially her work to make Sandia a more supportive workplace for transgender individuals. Photo by Lonnie Anderson



Economic impact

CONTINUED FROM PAGE 1

2021 Sandia Economic Impact brochure.

"Sandia National Laboratories continues to grow in employment and spending, and we are dedicated to working with businesses — especially small businesses — to support national security objectives."

Of all subcontract-related payments, totaling nearly \$1.37 billion, more than \$838 million — or about 61% — went to small businesses. Total subcontract-related payments increased \$37 million over fiscal year 2020.

Nearly 35% of all subcontract-related payments in fiscal year 2021 benefited New Mexico companies. Sandia also paid the State of New Mexico more than \$106 million in gross receipts tax, up nearly \$9 million from the previous fiscal year.

Sandia spent about \$485 million with New Mexico businesses in fiscal year 2021 that ended Sept. 30. That includes \$9.5 million in procurement purchases and \$475 million in subcontracts within the state. Of the New Mexico subcontracts, more than \$360 million — or approximately 76% benefited small businesses.

"Diverse small-business suppliers are vital to the success of Sandia Labs' national security missions," said Labs Director James Peery. "Their skills and hard work combined with ours are a powerful force in bringing cutting-edge technology to the marketplace. We are committed to partnering with small businesses and working together to promote innovation, achieve shared goals, and strengthen the local and national economies."

In addition to spending, Labs employment increased by more than 460 jobs over fiscal year 2020. Sandia's total employment across all sites is nearly 15,000, leading to more than \$2.3 billion in labor, including payroll, and nonsubcontract related payments. The largest Sandia site, located in Albuquerque, employs nearly 12,300.

Sandia awarded largest-ever subcontract to small business

Last year Sandia awarded an information technology subcontract up to \$700 ALL-TIME HIGH CONTRIBUTION

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Graphic by Lloyd Wilson

million over a possible seven years to Albuquerque small business Encantado Technical Solutions LLC.

"The subcontract with Encantado is one way Sandia proved its commitment to small business," said Paul Sedillo, Sandia's small-business program manager. "We are proud of how smoothly the contract transition went. By replacing several contracts with one, information technology efficiency increased throughout Sandia."

Under the contract, the company provides Sandia IT and telecommunications support for all Labs employees. This includes help desk and end-user support services, cloud-based solutions, software development, IT infrastructure services, data science and analytics, and automation engineering. The company employs nearly 500 people in New Mexico.

"As a lifelong resident of New Mexico, community stewardship is important to me and is a core value for Encantado," said Encantado General Manager Rodger Jones. "Encantado promotes and encourages our staff members to participate in local

OVERALI	NEW MEXICO	
\$1,369,484,000	Total Subcontract Payments	\$475,456,000
\$838,459,000	Total Small Business	\$360,118,000
\$384,063,000	Small Business*	\$131,873,000
\$222,242,000	Disadvantaged	\$128,011,000
\$173,092,000	Woman-Owned	\$81,680,000
\$132,438,000	Veteran-Owned	\$44,399,000
\$93,189,000	Service-Disabled Veteran-Owned	\$16,835,000
\$68,800,000	HUBZone	\$34,952,000

 SUBCONTRACT INCREASE — Sandia spent nearly \$1.37 billion on subcontracts in fiscal year 2021 with more than \$838 million going to small business

 es. Total subcontract-related payments increased \$37 million over fiscal year 2020.

 Graphic by Lloyd Wilson

professional and community-based organizations. Additionally, we take a percentage of our revenue to fund a local nonprofit, the Encantado Foundation, that supports STEM-based education and other programs across the state."

The nonprofit supports community needs, aiming to shape the next generation of leaders and foster learning through programs in the Albuquerque area.

Economic development programs support tech commercialization

Sandia manages economic development programs that combine people, innovations and the facilities of the Labs to deploy technology in support of Sandia's mission and create jobs.

During 2021, Sandia provided \$2.4 million in technical assistance to 133 small companies through the New Mexico Small Business Assistance program. In addition, Sandia currently has nine active projects in the Technology Readiness Gross Receipts Initiative, a technology maturation program that helps address a critical stage between technology development and commercialization when many companies need additional funding to ready products and services for the marketplace.

In the last fiscal year, there were 131 newly issued patents for Sandia technologies, 238 filed patent applications and 564 active commercial licenses.

Community Involvement supports nonprofits with \$1.4 million

Sandia Community Involvement teams continued to support K-12 educational success and family stability programs to address some of the greatest challenges faced in Albuquerque and Livermore. In calendar year 2021, Sandia contributed \$1.4 million to the local communities, including \$175,000 in the Livermore area.

Sandia employees generously committed \$4.7 million through the United Way of Central New Mexico to nonprofits throughout Albuquerque, Livermore and the nation during the Labs' annual Sandia Gives campaign. An additional \$85,000 was donated from employees to provide shoes, school supplies and holiday gifts for underserved children.

Sandia provided virtual STEM programs due to COVID-19 precautions. Offerings included Family STEAM Nights, Family Math Night, Kids Day at the Labs, Department of Energy Regional Science Bowls and the NM Electric Car Challenge. STEM in the Sun provided outdoor STEM activities for children attending Albuquerque community center programs.

"The last two years have challenged all of us due to the continuing COVID-19 pandemic," said Amy Tapia, manager of Community Involvement. "Sandia employees keep showing up to help our communities and it's inspiring to witness."

Sandia continues with aggressive small-business goals

The Labs have met and exceeded small business goals for five consecutive years. Sandia is already on track to meet all goals set for fiscal year 2022. The Labs focus on working with small businesses fitting the federal categories as small disadvantaged, woman-owned, veteran-owned, service-disabled veteran owned, and small businesses in impoverished, HUBZone areas.

"Sandia is determined to support small businesses and our teams are continuously thinking of new, creative ways to connect," Paul said. "The last two years have been especially difficult for many companies during the pandemic, and we're doing what we can to ease financial burdens."

Sandia teams seek small businesses through a variety of ways. During fiscal year 2021, the Labs hosted four virtual forums viewed by 1,800 suppliers. Through various efforts, Sandia worked with 500 small businesses during fiscal year 2021 that hadn't supported the Labs before.

For more information on doing business with Sandia, visit the **Procurement website** or email **supplier@sandia.gov** with questions.

U.S. Department of Labor recognizes Sandia for hiring veterans

Platinum award salutes businesses that recruit, hire and retain veterans

By Luke Frank

.S. Secretary of Labor Martin J. Walsh recently recognized Sandia as one of 849 recipients of the 2021 HIRE Vets Medallion Award during a virtual award ceremony presented by the Department of Labor. The Honoring Investments in Recruiting and Employing American Military Veterans Act Medallion Program recognizes employers who successfully recruit, hire and retain veterans.

Sandia's platinum designation — the highest category of award - honors the value the Labs has exhibited for the contributions of veterans in the workplace through a long-term career and growth plan that uses the diverse skills veterans acquired through their military service.

According to HIRE Vets, Sandia demonstrated rigorous employment and veteran integration assistance, including veteran hiring and retention percentages, availability of veteran-specific resources, leadership programming for veterans, dedicated human resource efforts, pay compensation and tuition assistance programs for veterans and more.

In 2020, Sandia hired 556 veterans and retained them for at least 12 months. In that same year, 10% of Sandia employees self-identified as veterans.

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Illustration by Dan Thompson

Mileposts





Daniel Stump



Elizabeth Lopez

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Matthew Cattaneo



Daniel McMurtrey

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Mark Higuera



Larry Shapnek 48



James Kajder



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Cindy Kajder



'Laney' Marie-Elena Kidd 35

Program helps speed up research of complex chemistry problems

By Michael Ellis Langley

successful partnership to help make aspects of chemistry research faster and more productive was recently renewed for another four years.

The Exascale Catalytic Chemistry project with Sandia, Argonne and Pacific Northwest national laboratories, as well as Brown and Northeastern universities, started in 2017 and brings together physical chemists and applied mathematicians to design computational tools to take advantage of the most powerful computers in the world to speed up understanding of heterogeneous catalysis, a complex chemistry problem.

Gas-phase molecules transformed on metal surfaces

Judit Zádor, the project's director, assembled the team of experts to develop faster, more reliable models for heterogeneous catalysis — reactions of gas-phase molecules that take place on metal surfaces.

"What this project brings to catalysis research, is that it tries to automate the creation of complicated models that are necessary to describe the complex chemistry between gases and the catalytic surface," Judit said. "Even for seemingly simple systems, like the hydrogenation of CO and CO2, there can be many dozens of reactions that take place on a simple facet of a metal. This can grow to hundreds or more if we con-sider larger molecules and more complex surfaces."

Chemists and engineers actively study these interactions in problems including the conversion of simpler, cheaper molecules to more useful, expensive ones. With the new tools developed, Judit's team at Sandia and beyond can create models and simulate these reactions more easily and systematically.

"People traditionally assemble these reaction mechanisms by trying to enumerate the relevant reactions manually the best they can, and then calculate the properties for each reaction individually. It's a slow process and can be error prone," Judit said.

"Our partners at Brown and Northeastern created a computer code that can enumerate the reactions and estimate their properties for you in a systematic way," Judit continued. "At Sandia we then create codes to systematically, yet automatically, study these reactions using quantum chemistry. We also made simulation and analysis tools to interpret the models as a whole. Pacific Northwest National Laboratory contributes by its expertise in the underlying quantum chemistry method, while Brown, Argonne and Sandia jointly develop new methods to improve the thermochemistry."

Improving chemistry one bit at a time

Besides uncovering interesting science about particular systems, an important goal of the project is to give other researchers tools that can more accurately predict their own systems of interest and eventually focus

experimental efforts on the most productive catalytic strategies. These systematic computations can more accurately predict which interactions will lead to a desired chemical reaction.

Judit said that finding which interactions are most important to model is akin to knowing which branch of a tree to prune to take the shape you want.

"On a catalytic surface there are always chemical pathways that end up where you do want, but there are pathways that end up with a product you don't want," she said. "If you imagine the tree, you can follow one branch to the right, and it leads to the right outcome, but follow to the left, and it leads to an undesirable outcome. If you have an automated tool and enough computational power, you can examine many more scenarios than traditionally theoretically or experimentally possible and help you understand what makes a catalytic reaction produce a given product."

A big reason why chemistry researchers

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that time, is composed of researchers from Sandia, Argonne and Pacific Northwest national laboratories, as well as Brown and Northeastern universities. Photo by Dino Vournas

NNSA Sandia Field Office manager ready to innovate, collaborate with Labs

By Kristen Meub

aryl Hauck became the manager of NNSA's Sandia Field Office in August, leading government oversight of Sandia, which is government owned and contractor operated. He also leads the daily operations of the field office and is responsible for the overall administration of the approximately \$3.9 billion per year Sandia contract.

As a federally funded research and development center, there is a special and trusting relationship between Sandia and the government, Hauck said. He described his role as representing government oversight of the safe and secure operations of Sandia while also providing stewardship of the Labs, championing efforts to update infrastructure and taking a governance approach to overseeing the Sandia contract.

"Given the scope of work, and the expertise of our partners, it is far more appropriate and effective to focus on collaboratively establishing and maintaining the Labs' assurance systems than it would be for the government to directly oversee daily operations," Hauck said. Hauck is a retired U.S. Air Force brigadier general and served as the program executive officer for stockpile modernization in NNSA's Office of Defense prior to becoming the field office manager.

The Lab News recently sat down with Hauck for an interview about his background and his new role at Sandia.

Lab News: Can you tell us about your background and what originally drew you to the U.S. Air Force Academy and the study of operations research, systems management and industrial engineering?

Hauck: I grew up on a steady diet of books like "Battle of Britain," "30 Seconds over Tokyo," "The Flying Tigers" and "The Right Stuff." I came to realize our history has been written by ordinary Americans who encountered extraordinary circumstances and rose to the occasion. Seeing a few airshows didn't hurt. I just knew I wanted to be around people like that, and that has proven to be true. My college undergraduate curriculum exposed me to a variety of topics, and I became interested in using quantitative methods to solve problems that were hard to define. Given the complexity of what we do now, understanding



NEW SANDIA FIELD OFFICE MANAGER — Daryl Hauck, Sandia Field Office Manager, at the new NNSA administration building. Photo by Tami Moore

the complete system as well as the environment in which we are operating is essential to arriving at solutions that will be effective.

Lab News: What are some of your proudest career achievements to date?

Hauck: While in the U.S. Air Force, I led the Intelligence, Surveillance and Reconnaissance portfolio, providing many rapid responses to joint urgent operational needs from U.S. Central Command

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Great Minds in STEM celebrates two Sandia engineers

By Luke Frank

andia systems engineer Kenneth Armijo has been named a 2021 Most Promising Engineer-Ph.D. at the Hispanic Engineering National Achievement Awards Conference. Sandia mechanical engineer Michael Omana was named a 2021 Most Promising Scientist-Master's Degree at the conference.

Kenneth, who holds a doctorate in mechanical engineering, leads molten salt, molten alkali metals and high-voltage arcfault research and development at Sandia's National Solar Thermal Test Facility. He also serves as an expert for molten salts, alkali metals, arc-fault safety technologies and reentry high-flux and high-temperature materials research and development for DOE and DOD programs.

Michael, a mechanical engineer and aerosol and filtration scientist, has spent the past year-plus serving as an aerosol and filtration science subject matter expert for numerous COVID-19 response efforts, while working with teams across the Labs and in industry on personal protective equipment development and testing.

Great Minds in STEM recognized both awardees at its annual conference in October. Each was selected from among the top candidates submitted in all professional categories as leaders working in any area of science, technology, engineering and mathematics, or STEM, who model the technical excellence and leadership that significantly impact an industry, a field of science or engineering, academia, the Hispanic community and the nation.

"Kenneth and Michael represent the best of Sandia National Laboratories both in their professional pursuits and their personal efforts to cultivate the next generation of STEM scientists within the Hispanic community," said Tobie Webb, acting senior manager and chief diversity officer at Sandia. "Their recognition is well-earned."

Ken Armijo – Alternative energy guru

A native of New Mexico, Kenneth serves as a principal investigator for a large DOE Solar Energy Technology Concentrating Solar Power Liquid-Pathway program. His duties include technical leadership and project management to develop the next generation of high-temperature concentrating solar power plants.

In addition to concentrating solar power, Kenneth's work includes aerospace and reentry materials research and development, photovoltaics and distributed-energy technologies, plasma reliability, thermal trends of photovoltaic technologies, inverter and power electronics reliability, and New Mexico Small Business Assistance Program projects. His work also spans other high-voltage and high-current direct-current power reliability applications, as well as applications in arc-fault safety in nuclear energy high-voltage applications.

Away from work, Kenneth is deeply involved with community outreach as vice president of the New Mexico Professional Hispanic Engineers organization. For the past eight years, he has volunteered through Sandia's Manos program and is also the co-founder and leader of Noche Ciencias, family science nights for middle and high school students and their parents, provided in both English and Spanish.

Candidates for Most Promising Engineer or Scientist-Advanced Degree must be an engineer or scientist with less than 10 years of work experience since earning a master's or doctoral degree in a STEM field. Award criteria include uniqueness or innovation of contributions to the organization; leadership abilities or initiative; professional and technical achievement; potential for advancement; and involvement within the Hispanic community nationally or internationally.

"I'm grateful to Sandia Labs for supporting my interest in alternative energy technologies and sustainability and my mentoring of young, aspiring scientists in the local community," Kenneth said. "This recognition comes from doing the things I love that give me professional and personal fulfillment."



ALTERNATIVE ENERGY GURU — Sandia systems engineer Kenneth Armijo has been named a 2021 Most Promising Engineer-Ph.D. by Great Minds in STEM at the Hispanic Engineering National Achievement Awards Conference. Photo courtesy of UNM Alumni Association

Michael Omana – COVID-19 response wrangler

Through numerous separate projects, Michael and his teams have rapidly produced personal protective equipment for frontline workers, determined the effectiveness of equipment sterilization techniques, provided independent performance testing of imported equipment and devised field tests to determine the spread of aerosols between medical exam rooms.

Michael was one of a team of 17 researchers who developed a disposable respirator early in the pandemic made from materials not already used in the supply stream to sidestep the shortage of medical-grade personal protective equipment available to healthcare workers. Additional work in mask development yielded a reusable respirator that filters both inhaled and exhaled air with easily replaced N95 filter material stored inside two disc-shaped cases, protecting wearers and patients.

In the community, Michael is a mentor to underrepresented students, often supporting community events held by the Society of Hispanic Professional Engineers. This includes conducting professional workshops, information sessions and tech talks for underrepresented student groups at the University of Texas, Austin. He also actively recruits diverse candidates as a member of Sandia's recruiting team.

Candidates for Most Promising Engineer or Scientist-Master's Degree must be engineers or scientists with less than 10 years of work experience and no higher than a



COVID RESPONSE WRANGLER — Sandia mechanical engineer Michael Omana was named Most Promising Scientist-Master's Degree by Great Minds in STEM at the Hispanic Engineering National Achievement Awards Conference. Photo by Bret Latter

master's degree completed. Award criteria include uniqueness or innovation of contributions to the organization; leadership abilities or initiative; uniqueness of accomplishments; professional and technical achievement; potential for advancement; and involvement within the Hispanic community nationally.

"The opportunity to team with this breadth and depth of experts in one place enables us to quickly develop solutions to emerging challenges," Michael said. "I'm honored to accept this award, but I understand how many professionals it takes working together to develop and advance important science."

Exascale

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need tools provided by high-performance computing is that there are so many possible reactions to measure or calculate.

"These days we can afford to do accurate computations not just for the top few most important reactions but for many more, and we get improved reaction rate estimates," Judit said. "The strategy of this project is to improve the models iteratively. You propose a mechanism, you select the most important but least known parts, you improve them and then you plug it back into the original mechanism. Now you have a better mechanism, and if it's still not good enough, you make another round. This circular improvement is a key concept of this project. If you go around enough times you ought to achieve your desired accuracy."

The next phase

Now that the Exascale Catalytic Chemistry project — funded by DOE's Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division — was renewed for another four years, Judit and her team want to study how the chemistry of a given molecule on a catalytic surface is altered The awards selection committee, composed of various Great Minds in STEM stakeholders, including many past award winners, evaluates the nominations and reports its recommendations to the selection committee chairs, who make the final award selections.

For 33 years, Great Minds in STEM has recognized the achievements of America's top engineers and scientists from the Hispanic community. These leaders, innovators and champions represent the best and brightest minds our nation has to offer. They are symbols of Hispanic contributions at the highest levels of academia, government, military and corporate America.

by the presence of other molecules on a surface.

"These so-called co-adsorbates change the outcome of the reactions, so they are important. However, setting up calculations for these systems leads to extreme complexity, because there are just too many ways in which these molecules can interact on a surface." Judit said. "You can't do that by hand, and it seems that you can't do that by sheer computer power only either. We will have to use machine learning to leverage our computational frameworks. It's an exciting challenge."

Read more about the Exascale Catalytic Chemistry project and its achievements.

HIRE Vets

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"I am proud of our efforts to attract military veterans and help them continue their service to the nation at Sandia Labs," said Labs Director James Peery. "We share a dedication to national security and a commitment to exceptional service. Veterans are a vital part of our workforce, and this Department of Labor platinum award recognizes that great things come from working with members of the U.S. Armed Forces who have steadfastly served us."

The HIRE Vets Medallion Award is earned by businesses that demonstrate unparalleled commitment to attracting, hiring and retaining veterans. There are different awards for large, medium and small employers that fit into two award tiers: platinum and gold.





Field Office

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in Operation Enduring Freedom. Culminating that career at the Air Force Nuclear Weapons Center, and now with NNSA, I am very proud of our progress in recapitalizing our strategic weapons, both delivery platforms and warheads, laying the groundwork for years to come.

Lab News: For people newer in their career at Sandia and the NNSA, how would you describe your role and your day-to-day work?

Hauck: My role is to enable the Laboratories' mission in a collaborative and responsive manner ... finding a way to quickly say, "yes," to the plans and programs that allow us to operate safely and securely, delivering the services and products our nation needs, and revitalizing our infrastructure to enable us to keep that promise in the future. Our bywords will be "innovate, collaborate and execute" as we partner with the Labs to deliver on our commitments. The complexity of our challenges and the caliber of our team makes this energizing and fulfilling.

Lab News: What has surprised you most about your current role as Sandia Field Office Manager?

Hauck: Probably the sheer volume of environmental

compliance reporting across multiple states. That said, it is vital to be good stewards of natural resources as we accomplish our important missions.

Lab News: Looking ahead, what are you most looking forward to at Sandia and the field office?

Hauck: It's exciting to gain the full perspective on all of Sandia's contributions. I would say I already have a strong appreciation of Sandia's role in the nuclear weapons stockpile, and it has been very interesting to see the entire "virtuous cycle" in play that leverages relevant technologies in a synergistic way.

Lab News: Would you like to share about your family and any interests outside of work?

Hauck: My spouse, Amy Lautenschlager, leads the Advanced Studies and Analysis Division at the Air Force Nuclear Weapons Center. We share a strong family commitment to strategic deterrence. I have also discovered an almost secret society of audiophiles in our complex, and it has been very enjoyable to rediscover music on equipment that reveals exquisite detail.

Lab News: Is there anything else you'd like to share?

Hauck: It has been a pleasure getting to know Labs Director James Peery. I'm really looking forward to continuing a great partnership with him and meeting more and more of the fantastic people making this Laboratory the crown jewel that it is.

Sandians give hundreds of gifts, coats to families in need

By Trina West & Paul Rhien

andians in California made sure dozens of families in need had coats during the cold winter months and holiday presents under their trees for children around the San Francisco Bay Area.

The Security Operations organization, in partnership with the U.S. Marine Corps Reserves, conducted this year's Toys for Tots campaign under the leadership of Dennis Baker and campaign organizers Jamie Duranleau and Kaela Angelo. The annual toy drive, which culminated in a collection by the Marines on Dec. 2, marks the eighth year that Sandia has supported the Toys for Tots mission of spreading joy by donating new toys to children who are less fortunate. Dennis reflected on how the campaign promotes a sense of community at Sandia and beyond.

"We're all in this together, and I'd like to extend my thanks to Sandians," said Dennis. "I'll be forever grateful for their generosity and for my opportunity to work with them."

The Protective Force installed toy collection boxes throughout the California site and encouraged donors to purchase toys from Amazon. They collected 287 toy donations.

Since 1947, the Toys for Tots program through the U.S. Marine Corps has distributed more than 604 million toys to more than 272 million children. The organization has also formed the **Toys for Tots Literacy** Program and the Toys for Tots Native American Program.

Krissy Galbraith from the communications group in California led the annual coat drive for the Livermore site. This was Krissy's 10th annual coat drive at Sandia and her 15th overall on behalf of **One Warm Coat**, a San Francisco-based nonprofit that provides people in need with free warm coats.

This year, in coordination with **Safe Passages**, Sandia/California donated 105 new and used coats to refugee and immigrant families from Central America living in Alameda County. The coats were distributed at two events hosted by the **Central American Refugee Committee**, a Safe Passages partner that impacts the lives of community members.

California staff donated from an Amazon Wish List, dropped off gently worn coats at the Livermore campus and made financial contributions.

"I didn't have the chance to stop by the

office during the campaign. So, when I came to collect the coats at the end of October, I honestly didn't know if there would be one or 50. I was elated to see the generosity of my peers and colleagues overflowing out of the



TOYS FOR TOTS — Dennis Baker, leader of Sandia/California's Toys for Tots campaign, poses with Santa Claus during the donation event on Dec. 2. Photo by Randy Wong



HEARTWARMING — Krissy Galbraith, right, delivered 105 new and used coats to the Central American Refugee Committee, a One Warm Coat partner in Oakland, California.

Photo courtesy Krissy Galbraith

bins. I was incredibly moved, and my heart was full. Sandians are truly some of the most big-hearted and giving people," Krissy said.

The Central American Refugee Committee is a grassroots organization dedicated to organizing and educating the Latino immigrant community to improve local social, economic and cultural conditions.

