LOS ALAMOS NATIONAL LABORATORY ◇ WINTER 2020

NATIONAL ★ SECURITY SCIENCE

THE COMPUTING ISSUE

Computing on the mesa: Since the Manhattan Project, Los Alamos has been on the front lines of computing

"We thank Miss Mary Tsingou": One of the Laboratory's first computer programmers gets the recognition she deserves

Computing for a cure: Los Alamos scientists use computers to fight the coronavirus pandemic

+PLUS:

The bizarre and promising world of quantum computing

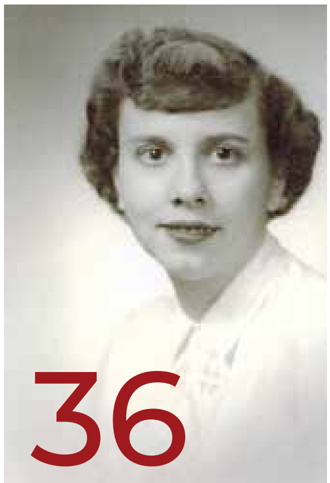
Superbugs are resistant to disinfectants—but not for much longer

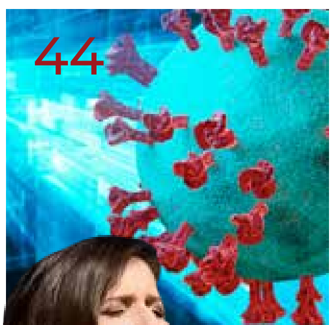
Scientists use machine learning to expose deepfake videos

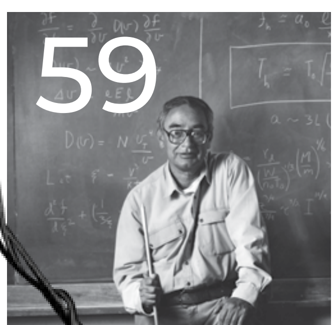
PHOTOBOMB

▼

Daniil Svyatsky of the Applied Mathematics and Plasma Physics group at Los Alamos National Laboratory demonstrates the power of Amanzi–ATS, a computer code that's used to simulate environmental systems. Shown here, a 3D Amanzi–ATS simulation models fractured porous material, such as rock, and the flow of chemicals through that material. Los Alamos scientists are particularly interested in the code's national security applications, such as studying how gases from an underground nuclear test flow through the earth. In 2020, Amanzi–ATS won an R&D 100 award—an "Oscar of Innovation." ★







About the cover: Using a computational fluid dynamics code, a supercomputer can produce a model that simulates turbulence when materials (such as gases, liquids, or metals) mix and change states. For example, when the cold water of Antarctica mixes with the warm Gulf Stream, the interaction produces turbulence, which is seen as vortices and curves and offers valuable information about material interactions.

IN THIS ISSUE

FEATURES

THE COMPUTING ISSUE

Los Alamos National Laboratory has led the way in developing and using computer simulations to understand the world around us.

JOHN SCOTT
DIRECTOR, OFFICE OF NATIONAL SECURITY AND INTERNATIONAL STUDIES

The world is made up of many physical systems—from natural systems, such as the formation of galaxies, to manmade systems, such as the detonation of a nuclear weapon. The experiments scientists conduct to understand physical systems provide us with knowledge essential for protecting the national interest, preventing disasters, finding cures for disease, and creating innovative, new technologies.

But what do scientists do when a physical system is too small, too large, too fast, too costly, too dangerous, or otherwise inaccessible for an experiment in a laboratory? Since the 1940s, scientists have increasingly relied on computer simulations to understand phenomena that cannot be experienced directly.

Computer simulations let scientists conduct virtual experiments using mathematical models—programs that attempt to replicate the natural behavior of an object or force. Virtual experiments open up new realms of research; for example, scientists can see a solar system evolve over eons. Virtual experiments also help us plan for complex situations, such as the need to avert an Earth-asteroid collision.

At Los Alamos, computing has been integral to our work since the Manhattan Project (see p. 16). In the early days, human computers—often the wives of scientists—performed calculations to support the development of the world's first atomic bombs. Over time, human computers were phased out and replaced with mechanical and then electronic computers, such as the MANIAC (see p. 23). Today, we use supercomputers that perform billions of calculations per second.

In the Laboratory's Weapons programs, scientists use this computing power to simulate nuclear explosions. The extreme conditions leading up to a nuclear explosion cause solid materials to flow and display instabilities and turbulence characteristic of fluids. Understanding the complex processes of instability and turbulence allows us to simulate with better accuracy the performance of America's nuclear deterrent.

The Laboratory's supercomputers are leveraged for non-weapons work, too. As you'll read on p. 44, our supercomputers are being used in the fight against COVID-19. We also use our supercomputers to better understand biology, climate, space, and just about any other area of study one can think of.

As we begin to say goodbye to Trinity (currently the world's seventh-fastest supercomputer, which is approaching the end of its useful life) and make plans to install its successor, Crossroads, we will continue to lead the world in computing power and drive the computing industry to develop ever-faster and more powerful computers. With our nation's best interests at heart, we will continue to use computers to help us simulate what we can only imagine. ★

MASTHEAD

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NSS STAFF SPOTLIGHT

In September 2020, story editor Eileen Patterson retired from the Laboratory after 28 years. Here, two-year-old Eileen (left) and her sister, Louise, kneel by their father, physicist and engineer Frank Tallmadge, shortly after he came to the Lab in 1948.

A NOTE OF CONFIDENCE

President Roosevelt lauds American science.

Less than a year into the Manhattan Project—the U.S. government's top-secret project to create the world's first atomic bomb to help end World War II—President Franklin Roosevelt wrote a letter of confidence and appreciation to Robert Oppenheimer, the project's scientific director. Working at a secret laboratory in Los Alamos, New Mexico, Oppenheimer's team of scientists and engineers would go on to detonate an experimental atomic device in July 1945 and partner with the military to drop two atomic bombs on Japan in August 1945. Roosevelt would have died by this time, but his confidence was justified, and his words remain true today: "Whatever the enemy may be planning, American science will be equal to the challenge." ★

THE WHITE HOUSE
WASHINGTON

Secret

June 29, 1943

My dear Dr. Oppenheimer:

I have recently reviewed with Dr. Bush the highly important and secret program of research, development and manufacture with which you are familiar. I was very glad to hear of the excellent work which is being done in a number of places in this country under the immediate supervision of General L. R. Groves and the general direction of the Committee of which Dr. Bush is Chairman. The successful solution of the problem is of the utmost importance to the national safety, and I am confident that the work will be completed in as short a time as possible as the result of the wholehearted cooperation of all concerned.

I am writing to you as the leader of one group which is to play a vital role in the months ahead. I know that you and your colleagues are working on a hazardous matter under unusual circumstances. The fact that the outcome of your labors is of such great significance to the nation requires that this program be even more drastically guarded than other highly secret war developments. I have therefore given directions that every precaution be taken to insure the security of your project and feel sure that those in charge will see that these orders are carried out. You are fully aware of the reasons why your own endeavors and those of your associates must be circumscribed by very special restrictions. Nevertheless, I wish you would express to the scientists assembled with you my deep appreciation of their willingness to undertake the tasks which lie before them in spite of the dangers and the personal sacrifices. I am sure we can rely on their continued wholehearted and unselfish labors. Whatever the enemy may be planning, American science will be equal to the challenge. With this thought in mind, I send this note of confidence and appreciation.

Though there are other important groups at work, I am writing only to you as the leader of the one which is operating under very special conditions, and to General Groves. While this letter is secret, the contents of it may be disclosed to your associates under a pledge of secrecy.

Very sincerely yours,

Franklin D Roosevelt

LISTEN UP

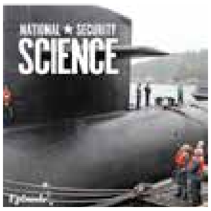
National Security Science magazine now has a podcast!

The National Security Science podcast, a spin-off of this magazine, brings you stories from the Weapons programs at Los Alamos National Laboratory—stories that show how innovative science and engineering are key to keeping America safe. Or, as we like to say, better science equals better security.

The first three episodes highlight different branches of our nuclear triad—the land, air, and sea-based components of America's nuclear deterrent. Listen and subscribe anywhere you download podcasts. ★

EPISODE 1 "A wealth of stealth" is written and read by Lieutenant Colonel Geoffrey Steeves, a senior Los Alamos Air Force Fellow and B-2 bomber pilot. Most of the nuclear weapons a B-2 can carry were designed at Los Alamos.

EPISODE 2 "A moment of glory" features Los Alamos Air Force Fellow Major Nicholas Edwards. As part of the Air Force's 576th Test Squadron, Edwards test-launched unarmed Minuteman III intercontinental ballistic missiles.

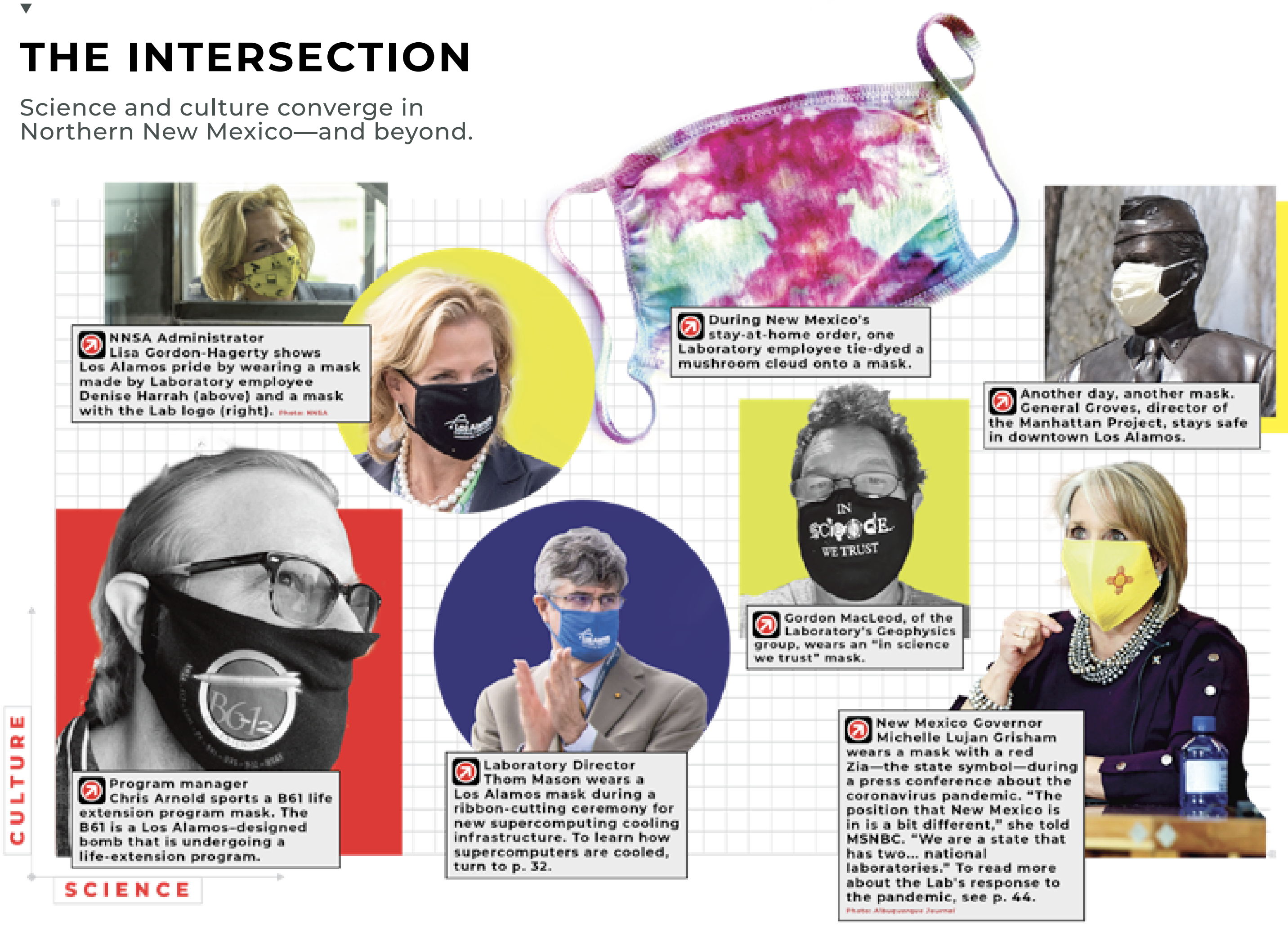


EPISODE 3 "Salt life" is written and read by Navy veteran and former Los Alamos employee Mark Levin. Learn what it's like to serve on board an Ohio-class submarine that has the ability to launch Los Alamos–designed nuclear weapons.

INFOGRAPHIC

THE INTERSECTION

Science and culture converge in Northern New Mexico—and beyond.



NNSA Administrator Lisa Gordon-Hagerty shows Los Alamos pride by wearing a mask made by Laboratory employee Denise Harrah (above) and a mask with the Lab logo (right). Photo: NNSA

During New Mexico's stay-at-home order, one Laboratory employee tie-dyed a mushroom cloud onto a mask.

Another day, another mask. General Groves, director of the Manhattan Project, stays safe in downtown Los Alamos.

Gordon MacLeod, of the Laboratory's Geophysics group, wears an "in science we trust" mask.

Program manager Chris Arnold sports a B61 life extension program mask. The B61 is a Los Alamos–designed bomb that is undergoing a life-extension program.

Laboratory Director Thom Mason wears a Los Alamos mask during a ribbon-cutting ceremony for new supercomputing cooling infrastructure. To learn how supercomputers are cooled, turn to p. 32.

New Mexico Governor Michelle Lujan Grisham wears a mask with a red Zia—the state symbol—during a press conference about the coronavirus pandemic. "The position that New Mexico is in is a bit different," she told MSNBC. "We are a state that has two… national laboratories." To read more about the Lab's response to the pandemic, see p. 44. Photo: Albuquerque Journal

Photo: U.S. Air Force

DELIVERY SYSTEM

QUALIFIED FOR DELIVERY

The F-15E fighter jet is equipped to carry the updated B61 gravity bomb.

A mock version of the B61-12 gravity bomb, designed by Los Alamos and Sandia national laboratories, has been successfully tested on the F-15E, making the aircraft the first fighter jet to be officially compatible with this nuclear weapon.

Two test flights were flown in March at the Tonopah Test Range in Nevada. During one flight, a mock weapon was released at about 1,000 feet and nearly the speed of sound, while a higher-altitude test occurred at around 25,000 feet. Both test drops hit the target. These flight tests are one important milestone in the overall weapon certification program.

With the first production unit scheduled for completion in November 2021, the B61-12 will ultimately replace the B61-3, -4, -7, and -10 nuclear gravity bomb variants. This modern variant will be qualified for delivery on the F-15, as well as on the F-16 and the B-2 bomber. ★

ASK A PHYSICIST

Three questions for Charlie Nakhleh, the new Associate Laboratory Director for Weapons Physics.

BY ARTHUR BISHOP

In May, weapons designer and physicist Charlie Nakhleh became the Associate Laboratory Director for Weapons Physics (ALDX). ALDX develops and applies cutting-edge theory, computational models, large-scale weapon simulation codes, and state-of-the-art experiments for the design, certification, and assessment of U.S. nuclear weapons.

"I'm really excited to be in my new role," says Nakhleh, who started at the Lab in 1996. "Working at the Laboratory has been one of the most profound privileges of my life—and it hasn't gotten boring yet."

The Lab's Public Affairs Office staff sat down with Nakhleh to talk about his leadership style and what's next for him in his new role.

What do you think are the Lab's strengths right now?

We have many, but one of our biggest strengths is our intellectual honesty. Sometimes we get into cantankerous arguments over where the truth lies. But the commitment to finding objective truth in our work is one of the great foundational strengths of the Laboratory.

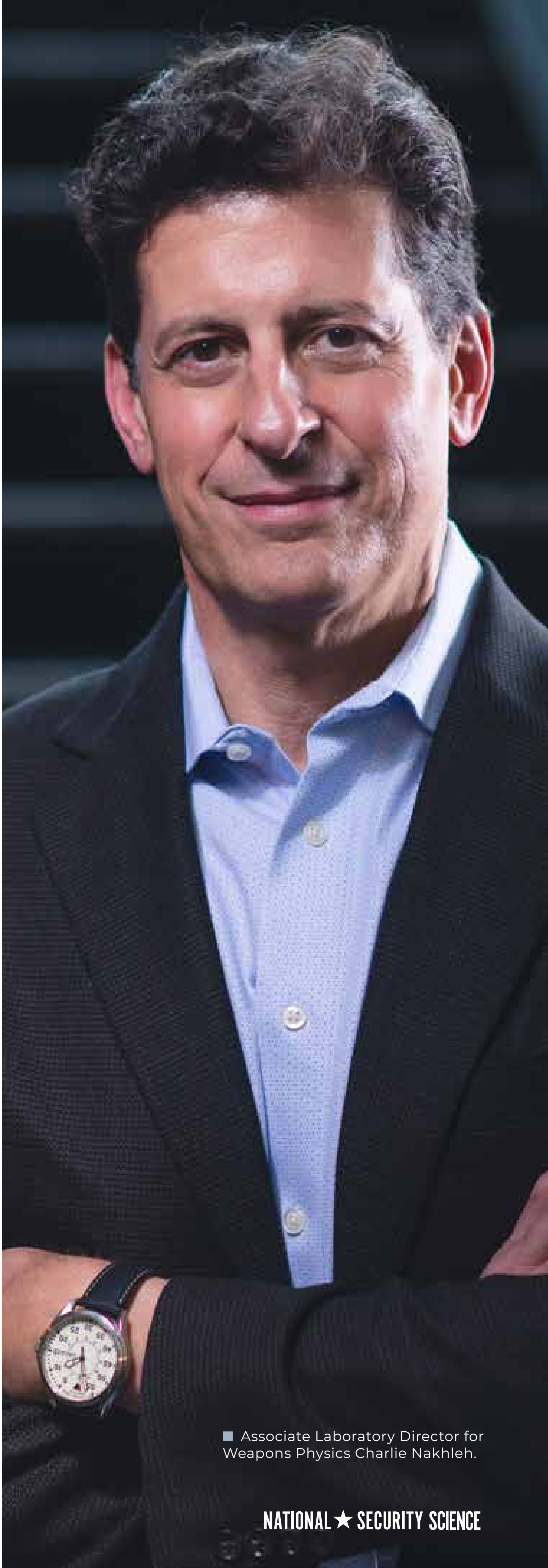
What is a particular strength of ALDX?

ALDX has a leading intellectual role to play in the debate about what it means to have a strong and resilient nuclear deterrent in an uncertain world. We don't know what the future of the deterrent is going to look like, so we have to provide the government with options that enable the country to maintain a resilient deterrent in an affordable, responsive way. And we have to be poised to do so quickly and creatively.

I want all the people in my organization to be free with their ideas and open to discussion. When I was designing experiments, I always made sure to talk to most of the people who touched the experiment. You should always talk to the technicians. You have to understand how they make the hardware because they have local knowledge that you don't have and couldn't possibly know. You can then incorporate that into your work. You have to talk to the experimental physicist and the diagnostician and ask how and why they're doing what they're doing. You can't sit in your office and do that—you have to tap into the knowledge network that's out there.

What's a recent experience that's prepared you well for your new role?

One of my most formative career experiences was the nearly six years I spent at Sandia National Laboratories. The time that I spent there helped me fill in some gaps in my professional experience and allowed me to see my home laboratory from a distance, as it were. I could also see up close how a different lab functioned. I learned that, while all of the labs are different, Los Alamos, Sandia, and Livermore are more similar than they are different. They're all national security labs that value cutting-edge science and engineering. ★



■ Associate Laboratory Director for Weapons Physics Charlie Nakhleh.

COMPUTING

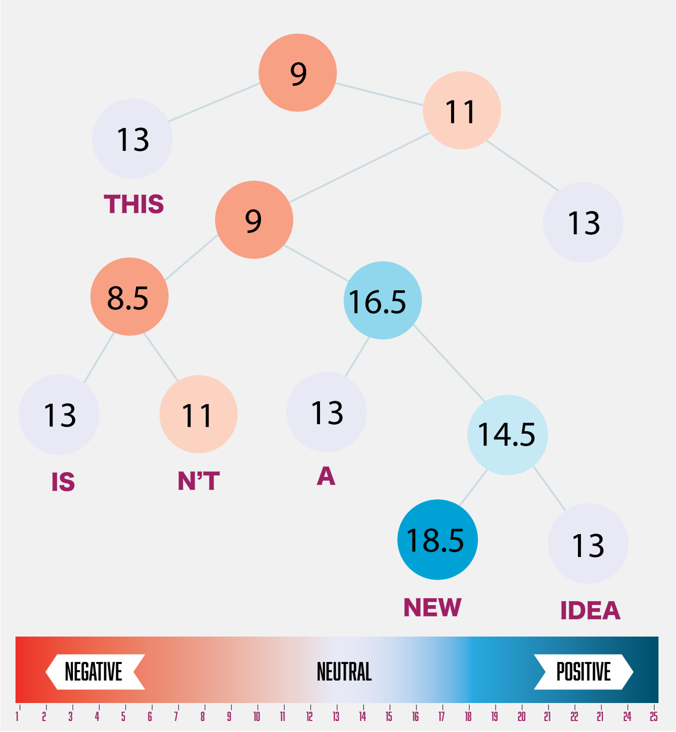
THE POWER OF SOCIAL MEDIA

By analyzing social media, governments can "poll" remote areas to better gauge policy decisions.

BY J. WESTON PHIPPEN

Social media is where people express opinions about many topics, including movies, vacations, meals, and major political events. Of course, scientists at Los Alamos National Laboratory are not the first to recognize this. But now researchers at the Lab are using social media platforms—instead of traditional polling—to quickly gauge public sentiment on matters of national and global importance.

Traditional polling involves an interested party hiring workers to ask peoples' opinions about a particular issue. But this can be expensive. It can also take a lot of time to write objective questions, to prep a team for interviews, and, for in-person polling, to have pollers knock on doors.



▲ The CoreNLP language-analyzing software scores each word in a sentence and then assigns the sentence a value.

In some countries, pollers could have difficulty or face danger when trying to reach some parts of the population, such as people living in the jungles of Colombia. Since the 1960s, remote regions of Colombia have been controlled by dangerous Marxist rebel groups, including the large and powerful Revolutionary Armed Forces of Colombia (FARC). During its 50-plus-year existence, FARC has kidnapped and killed thousands of people. Even so, in the years leading up to the 2016 peace deal between FARC and Colombia, the country's citizens had mixed reactions.

"During peace negotiations, people from all over Colombia were on social media, posting publicly about how they felt," says Ashlynn Daughton, an information scientist at the Lab. "It was such a rich set of data, and it wasn't being explored. And from the past we know it's absolutely necessary that the public support these kinds of talks, or they'll eventually fail."

In 2020, Daughton decided to see if public sentiment could be polled via social media. Her team created a timeline of pivotal events during the Colombia peace-deal talks. Daughton then overlaid that timeline with 720,915 public tweets, posted between 2010 and 2018, by Twitter users in Colombia. To weed out irrelevant tweets, her team used unsupervised machine learning to group hashtags and peace talk–related Spanish words, such as the names of politicians or groups involved in the peace talks, and other words commonly associated with the negotiations. Daughton's team then analyzed each tweet using Stanford University's CoreNLP language-analyzing software.

CoreNLP dissects a sentence and creates a "sentiment tree branch" that assigns each word and group of words a score from "very positive" to "very negative." The entire sentence is then assigned a value. With this new system, Daughton found that she could gauge the country's sentiment toward the peace talks immediately following important events during the negotiation process—such as the shooting of 11 government soldiers in 2015, a major setback to the peace talks.

When compared with polls at the time, Daughton's method was just as accurate (although it's important to note that polling data is rare, so Daughton's findings cannot be fully validated). And although this study re-created past events, it proved that, going forward, social media provides a valuable data set that, when combined with traditional polling data, may help future governments reach peace deals more quickly with more calculated steps. ★

▼ Colombians protest against FARC in 2008. Photo: Flickr/xmascarol

▲ Computer scientists Pat McCormick (left) and Galen Shipman inspect a task graph for a supercomputing application. Task graphs indicate which tasks are dependent on others and which tasks can run simultaneously.

COMPUTING

AUTOMATING AT EXASCALE

A new parallel programming system boosts supercomputing performance and efficiency.

BY KATHARINE COGGESHALL

Supercomputing is on the verge of a breakthrough—computing at the exascale, where a billion billion calculations per second will be the norm. That's 10 times faster than current supercomputing speeds. Before that milestone can be met, supercomputing applications—essentially souped-up versions of phone apps—need to become much more efficient.

Whereas your phone apps keep you posting and swiping, supercomputing applications help simulate molecule interactions, fluid dynamics, and other physical phenomena. There's a profound difference in the level of complexity here, but surprisingly little difference in the inner application workings. All applications, whether for a phone or a supercomputer, rely on coded commands (or tasks) that instruct the computer how to run the application. Applications can have millions of tasks, and those tasks can be executed in tens of thousands of different processors (the physical locations for data crunching). Designating the "what" and "where" for all of those tasks is currently hampering computing speed and efficiency.

Right now, these applications depend on their human developers for scheduling tasks and moving the corresponding data. This hands-on coding isn't realistic at the exascale—where the aim is to more accurately simulate real-world mechanisms and behaviors, which are inherently complex. In the most complex cases, there are too many choices to be evaluated and implemented by hand. Therefore, the ability to harness the full power of modern supercomputers depends on replacing this hands-on coding with something more efficient, something automated.

"We wanted to improve the process of finding ways to keep a computer system as busy as possible and assist in scheduling application tasks and data movement," says Pat McCormick, a computer scientist at Los Alamos National Laboratory.

So, Los Alamos scientists, along with colleagues at five other institutions (the Nvidia corporation, the University of California–Davis, Stanford University, SLAC National Accelerator Laboratory, and Sandia National Laboratories) created a parallel programming system to do just that. The system, called Legion, sifts through an application to determine which tasks can run in parallel, or simultaneously, to save time and boost computing efficiency. Legion can also determine which processor should run each task in order to maximize resources.

This is harder than it sounds because not all applications and processors speak the same language. Application developers have had to become experts in switching syntax, jumping between C++, Python, and Fortran codes as needed. This was an obvious area for improvement, so the Legion creators came up with a universal language instead. They named it Regent.

Now, application developers can write a single set of instructions in Regent, and Legion will automatically decide how best to run the application and move the data. Legion has been shown to improve efficiency up to 10-fold.

"We've demonstrated Legion on top supercomputers, such as Trinity at Los Alamos and Sierra at Lawrence Livermore National Laboratory, for physics simulations that support the stockpile stewardship program," says Galen Shipman, Los Alamos Legion co-developer, "and we will demonstrate it on Crossroads, the new supercomputer coming to Los Alamos, when it's up and running."

Legion is already a foundational part of the Department of Energy's Exascale Computing Project, and researchers from academia, other national laboratories, and industry have started using Legion to boost the performance and scalability of their supercomputing applications. As open-source software, Legion is available to anyone, which will allow swaths of scientists to study systems that otherwise would be impractical or impossible to investigate in the real world. ★

INFOGRAPHIC

NOT YOUR AVERAGE TRASH DAY

The Laboratory's current weapons work results in transuranic waste, which is carefully shipped offsite.

BY VIRGINIA GRANT

The term "transuranic" describes the elements that come after uranium on the periodic table—radioactive elements that aren't naturally occurring, such as plutonium. Use of these elements results in transuranic (TRU) waste, which has to be disposed of in very careful and specific ways. ★

1,233

Total number of TRU waste drums included in shipments to WIPP in fiscal year 2020 (October 2019–September 2020).

41

Number of TRU waste shipments sent from Los Alamos to the Waste Isolation Pilot Plant (WIPP), near Carlsbad, New Mexico, from October 2019 to September 2020.

315

Approximate miles from Los Alamos to WIPP.

51 %

Reduction of the Lab's TRU waste at Technical Area 55, home of the Lab's Plutonium Facility, in fiscal year 2020 (compared with fiscal year 2019).

3

Times the amount of TRU waste shipped to WIPP in fiscal year 2020 compared with the previous fiscal year.

12,705 lbs.

The weight of an empty TRUPACT-II (Transuranic Package Transporter Model 2), the container used to transport TRU waste.

385 g.

The force that TRUPACT-II waste containers can withstand in a collision with concrete; that's 385 times the force of gravity (g). For comparison, a car hitting a barrier at 30 mph creates a force of about 20 g.

26,975

Number of waste drums shipped from Los Alamos to WIPP since 1999, in a total of 1,447 shipments.

55

Gallons of TRU waste that a typical drum can hold.

14

The number of 55-gallon waste drums that can be held by a TRUPACT-II container.

1999

Year of the first-ever shipment from Los Alamos to WIPP, on March 26.

LITERATURE

MUST-READ BOOKS ABOUT LAB HISTORY

Five favorites from members of the Lab's National Security Research Center.

BY BRYE STEEVES

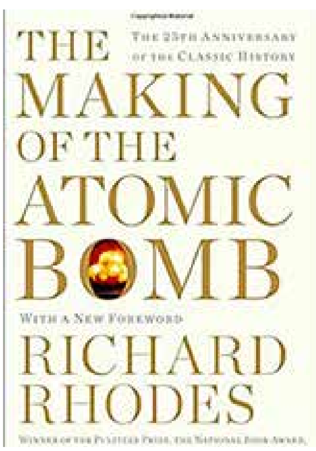
October is National Book Month, and members of the National Security Research Center (the Lab's classified library) know a thing or two about books. NSRC Director Riz Ali and Senior Historian Alan Carr share their top picks on Los Alamos and atomic bomb history. ★

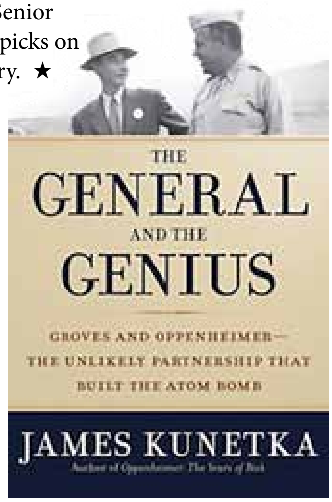
The Making of the Atomic Bomb

By Richard Rhodes

This Pulitzer Prize-winning book begins with early discoveries leading to the science of nuclear fission, through the Manhattan Project, and then the bombings of Hiroshima and Nagasaki.

Carr says: "If you only read one book on the Manhattan Project, make it this one."



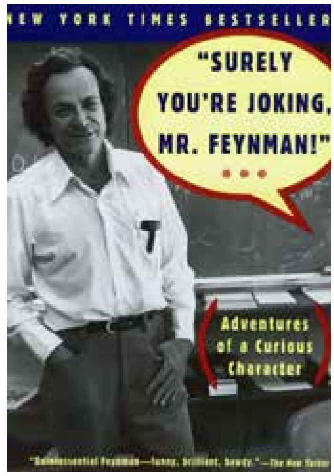


The General and the Genius: Groves and Oppenheimer—The Unlikely Partnership That Built the Atom Bomb

By James Kunetka

The story of how two extraordinary, yet opposite in nearly every way, men partnered to create the world's first nuclear weapons and help end World War II.

Carr says: "This is the first book-length study of the Groves-Oppenheimer partnership, and it's fascinating. The author, who was a visiting scientist at the Lab years ago, did a nice job."



"Surely You're Joking, Mr. Feynman!": Adventures of a Curious Character

By Richard Feynman, et al.

A book of eccentric anecdotes from Feynman, a Manhattan Project physicist and Nobel Laureate, including trading ideas on atomic physics with Einstein and cracking the uncrackable safes with the most deeply held nuclear secrets.

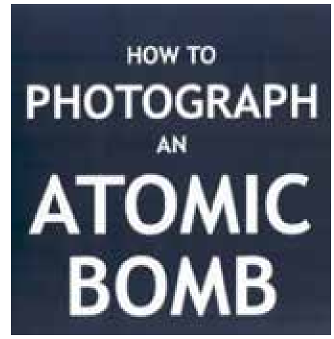
Ali says: "This is the funniest autobiography I have ever read. A side note: the NSRC has Feynman's classified Lab notebook. I didn't understand any of the scientific things he wrote in there, but I noticed that his handwriting was incredibly neat."

American Prometheus: The Triumph and Tragedy of J. Robert Oppenheimer

By Kai Bird and Martin Sherwin

A Pulitzer Prize-winning biography that examines the life of one of the most iconic scientists of all time and how he led the effort to build the first atomic bomb.

Carr says: "I often refer to this book as, 'the everything you wanted to know about Oppenheimer and so much more' biography."

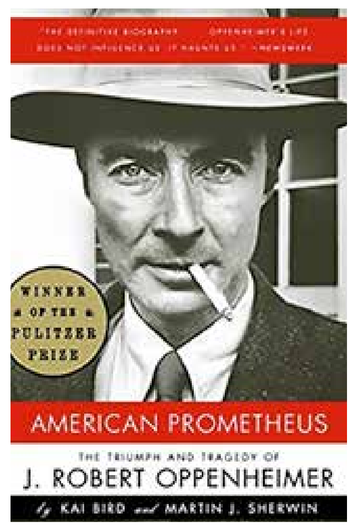


How to Photograph an Atomic Bomb

By Peter Kuran

A compilation of photos and technical details about the stories and techniques behind atomic bomb photography, including declassified pictures from U.S. atomic weapons tests.

Ali says: "This book offers insight on how early nuclear photographers learned their craft through technical prowess and ingenuity, as well as trial and error. The author is now collaborating with Lab historian Alan Carr on a book about the history of above-ground nuclear testing, which the NSRC will publish next year."

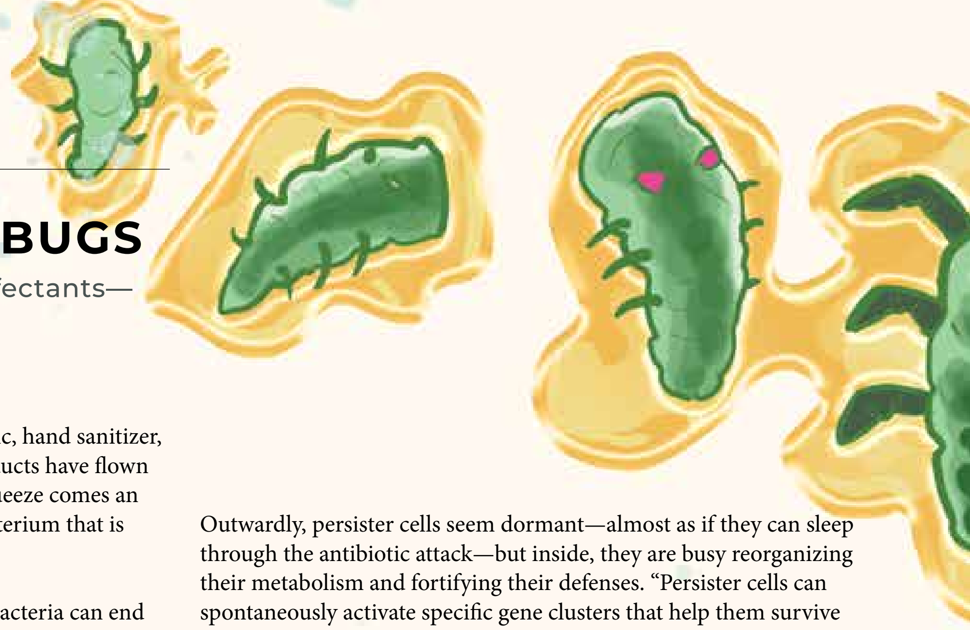


"High-performance computing is critical to maintaining peace and assessing the national nuclear stockpile to ensure safety and security. That's part and parcel of, and centrally located at, Los Alamos National Laboratory."

—NNSA Administrator Lisa Gordon-Hagerty during her July 16 visit to Los Alamos. Gordon-Hagerty cut the ribbon for the Lab's new Exascale-Class Computer Cooling Equipment project, which will support next-generation supercomputers. To learn more about this sophisticated cooling equipment, turn to p. 32.

ABSTRACTS

BIOLOGY



SQUASHING SUPERBUGS

Some bacteria are resistant to disinfectants—but not for much longer.

BY KATHARINE COGGESHALL

Since the outbreak of the novel coronavirus pandemic, hand sanitizer, antibacterial soap, and bacteria-killing cleaning products have flown off supermarket shelves. But with each spritz and squeeze comes an opportunity for the emergence of a superbug—a bacterium that is resistant to antibacterial agents.

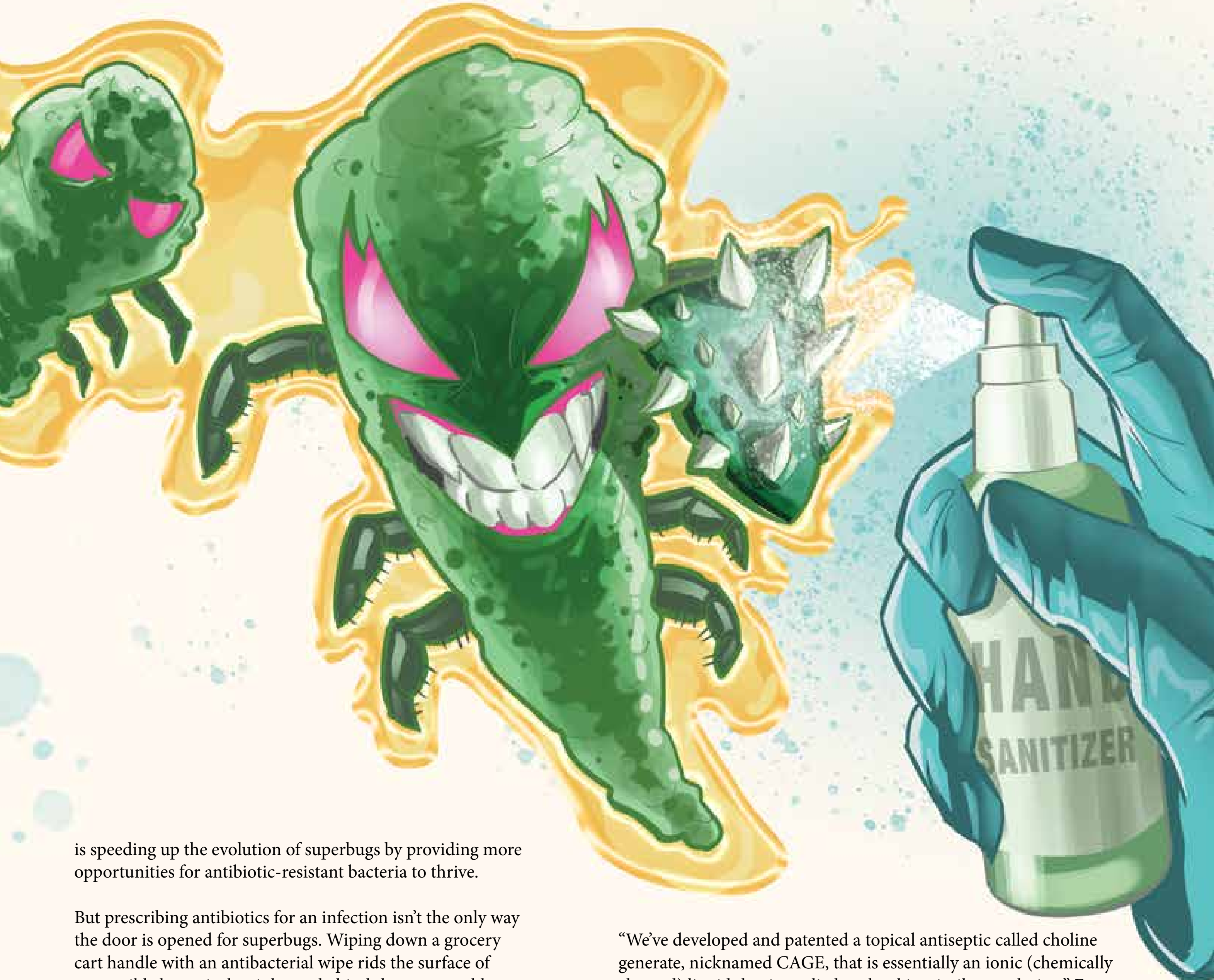
How is it possible that using products meant to kill bacteria can end up making some bacteria stronger? It comes down to percentages and evolution. When antibacterial soaps and cleansers are used to kill bacteria, they never kill 100 percent of the population. Some germs don't die because they possess a helpful genetic mutation (such as a gene that enables antibiotic resistance) or they've achieved what's called a persister state, which allows them to ride out the environmental inconvenience of an antibiotic without getting killed.

This persister state isn't well understood, but it is documented. "Persister cells are genetically identical to the susceptible bacterial cells in a population," says Sofiya Micheva-Viteva, a bioscientist at Los Alamos National Laboratory, "but they are able to persist when an environmental stressor (such as an antibiotic) is present."

Outwardly, persister cells seem dormant—almost as if they can sleep through the antibiotic attack—but inside, they are busy reorganizing their metabolism and fortifying their defenses. "Persister cells can spontaneously activate specific gene clusters that help them survive environmental stress," Micheva-Viteva continues. Even though the rest of the bacterial cells possess the same genes, they don't turn them on the way the persister cells do.

So, how much of a given bacterial population is considered persistent? This trait is actually quite rare, with fewer than one percent able to resist antibiotics. But that little amount is enough to create a big problem, especially during a pandemic. Not only are people over-cleaning with unnecessary antibacterials—good old soap and water will get the job done—but more antibiotics are being prescribed as a result of the pandemic (often, when people get sick from coronavirus, bacteria cause a secondary infection, such as bacterial pneumonia, which is treated with antibiotics). This rampant antibacterial use

◆ David Fox demonstrates how his patented antiseptic kills methicillin-resistant *Staphylococcus aureus* (aka the MRSA superbug) in less than 30 seconds.



is speeding up the evolution of superbugs by providing more opportunities for antibiotic-resistant bacteria to thrive.

But prescribing antibiotics for an infection isn't the only way the door is opened for superbugs. Wiping down a grocery cart handle with an antibacterial wipe rids the surface of susceptible bacteria, but it leaves behind the unstoppable persister cells. The superbugs can now reproduce at will, creating larger populations of antibiotic-resistant germs.

This scenario gets worse as these superbugs find new homes on skin and particularly in wounds, where superbugs are protected by a slimy matrix of bacterial cells, sugars, and proteins. "Antibiotic-resistant bacteria in wounds can be really detrimental," says David Fox of the Laboratory's Actinide Analytical Chemistry group. "It can lead to amputation of a limb or even mortality."

Fox has studied several superbugs that fall into a pathogen category known as ESKAPE. ESKAPE is a known grouping of six multi-drug-resistant bacteria: *Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and the Enterobacter species. These pathogens are extremely resistant to traditional therapeutic agents. In other words, they are superbugs, noted by the World Health Organization as high priority in terms of urgently requiring the development of new antibiotic treatments. Fox has been working on just that.

"We've developed and patented a topical antiseptic called choline generate, nicknamed CAGE, that is essentially an ionic (chemically charged) liquid that is applied to the skin, similar to a lotion," Fox explains. "It can penetrate the biofilms these superbugs make and thin their cell membranes."

In other words, Fox has discovered a treatment that can kill the unkillable ESKAPE pathogens, and it's a fair bet that CAGE could also be effective against new superbugs. However, CAGE still needs approval from the U.S. Food and Drug Administration (FDA) before it's ready for widespread human use. Once CAGE is FDA approved, Fox envisions it as being available with a simple doctor's prescription, and eventually CAGE could be an over-the-counter treatment similar to Neosporin (but far more effective against resistant bacteria).

In studies with mice, CAGE was nontoxic and not irritating, which Fox says is because the antiseptic is made from FDA-approved GRAS (generally recognized as safe) ingredients. Since the mouse studies, CAGE has been patented and is ready for human testing. Fox is now collaborating with Northern Arizona University to build CAGE into a form that can be used on a bandage. Which means that hopefully, in the not-too-distant future, squashing superbugs will be as easy as slapping on a Band-Aid. ★

COMPUTING

WORKING SMARTER

Expanding the computer codes that are used to simulate how nuclear weapons work will help scientists think about how to update weapons.

BY KATHARINE COGGESHALL

Nuclear weapons have a life cycle—just like a car or computer, they are designed, developed, produced, and maintained. And just like cars and computers, weapons won't last forever. Currently, America's nuclear weapons are being updated and refurbished—which sounds straightforward but can be complicated.

For one, the manufacturing facilities that produced our nation's nuclear weapons decades ago may run into roadblocks, such as new environmental regulations that make manufacturing certain parts or using certain materials impossible. And two, much of the workforce that created our aging weapons has retired, leaving the task to a new generation—one with no experience designing a weapon from start to finish. What would the U.S. government do if new threats necessitated an improved weapons system?

Because the United States no longer tests nuclear weapons, it maintains its weapons through science-based stockpile stewardship, which uses old testing data, data from current small-scale experiments, and supercomputer simulations of how a weapon works.

The supercomputers use computing codes that have been fine-tuned over the years for existing weapons systems. But recently, with the anticipation of someday needing improved weapons, a team at Los Alamos has begun to essentially expand the codes to enable the exploration of weapon designs.

"We wanted our engineers and scientists to exercise every part of a weapon's life cycle," says weapons design engineer Matthew Tucker.

▲ A B-2 Spirit stealth bomber drops a mock-B61 gravity bomb. The B61 is a Los Alamos–designed weapon that's currently undergoing a life extension program. Photo: U.S. Air Force

But the team quickly realized that focusing on all the phases of a weapon's life cycle is a lot more work than focusing on the "maintain" portion of the life cycle. To address their self-inflicted colossal workload, the team members introduced functional data analysis (FDA) for certain tasks.

FDA is a statistical computer program that "learns" what a designer is attempting to accomplish, such as selecting the best data out of a huge set of possibilities. As statistician Joanne Wendelberger explains, "What used to take a designer 200 runs of computer code, with each runtime at approximately 30 minutes, can be cut down to only 20 runs of code."

Using FDA allows weapons designers to explore more innovative aspects of weapons physics. One such success was demonstrated with a recent hydrodynamic (hydro) experiment—a test of a nuclear weapon design that uses nonnuclear materials. The data from this hydro, when cross-referenced with simulations from the expanded codes, provided physical proof that the codes will be useful for weapon design.

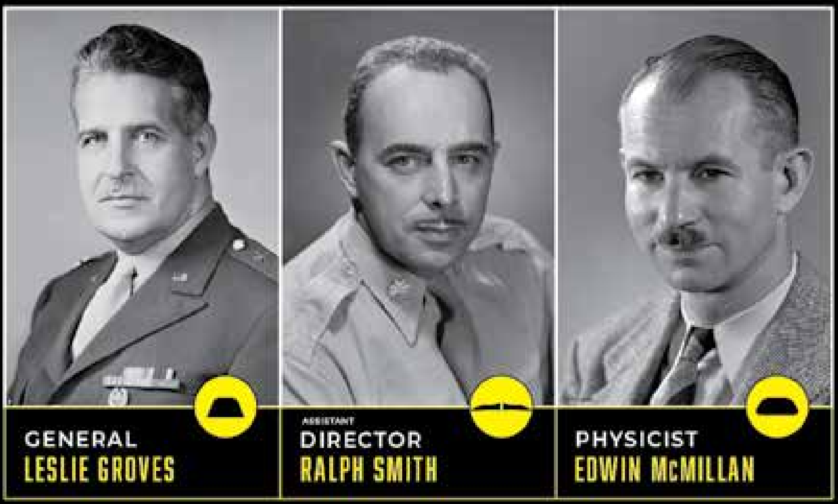
"These expanded codes are really important as we move forward as a nation," Tucker says. "They allow us to quickly respond to adversary actions and fill in gaps that could lead to vulnerabilities in the current stockpile." ★

CULTURE

NO-SHAVE NOVEMBER

Lose the razor to support men's health.

During No-Shave November (also called Movember for mustache + November), some men choose to grow 'staches to raise awareness of cancer and mental health issues. If you're going for a new look this month, take some inspiration from these past and current Los Alamos employees. ★



DETECTING DEEPFAKES

Scientists use machine learning to expose deceptive, sometimes dangerous, videos.

BY OCTAVIO RAMOS

Since the 1950s, filmmakers have used computer-generated imagery (CGI) to produce breathtaking special effects for blockbuster films. Over time, CGI has become more sophisticated and easier to produce, creating fantastic creatures like the dragon in *The Hobbit* trilogy and crafting realistic models of actual human beings.

Today, what used to take months of intense labor, multiple computing systems, and millions of dollars to produce can now be done on a home computer in a matter of hours. Thanks to advances in artificial intelligence technology, anyone can create startling videos by using sophisticated but surprisingly accessible and cheap software programs. These programs have led to a phenomenon known as a "deepfake."

"A deepfake is a manipulated video recording, either doctored footage or completely fabricated performances," explains Juston Moore of the Advanced Research in Cyber Systems group at Los Alamos National Laboratory.

The most common type of deepfake is a video portrait. "A source actor is filmed speaking, and then special software transfers the target's (say Barack Obama's or Donald Trump's) facial mannerisms—including head position and rotation, eye gaze, and lip movement—over the source actor," Moore explains. New audio is provided by an actor capable of mimicking voices. The end result is a video of a target saying something they never actually said.

"The sophistication of this technology continues to evolve quickly," Moore says. "It's getting to the point that we will no longer be able to trust our own eyes."

Deepfake technology has been used to create amusing videos, such as one with Gene Kelly's head replaced by that of Nicolas Cage for a "Singing in the Rain" dance sequence. But deepfakes can be insidious, posing a threat to national security.

Imagine a convincing deepfake of a world leader declaring war or a well-liked actress making a terrorist threat. To demonstrate quickly that such videos are frauds, a team of Los Alamos researchers is exploring several machine-learning methods that identify and thus counter deepfakes.

Garrett Kenyon, a member of Moore's team, is working on an approach inspired by models of the brain's visual cortex. In other words, Kenyon's models recognize images much like the brain does.

"Our detection technology consists of cortically inspired algorithms," Kenyon explains. "Think of these cortical representations as pieces of a jigsaw puzzle. Our algorithms are so powerful that they can reconstruct the same jigsaw puzzle—the video portrait—in an infinite number of ways."

The team discovered that the jigsaw pieces used to reconstruct real video portraits are different from the ones used to reconstruct deepfakes. The disparities are what enable the software under development to tell the difference between a real video portrait and a deepfake one.

Kenyon notes that better, more realistic deepfakes are under constant development. For example, one new target for deepfakes is body manipulation—videos that show, for example, couch potatoes playing professional sports, performing advanced martial arts, or executing 100 chin-ups with ease. Although full-body manipulation is still in its infancy, the age of the "digital puppeteer" is here.

"We are up against a rapidly moving target," Kenyon says. "Thus, we are constantly working on speeding up and improving our algorithms. Advanced deepfakes may fool the brain, but we're working to ensure that they don't fool our algorithms." ★

HAPPY ANNIVERSARY!

In 2020, 11 employees in the Laboratory's Weapons program celebrated 30, 35, and even 45 years of service to the Laboratory.

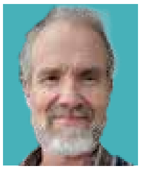
Larry Avens — **30 years**

Avens recalls what a Washington official once told him: without nuclear weapons, we'd be at the mercy of those who have no mercy. "I've been a big fan of nuclear weapons ever since," he says.

Rita Galvan — **30 years**

Michael Haertling — **35 years**

Nelson Hoffman — **45 years**



Hoffman began his career testing nuclear weapons underground in Nevada. "I remember riding on an underground railcar for miles under Pahute Mesa with a 10-kiloton bomb on the car right in front of me, thinking 'I hope we make it back,'" he recalls.

Lynne Kroggel — **30 years**

In 2000, Kroggel began working as a quality engineer on the W88 mission. "This involvement was one of greatest endeavors of the Laboratory," she says. "It was a time of work, synergy, and patriotism."

Lesley Lacy — **30 years**

Derrick Montoya — **30 years**

Montoya led the Lab's detonator group for nine years. "The good thing about detonators," he says, "is that everybody needs them. Every single experiment needs a detonator."

Bruce Trent — **35 years**

Darrell Vigil — **30 years**

Chuck Wilkerson — **30 years**

"We are scientists because we want to understand nature, but it is our human interactions that make the quest for understanding vital and rewarding."

William Wingfield — **30 years**

◆ German-born British physicist Rudolf Peierls (far left) observes the installation of the x-ray detector post at P-Site, part of the wartime Laboratory (Project Y), in the early 1940s.

▲ Deputy Laboratory Director for Weapons Bob Webster (left) and Weapons Executive Officer John Benner inspect the 1940s-era x-ray detector post at P-Site in July 2020.

A BLAST FROM THE PAST

A 1940s-era explosives site is now a protected archaeological site.

BY WHITNEY SPIVEY

In October 2016, engineers John Benner and Jonathan Morgan were driving around a remote part of Los Alamos National Laboratory. A new road had recently been cut along the edge of a canyon to provide access to groundwater-monitoring wells, and they wanted to see if it encroached on the areas where high-explosives experiments take place. "We wanted to verify that all road access to these areas had appropriate warning signs and locked entry gates," Morgan remembers.

Looking out the passenger window, Benner saw a large, rusted steel post lying on the ground. "I said 'Stop!'" Benner remembers. "'That looks really old!'"

The two got out to inspect the post, the top of which was in the shape of a cross. "We could tell it was designed to withstand blasts and that it had experienced blasts," Benner says. Beyond that, he wasn't quite sure what the post was … until a Laboratory historian recalled a Manhattan Project photo of the very same post being suspended by a crane.

During the Manhattan Project, scientists wanted to study implosion—compressing a plutonium core by detonating high explosives around it, which results in a nuclear explosion. Small Geiger counters (instruments used to detect radiation) were used to detect x-rays passing through the high explosive. Several Geiger counters, each about an inch in diameter, were placed inside the post (a hollow construction) and arranged in a grid on the inner-back surface of the heavily reinforced cross-shaped section. The post was strong enough to survive nearby explosions while allowing x-ray penetration to the detectors inside it. The resulting data was used to study components of the implosion device, although this particular method did not work as well as scientists had hoped and was abandoned in March 1945.

The x-ray detector post, and all of P-Site, where this and other explosives work had taken place, was also quite literally abandoned. The remote 10-acre area was seemingly forgotten until 2005, when the Laboratory decided to demolish the remaining buildings, which were old and unsafe.

Even then, it was another decade before Benner and Morgan stumbled upon the post. The men went back to P-Site with some colleagues on October 31, a few days after their initial discovery. "By sticking a phone camera inside the structure, we were able to get a picture of all the electrical cabling that tied the detectors together into an array," Morgan says. "As we left the site on Halloween, the team had a pretty good idea that this was a setup to radiograph detonating high-explosives objects and measure the wave shape in the cruciform x-y directions."

Laboratory archaeologist Jeremy Brunette explains how fortuitous it was that Benner and Morgan were the ones to find the post. "Due to their extensive experience in the Weapons programs, they knew what they were looking at, and could convey the significance of what they found," Brunette says. "The detector post sits right next to a seldom-used road, but to most people—myself included—it doesn't look like anything special. It really took people who understand the science and engineering components of the Manhattan Project to understand what it was."

Shortly thereafter, the Laboratory's cultural resources staff surveyed P-Site and submitted documentation to the New Mexico State Historic Preservation Office, which then declared the area an archaeological site. "The fact that it is now an archaeological site is helping to protect the site and is a critical part of the preservation of the site," Brunette explains. "My hope is that we can make progress on the archaeology of P-Site so that it's more formally recognized as contributing to the Manhattan Project. Many areas of the Laboratory are already part of the Manhattan Project National Historical Park, but P-Site is not one of them—yet."

In the meantime, Brunette and his fellow archaeologists are trying to decide what to do with the x-ray detector post. "I would like to see it displayed at P-Site, at the Laboratory's Bradbury Science Museum, or near the Lab's Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility, which is where the Lab does implosion experiments today," he says, noting that any option will require quite a bit of effort: "At probably more than 3,000 pounds, the post is very heavy!" ★

▲ Today, the Laboratory's DARHT facility is a much improved descendant of the 1940s-era x-ray detector post. DARHT consists of two large x-ray machines that produce freeze-frame radiographs (high-powered x-ray images) of mock-nuclear weapons that implode at speeds greater than 10,000 miles an hour. Completed in April 2020, a new weather enclosure (pictured) around the site's firing point (where implosions take place) keeps experiments on schedule and improves worker safety.

BETTER SCIENCE = BETTER SECURITY

For more than 75 years, computers—from human computers to supercomputers—have been **an integral part of solving national security challenges.**

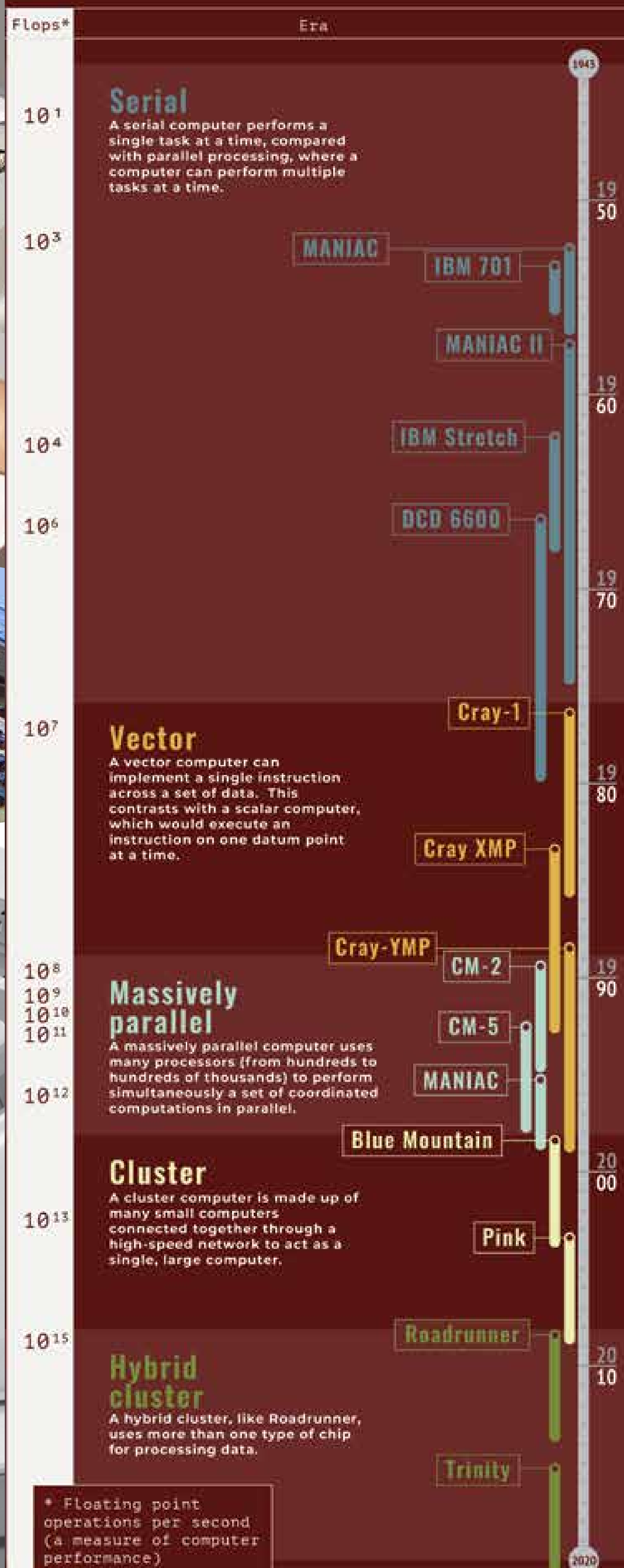
COMPUTING ON THE MESA

1943 TO TODAY

Since the Manhattan Project, scientists' need to process, store, and visualize large quantities of numerical data to simulate physical phenomena has kept Los Alamos on the front lines of computing.

BY NICHOLAS LEWIS AND WHITNEY SPIVEY

77 years of computing at Los Alamos



I

If you've seen the 2016 Academy Award–nominated film *Hidden Figures* or read the book of the same name, you know that human computers were employed by NASA in the 1960s. These computers, usually African American women, performed mathematical calculations to help the United States stay competitive in the Space Race.

But nearly two decades before the Space Race, human computers were helping to win another race—the race to create the world's first atomic bomb. This race took place in various capacities all across the United States, but much of the action occurred at a mesa-top laboratory in Los Alamos, New Mexico. This laboratory, known as Project Y, was established in 1943 with the singular goal of creating an atomic bomb to help end World War II.

At the time, scientists had a theoretical understanding of such a bomb, but to make it a reality, they needed to better understand how its components might work and how certain materials might behave. Uranium and plutonium, two actinide metals that are key to a nuclear explosion, weren't well-understood at the time. Having been discovered only in 1940, plutonium was particularly mysterious.

Scientists could hypothesize what these materials and components might do at extreme scales and speeds, and these hypotheses could be written out as elaborate mathematical calculations—so elaborate, in fact, that the math took months to do by hand.

The wives of scientists, members of the Women's Army Corps, and local civilians were recruited to perform these calculations on mechanical calculators from two California-based companies, Marchant and Friden, and the New Jersey–based Monroe Calculating Machine Company. These calculators were similar in shape, size, and operation to old typewriters; the women could add, subtract, multiply, and divide by punching numbers on a keypad. These women—along with some of the theoretical physicists who used the machines—were the first "computers" at Project Y.

Punched-card machines

IBM's punched cards were standardized in the 1920s and remained in regular use for more than half a century. These 62,000 punched cards equal roughly five megabytes of data—that's about one iPhone photo.

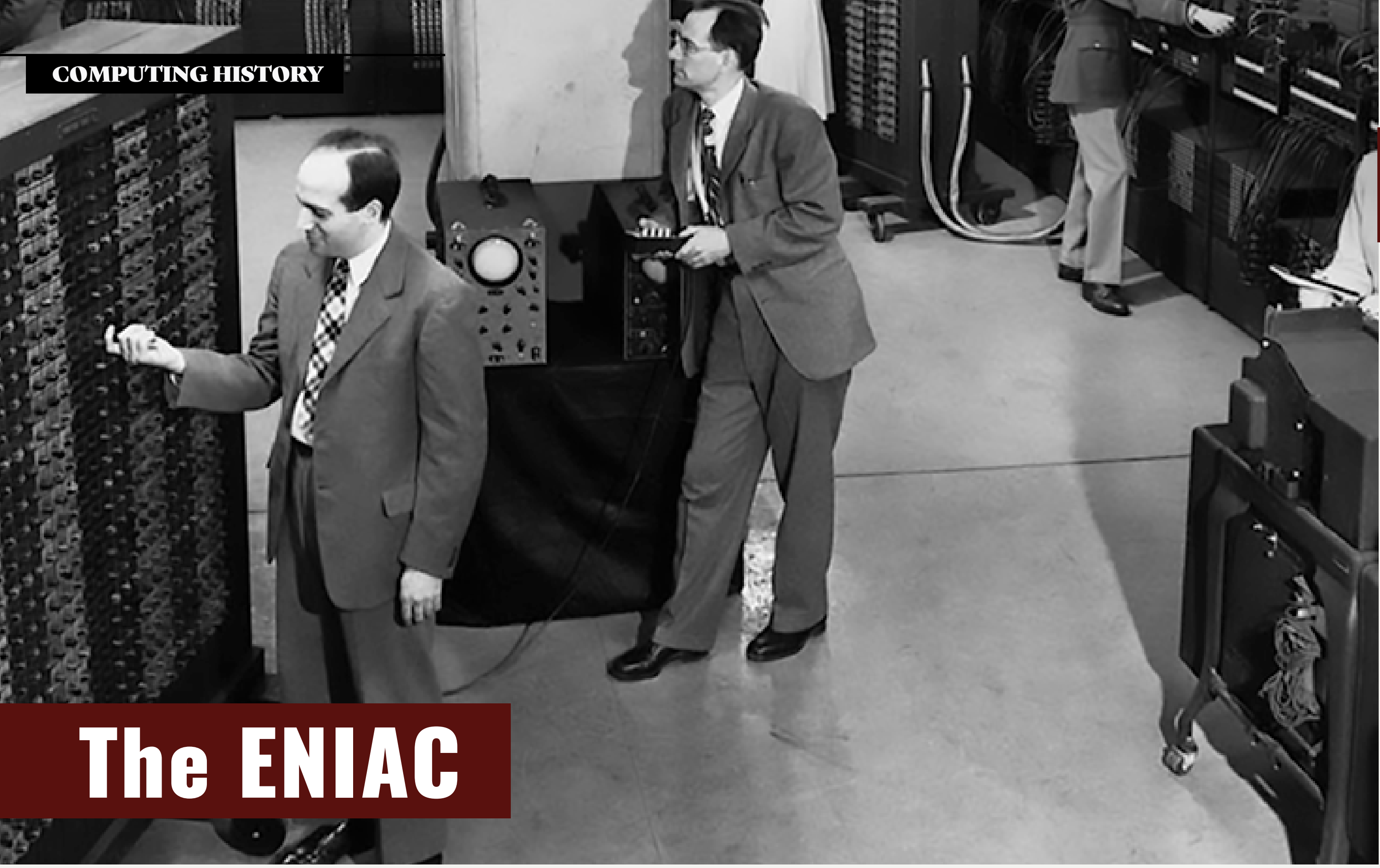
Physicist Dana Mitchell was in charge of equipment procurement at Project Y. He'd previously worked at Columbia University, and from that experience, he was aware that New York–based International Business Machines Corporation (IBM) made accounting machines. These machines used paper cards in which holes had been punched to represent data. The punched cards were then fed into the accounting machines (and later, into early electronic computers), which could perform calculations faster than human computers.

Mitchell persuaded Project Y's governing board that the IBM machines would be a good addition to the computing group. Upon arrival, the punched-card machines were modified to perform implosion simulations. (Implosion—when high explosives compress the plutonium core of a bomb to create a nuclear explosion—was scientists' hope for an atomic weapon.)

The first implosion calculation took three months to complete, but theoretical physicist Richard Feynman's refinement of the process reduced the calculating time to less than three weeks.

On July 16, 1945, the Trinity test—the detonation of the Gadget, the world's first implosion device—corroborated the results of the massive calculation effort and demonstrated the utility of the computational models the effort employed. Just 24 days later, a second implosion device—the Fat Man bomb—was dropped over Nagasaki, Japan, contributing to the end of World War II.

Operators translate problems into punched cards to be fed into the computers at Los Alamos, circa 1955.



The ENIAC

To continue its weapons work after the war, Los Alamos Scientific Laboratory (previously Project Y) needed more-powerful computational tools, particularly as scientists began to develop hydrogen (thermonuclear) weapons.

As the Laboratory began to search for these tools, John von Neumann, a Hungarian-born mathematician who consulted at Los Alamos, recalled the ENIAC project, which had been built between 1943 and 1945 at the Moore School of Electrical Engineering at the University of Pennsylvania.

"The Eniac [sic], known more formally as 'the electronic numerical integrator and computer,' has not a single moving part," according to a 1946 *New York Times* article. "Nothing inside its 18,000 vacuum tubes and several miles of wiring moves except the tiniest elements of matter-electrons. There are, however, mechanical devices associated with it which translate or 'interpret' the mathematical language of man to terms understood by the Eniac, and vice versa. … [I]ts inventors say it computes a mathematical problem 1,000 times faster than it has ever been done before."

The ENIAC occupied more than 1,000 square feet and weighed 30 tons. Even though programming the machine was tedious—wires and switches had to be rearranged for each calculation—the machine is believed to have done more calculations in 10 years than all of humanity had done until that time, according to the Computer History Museum in Mountain View, California.

In early 1945, von Neumann brought word of the ENIAC to Los Alamos, and that summer, he began working alongside physicists Stanislaw Ulam and Nicholas Metropolis to formulate a calculation for the ENIAC to test the viability of a thermonuclear bomb. The results of the test calculation, which was programmed at Los Alamos by Stanley Frankel but performed in Pennsylvania, were largely inconclusive but served as the first practical use of a general-purpose electronic digital computer.

A calculation that required 20 hours for a human computer could be performed by the ENIAC in 30 seconds.

Monte Carlo method

In 1946, Ulam was recovering from an illness and playing cards when he wondered: "What are the chances that a Canfield solitaire [which is very difficult to win] laid out with 52 cards will come out successfully?"

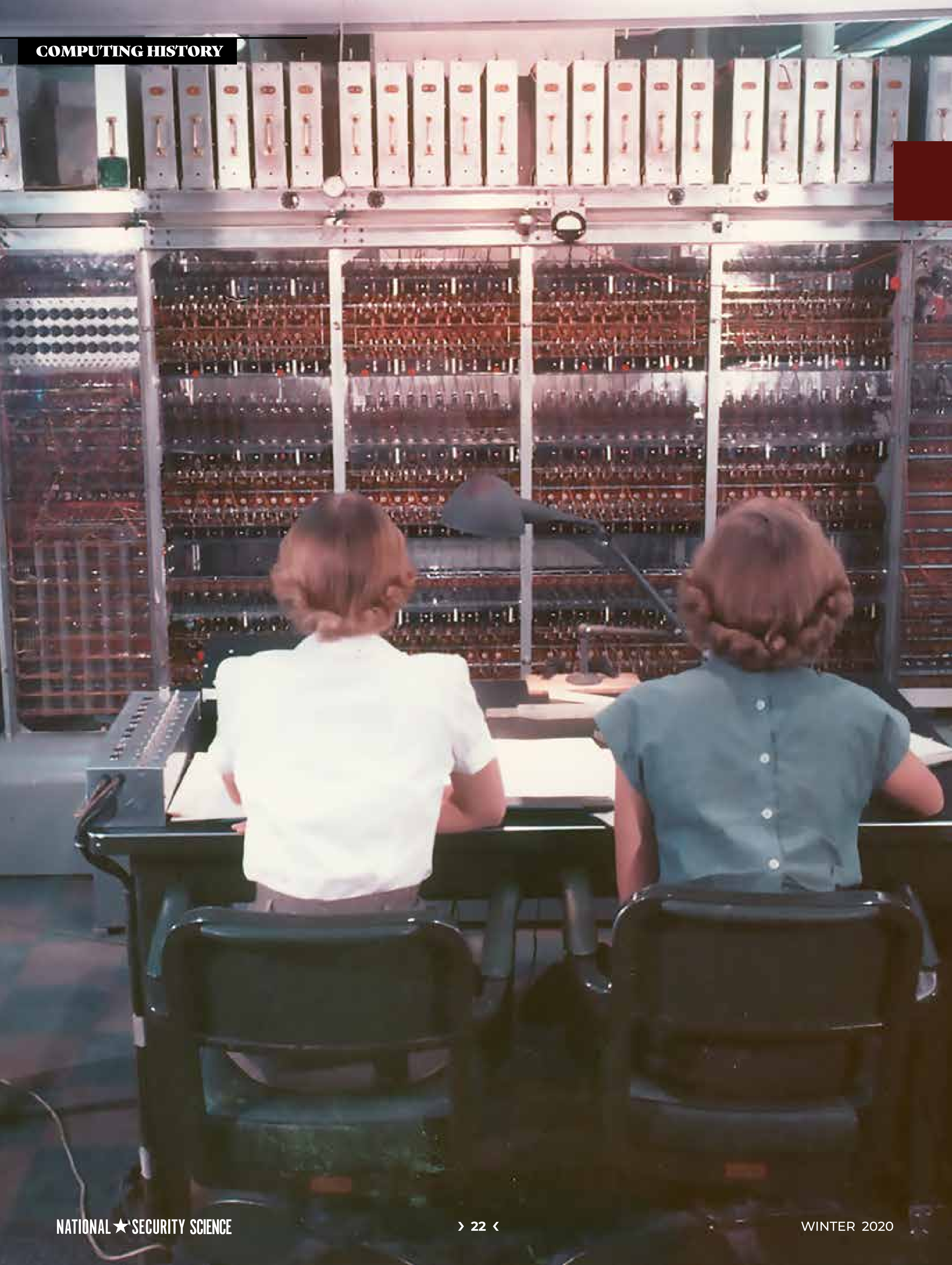
As Ulam tried to calculate the odds, he wondered if a more practical approach might be to lay out the cards 100 times and simply observe and count the number of successful plays. "This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations."

This idea—essentially using randomness to solve problems that might be deterministic (not random) in principle—became known as the Monte Carlo method. In 1946, Ulam described the idea to von Neumann, and they began to plan actual calculations. The ENIAC ran the first Monte Carlo calculation in 1947. By the 1950s, Monte Carlo methods were being applied to the hydrogen bomb effort.

"Statistical sampling had been known for some time, but without computers the process of making the calculations was so laborious that the method was seldom used unless the need was compelling," explained physicist Herbert Anderson in the fall 1986 issue of *Los Alamos Science*. "The computer made the approach extremely useful for many physics problems." In fact, the Lab maintains an entire group of Monte Carlo scientists today.

Polish-American scientist Stanislaw Ulam realized that computers could apply statistical methods to problems without known solutions.

> **"What are the chances that a Canfield solitaire [which is very difficult to win] laid out with 52 cards will come out successfully?"**
>
> **—Stanislaw Ulam**

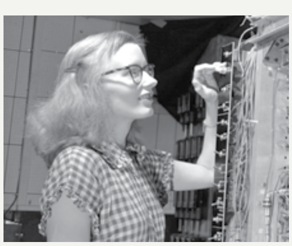


The MANIAC

The MANIAC computer, built at Los Alamos in 1952, was one of the first electronic digital computers and could perform up to 10,000 operations per second. The MANIAC powered Monte Carlo and other simulation techniques invented at Los Alamos.

MANIAC operators sat directly in front of the machine and grew to know it so well that they could debug code by ear, using a radio to listen to the interference patterns the computer generated.

The MANIAC was used to carry out calculations necessary for hydrogen bomb research as well as studies of thermodynamics, simulations using the Monte Carlo method, and attempts to decode DNA.



With each calculation, the ENIAC demonstrated the feasibility of quickly and accurately translating real-world phenomena into computable problems. But the ENIAC had three major problems: it had to be rewired for each new problem, its memory was limited, and it wasn't located at Los Alamos.

So, scientists were thrilled when the MANIAC (Mathematical Analyzer, Numerical Integrator, and Computer) was built at Los Alamos from 1949 to 1952. The MANIAC was an early example of what came to be known as "von Neumann architecture"—instead of the computer being programmed using wires and switches, it was programmed using the same media that contained the input data, such as punched cards or paper tape (a long strip of paper in which holes are punched to represent data). This process greatly reduced both the amount of time required to program the computer and the amount of human intervention needed during a computation.

The timing could not have been better. On August 29, 1949, the Soviet Union detonated its first atomic bomb. Many believed a Soviet thermonuclear weapon was imminent and that the United States should be ready with one of its own. "It is part of my responsibility as commander in chief of the Armed Forces to see to it that our country is able to defend itself against any possible aggressor," President Harry Truman said in January 1950. "Accordingly, I have directed the Atomic Energy Commission [which oversaw Los Alamos Scientific Laboratory] to continue its work on all forms of atomic weapons, including the so-called hydrogen or superbomb."

Computers such as the MANIAC were deemed essential tools in the development of these bombs. But although the MANIAC began to displace the IBM accounting machines and human computers at Los Alamos, it did not replace either one of them immediately. Human computing was a well-established form of computation, while electronic digital computing was still enormously expensive and technically challenging.

But using this hybrid system of electronic and human computers, Los Alamos inched its way closer to developing a thermonuclear weapon, and on May 8, 1951, Laboratory scientists demonstrated thermonuclear fusion with the George test at Eniwetok Atoll in the Pacific Ocean. With a 225-kiloton yield (the equivalent of 225,000 tons of TNT), George was the largest nuclear explosion up to that time.

The IBM era

A woman works on the IBM 704, the first commercially available floating-point computer and the first computer equipped with magnetic core memory. Los Alamos operated three IBM 704s in the late 1950s.

The Laboratory's four IBM 601 Multiplying Punch machines were the computational workhorses behind the implosion calculations needed for the Trinity device. Two of the four 601s pictured were capable of division and were unique to Los Alamos.

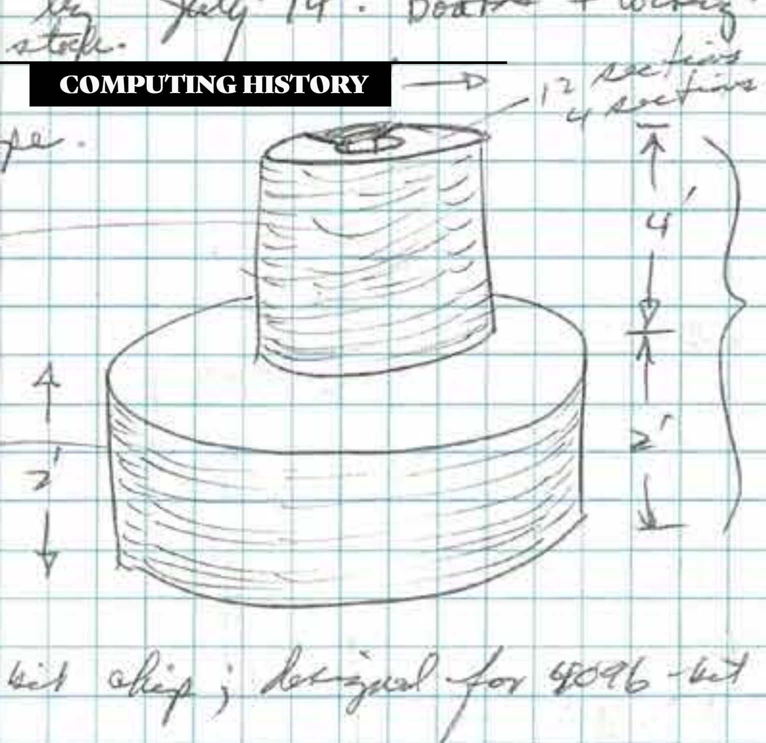
In the early 1950s, IBM developed its first commercial computer, the 701 Electronic Data Processing Machine. Also called the Defense Calculator, the 701 was a powerful digital computer based on von Neumann's architecture. In 1953, Los Alamos leased the first commercially available 701, beginning a long relationship between IBM and Los Alamos and a tradition of collaboration between the Lab and commercial vendors that has continued, in various forms, to the present.

The Los Alamos–built MANIAC edged out the 701 in performance, but IBM's successor to the 701, the 704, proved to be more capable and reliable than the MANIAC's successor, the MANIAC II. While the MANIAC II would remain in service for 20 years, it was the last of the Los Alamos–built computer systems. The cost of developing and producing digital computers meant that by the mid-1950s, purchasing or leasing a computer offered greater value than building one.

Despite opting to exclusively purchase computers following the MANIAC II, Los Alamos did not remain outside the computer development process and worked with a multitude of vendors and government and academic institutions to influence, fund, and promote developments in scientific computing.

The first major collaboration involved the IBM 7030, also known as Stretch because it was intended to "stretch" IBM's capability with computing technology—IBM pledged the computer would have 100 times the power of the 704. The new machine, however, did not live up to this lofty projection, offering closer to 35 times the power of the 704. Even so, Stretch—arguably the world's first supercomputer—was by far the most powerful computer in the world when delivered to Los Alamos in 1961.

Through the mid-1960s, Los Alamos remained an "IBM shop," making extensive use of high-end IBM computers and equipment for both weapons and administrative work. During this period, "batch processing" dominated computer use at Los Alamos. Computer users typically brought their pre-coded data and programs, in the form of punched cards or paper tape, to professional operators, who scheduled time for the user's code to run on the computer. Shorter jobs ran during the day, while longer jobs ran at night and on the weekends.



Control Data Corporation era

In an April 1974 meeting with Cray Research, Jack Worlton, who was involved with Laboratory procurement, sketched the computer that would eventually be known as the Cray-1. Los Alamos eventually had five Cray-1 computers.

The Partial Test-Ban Treaty of 1963 prohibited nuclear tests in the atmosphere and under water, which forced nuclear testing to be conducted underground. The added cost of underground testing increased the reliance on computer simulation. By first using a computer to simulate a nuclear test (largely using data from previous nuclear tests), scientists hoped to avoid expensive test failures.

As reliance on computers increased, the Lab hired more and more people to operate the machines around the clock. But it soon became obvious that what Los Alamos needed was a better computer, one that was at least as powerful as Stretch, with plenty of memory and storage to cope with the demands that increasing numbers of users and the growing complexity of weapons codes were placing on the computers.

After reviewing proposals from several manufacturers, a selection committee narrowly voted to remain with IBM. IBM's proposal, a series of larger computers that would be traded repeatedly as newer models became available, did not offer a significant jump in computing power at Los Alamos but promised to keep step with the projected computing demands.

The other serious contender in the search was from the relatively new Control Data Corporation (CDC) with its CDC 6600 supercomputer. The CDC computer, the most powerful in the world in 1965, offered four to six times the performance of Stretch. But it was rejected because it was extraordinarily difficult to program and could not recover automatically from a programming error. In addition, its parent company did not, at the time, offer the support, software, or range of disc storage that IBM provided. IBM was the safer—and cheaper—option.

In late 1965, however, IBM backpedaled on its agreement, and Los Alamos signed a contract with CDC, whose 6000-series of computers had by that time been improved in performance and reliability. The first of several 6600s arrived at the Lab in August 1966. What began as the second choice in a botched agreement with IBM developed into a new era of computing at Los Alamos, and an even longer relationship with Seymour Cray, the CDC designer behind the 6600.

The CDC machines offered considerable leaps of performance with each generation. The successor to the 6600, the CDC 7600, went on the market in 1969 and offered approximately 10 times the performance of the 6600. Los Alamos ultimately purchased four 7600s, which formed the bulk of the Lab's production capacity for nearly a decade.

The 7600s allowed for time-sharing—multiple users accessing a single computer's resources simultaneously. Time-sharing meant that, while some of the machine's processing power was invested in swapping between simultaneous users, rather than focusing entirely on processing code, users would not have to wait for machine access.

In 1972, Seymour Cray left Control Data to form his own company, Cray Research, Inc. Cray's first computer, the Cray-1, was completed in 1976 and went to Los Alamos for a six-month evaluation at no cost to the Lab. Despite the machine's extraordinary speed, it lacked error-correcting memory—the ability to detect changes in data due to mechanical or environmental problems and then correct the data back to its original state. Los Alamos returned it at the end of the evaluation period.

The evaluation at Los Alamos provided Cray Research more than technical assistance. The fact that Los Alamos, with its long history of computing expertise, was willing, even eager, to evaluate and use the company's first computer was important for the image of the new company.

Cray Research modified subsequent Cray-1 computers to incorporate error-correcting memory, and five of them went to Los Alamos. The Cray-1 was the first commercially successful vector machine, meaning that the computer's processor (essentially its brain) could execute a single instruction on multiple pieces of data simultaneously. Vectoring stood in contrast with scalar processing, in which a computer could execute only a single instruction on a single piece of data at a time.

The enormously successful Cray-1 was followed by a series of machines, including multiprocessor computers. The 1982 Cray X-MP possessed two central processors, while its successor, the Y-MP, featured up to eight. These machines formed the bulk of the Lab's computing capacity into the early 1990s.

The Lab employed nine Cray Y-MPs between 1989 and the late 1990s.

Stockpile stewardship

Visualization is an important tool for the understanding of complex data. The creation of a 3D visual representation in the CAVE enables the human visual system to detect, among other things, trends, correlations, anomalies, and unexpected events in the data.

As the 1980s drew to a close, Los Alamos continued to drive the evolution of computing. The Lab worked with Thinking Machines Corporation to develop the massively parallel Connection Machine series, which focused on quantity over quality: using thousands of microprocessors (not more powerful ones) to perform numerous calculations simultaneously. This took Lab computing into the gigaflop zone (1 billion floating-point operations, or calculations, per second) by 1990.

But then the Cold War came to an abrupt end in 1991, and nuclear weapons testing stopped in 1992. A science-based stockpile stewardship program (SSP, see p. 54) was implemented to ensure the continued safety, security, and effectiveness of the nation's nuclear deterrent. SSP would use data from past nuclear tests and data from current small-scale (nonnuclear) experiments to make three-dimensional (3D) computer simulations that would gauge the health of America's nuclear weapons.

Now a crucial part of how Los Alamos fulfills its mission, computer simulations allow Laboratory scientists to virtually detonate weapons systems and monitor what is happening inside the nation's aging deterrent—most nuclear weapons in the U.S. stockpile were produced during the 1970s and 1980s and were not designed or intended to last indefinitely.

Baseline simulations of historical nuclear tests are used to compare against real historical test data to verify the correctness of the simulation tools. Then these simulation tools, including applications, codes, and more, are used to explore weapons virtually in circumstances different from the original test to determine unseen aspects of the weapon, such as the effects of aging.

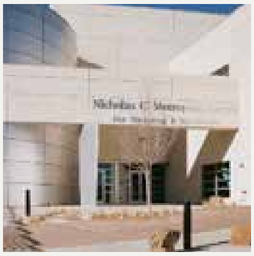
"The codes model every piece of physics involved in a weapon—these codes are very complicated and unique compared with most science codes," says Bill Archer, Lab scientist and former program director for Advanced Simulation and Computing.

The extensive use of simulations made it necessary to rapidly develop supercomputers powerful enough to replace real-world nuclear testing with virtual testing. Increasing computer speed was important, but having 3D simulations with high resolution and accuracy was even more important. To achieve high-fidelity 3D simulations, computing would need to make incredible technological leaps: gigaflops to teraflops (trillions of calculations per second, which happened in 1999), teraflops to petaflops (quadrillions of calculations per second, which happened in 2008), and petaflops to exaflops (quintillions of calculations per second, coming soon).

Accelerated Strategic Computing Initiative

Installed in 2008 and named for New Mexico's state bird, Roadrunner was the first large-scale hybrid cluster computer and the first to break the petaflop barrier.

The Laboratory's Nicholas C. Metropolis Center (also known as the Strategic Computing Complex) is a 300,000 square-foot advanced computing facility that supports DOE's Accelerated Strategic Computing Initiative.
Photo: Sears Gerbo Architecture



As Department of Energy (DOE) laboratories—including Los Alamos, Lawrence Livermore, and Sandia—pivoted to stockpile stewardship, they had to rely more heavily on computer-based simulations to verify the health of America's nuclear weapons. The DOE's Accelerated Strategic Computing Initiative (ASCI, now ASC) began in 1995 as a joint effort among the laboratories to provide the computational and simulation capabilities needed for stockpile stewardship.

ASCI was intended to promote industry collaboration and meet progressive performance goals. The initiative emphasized hardware and software solutions that could leverage existing commodity products, such as cluster computers—collections of small computers linked by a network to operate as a single, large computers.

In 1998, Los Alamos collaborated with Silicon Graphics to install the ASCI Blue Mountain cluster—the first large-scale supercomputer to emerge from this effort. "A considerable challenge in the deployment of the ASCI Blue Mountain system is connecting the 48 individual machines into an integrated parallel compute engine," states a Laboratory leaflet from 1998. But once installed, "in its full configuration, the Blue Mountain system is one of the most powerful computers installed on-site in the world."

By the early 2000s, the cluster was the dominant type of supercomputer. But Los Alamos computing planners realized that ever-larger clusters would eventually become unsustainable, needing too much electricity and too much cooling to be affordable and reach exaflop-level performance. In concept, "hybrid" clusters—using more than one type of processing chip—offered the performance and efficiency the supercomputing field needed, but only Los Alamos and its co-developer, IBM, were willing to put the radical new hybrid approach to the test.

In 2008, Los Alamos and IBM co-designed the Roadrunner supercomputer and proved enhancing performance did not mean sacrificing energy efficiency. Based on what was considered a radical approach at the time, Roadrunner was the first large hybrid supercomputer. This meant that Roadrunner had multiple kinds of processing chips, rather than just one type of microprocessor. With careful programming, Roadrunner used the chip best suited for a task; either its conventional AMD microprocessors—like those in a desktop computer—or its energy-efficient Cell accelerator chips from IBM—similar to the Cell chip found in the Sony Playstation 3. This hybrid approach (rather than a "one-chip-fits-all" approach) made Roadrunner the fastest computer in the world and extremely efficient, using only one-third the power of equivalent, nonhybrid supercomputers. Ever since Roadrunner pioneered the concept, hybrid supercomputers have become the norm.

On May 26, 2008, Roadrunner became the first supercomputer to exceed a sustained speed of 1 petaflop/s—a million billion calculations per second. How fast is a petaflop? Imagine that a normal desktop computer was the fastest human sprinter alive, running at about 28 miles per hour. At full speed (and without stops), that sprinter could run from Los Alamos, New Mexico, to New York City in 72 hours. Roadrunner, a 1-petaflop supercomputer, would make the same journey in only 25 seconds. A 1-exaflop supercomputer would reach New York in only 2 seconds.

Trinity and Crossroads

In 2002, the 300,000-square-foot Strategic Computing Complex was built to house the Lab's ever-expanding fleet of high-performance computers. The floor of the supercomputing room is 43,500 square feet, nearly the size of a football field. The largest computer there, named Trinity after the 1945 Trinity nuclear test, enables (among other things) large-scale data analysis and visualization capabilities in two of the building's special facilities: the Powerwall Theater and the Cave Automatic Virtual Environment (CAVE), an immersive virtual reality environment powered by computers.

In the CAVE, users wearing special glasses can interact with virtual 3D environments of everything from nuclear detonations to the birth of galaxies. Weapons scientists must produce high-resolution simulations of real events, and interacting with visualizations helps scientists test their hypotheses and their solutions to problems.

The tri-lab computing community at Los Alamos, Lawrence Livermore, and Sandia National Laboratories share Trinity, an Advanced Simulation and Computing Advanced Technology System (ATS) supercomputer, for their largest-scale weapons-computing needs. Los Alamos uses Trinity primarily to study weapons performance, Sandia to study weapons engineering, and Livermore to quantify uncertainty (to study the likelihood of a certain outcome if some aspects of the problem are not known).

Trinity, however, is approaching the end of its useful lifetime. Even though it's only five years old, soon parts will no longer be available because they're already considered dated—that's how fast the computing world moves.

In 2022, the Lab will acquire a new computer, Crossroads, named for Operation Crossroads, the 1946 series of nuclear tests in the Marshall Islands. Hewlett Packard Enterprise (HPE) was awarded the $105-million contract to deliver Crossroads to Los Alamos.

"We can only purchase and build these big world-class computers one at a time," says Jim Lujan, a program manager in the High Performance Computing division. "The three labs share NNSA [National Nuclear Security Administration] codes and computing time on these unique resources, and it's typically two and a half years before an increase in capability is needed, requiring the next system." The location for the ATS-class supercomputers alternates between Los Alamos and Livermore.

Crossroads' design is focused on efficiency in performance, workflow, and porting. Performance efficiency means that more usable computing power is available to the applications than on previous systems. Workflow efficiency aims to decrease the total time-to-solution of the entire problem, including all steps like data input, computing, data output, and analysis. Porting efficiency refers to the ease with which existing computing codes can be enhanced to take advantage of the new capabilities of the Crossroads system.

"This machine will advance our ability to study the most complex physical systems for science and national security," says Jason Pruet, Los Alamos' program director for the Advanced Simulating and Computing (ASC) program. "We look forward to its arrival and deployment."

At Los Alamos' Strategic Computing Complex, installation of the cooling infrastructure to support the Trinity supercomputer is underway in June 2015.

Following its two-stage installation between 2015 and 2016, Trinity was the first platform large and fast enough to begin to accommodate finely resolved 3D calculations for full-scale, end-to-end weapons calculations.

The computer operations center at the Laboratory's Strategic Computing Complex, where some supercomputers are located.

Looking forward

The Los Alamos tradition of adapting and pushing the boundaries of what's possible in high-performance computing, which began with human computers, now continues with the use of multi-petaflop clusters and the exploration of quantum computing (see p. 34).

Although the technologies have changed, the talent for creating and innovating where few, if any, have trod before, has remained consistent. Although the future of computing is difficult to predict, Lab history demonstrates that Los Alamos will be a driving force in the decades to come, helping to turn big ideas into the commonplace. ★

*Author **Nicholas Lewis** has compiled a history of computing at the Laboratory. To learn more about his work, email HPChistory@lanl.gov.*

COOL COMPUTING

Warm water mixed with a little detergent keeps supercomputers from overheating.

BY CRISTINA OLDS

When your iPhone overheats, it shuts off or even becomes permanently damaged. A supercomputer—which is approximately 200,000 times more powerful and 192,000 times bigger than an iPhone—is no different, except that the consequences are greater because a supercomputer is expensive (millions of dollars) and the data it's crunching may have national security implications. Therefore, it's imperative that supercomputers are cooled properly.

Crossroads, the new supercomputer coming to Los Alamos National Laboratory in 2022, will be direct-liquid cooled—heat from this supercomputer will be removed by a liquid coolant that's a mix of treated wastewater, detergent, and Nalco 460 CCL 100. The detergent helps prevent corrosion of the cooling pipes, and Nalco is a chemical that prevents algae growth.

Liquid cooling was used in the 1980s before air cooling became popular in the '90s. Now the pendulum is swinging back to liquid because recent advances in liquid cooling have made it more efficient than air cooling. Liquid carries away more heat from the computer's core than air, and liquid directly removes heat, which is more effective than blowing cool air over a supercomputer.

A direct-liquid cooling system circulates 75-degree liquid coolant through a closed system that directly contacts the areas in the supercomputer where the most heat is generated. Unlike the 60-degree coolants used in previous generations of cooling systems, the warmer, 75-degree coolant in the current system uses less energy to do its job. The coolant carries the heat away from the computer, allowing the machine to operate at a viable 110 degrees.

The coolant, now warmer because of its contact with the computer, flows through a series of loops inside large towers to cool off. The water in the towers is evaporated to expel heat into the atmosphere. The number of times the coolant runs through these loops is called the cycles of concentration (CoC).

With each CoC, some of the water evaporates, so after several CoCs, new water is needed. Any remaining old water is tested for environmental safety and released into a nearby canyon. New treated wastewater from the Laboratory is used to replace the spent tower water.

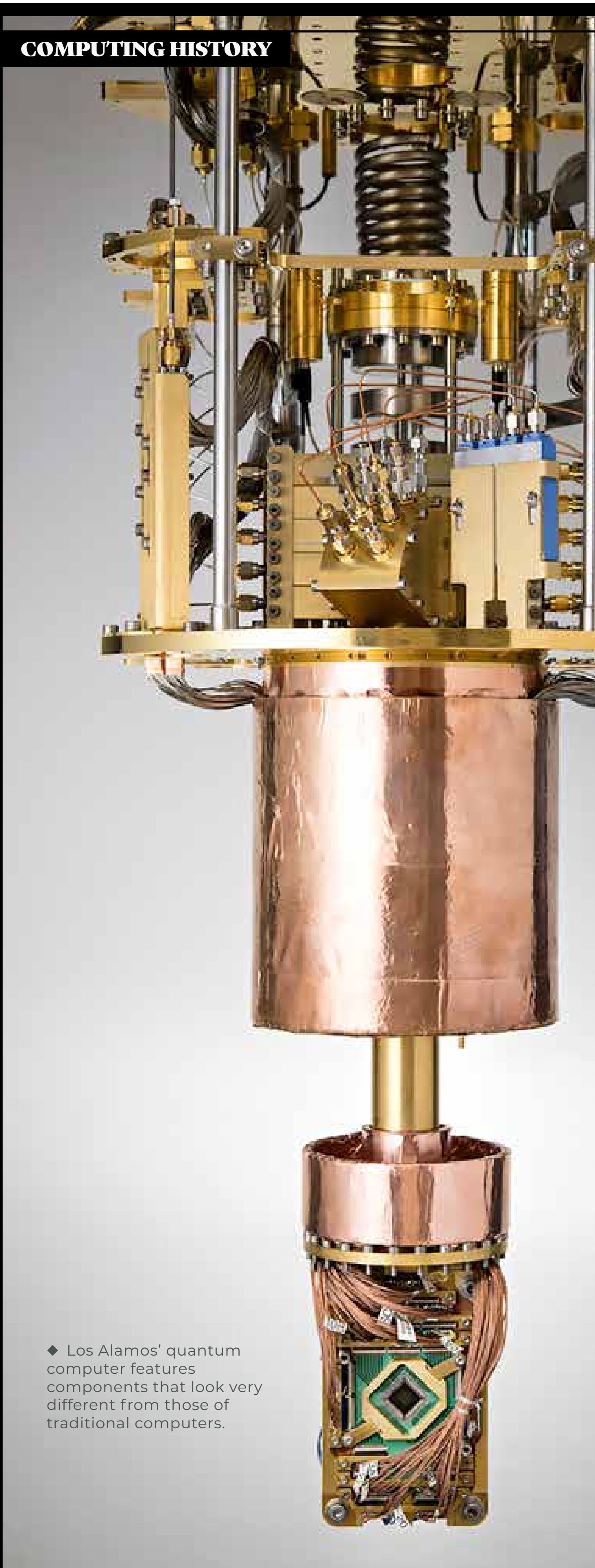
◆ From left: John Sarrao, Thom Mason, Gabriela Lopez-Escobedo, Lisa Gordon-Hagerty, John Gallegos, Kathye Segala, Michael Weis, and Gary Grider cut the ribbon in front of the new cooling towers at the Laboratory's Nicholas C. Metropolis Center for Modeling and Simulation on July 16.

The higher the CoC, the more times water circulates before it needs to be replaced. Higher CoCs use less water for the same job. One way to increase the CoCs is to improve the quality of water being used. Well water, for example, has a CoC of 2.5—meaning it can circulate in the towers 2.5 times before new water is needed.

The water cooling the Laboratory's Strategic Computing Complex's supercomputers is repurposed water from the Lab's Sanitary Effluent Reclamation Facility (SERF). In 2019, SERF improved its water purification process, which gave the Lab's treated wastewater a CoC of six and greatly reduced the total amount of water necessary to cool the Lab's current supercomputer, Trinity. Instead of using 88,000 gallons daily, Trinity now uses 50,000 gallons. Crossroads, which will be even more of a workhorse than Trinity, is estimated to use 90,000 gallons—far less than it would have without the sustainability project.

Less environmental impact plus a "large jump in efficiency," makes direct-liquid cooling a big win, according to High Performance Computing Division Leader Gary Grider. But those aren't the only perks. "The machine is super quiet since there are no fans and just pumps," says Grider, who was at the Lab in the '80s and can remember the original liquid-cooling technology. "It's been a long, long time since the systems were cooled with just water." ★

▲ Completed in May 2020, the Exascale-Class Computer Cooling Equipment project increased the existing water-cooling capability at the Laboratory's Strategic Computing Complex, where the new supercomputer, Crossroads, will reside. Crossroads is due at the Laboratory in 2022.



◆ Los Alamos' quantum computer features components that look very different from those of traditional computers.

THE BIZARRE AND PROMISING WORLD OF QUANTUM COMPUTING

Quantum computers derive their (potentially) extreme speeds from the mysterious properties of quantum physics.

BY VIRGINIA GRANT

Quantum computing, first discussed abstractly in the 1980s by physicists Paul Benioff and Richard Feynman, is gaining momentum, and significant advancements in this strange frontier are coming out of Los Alamos' Theoretical (T) Division. In 2015, Los Alamos acquired a quantum computer (and updated it in 2019), and a number of theoretical physicists are working to find ways to unleash the potential of this strange machine.

Quantum computers use the properties of quantum physics to find shortcuts in computing by taking unconventional routes to perform operations. The individual operations are not faster than those of classical computers—they might, in fact, be slower. But, for some types of problems, a quantum computer can reach a result with many fewer operations than a classical computer.

In classical computers, binary code—a language of ones and zeros—tells the computer what operations to perform by turning transistors (electronic signals) on and off. But what could a computer do if the transistors could be on and off and in between, all at the same time?

Physicist Erwin Schrödinger posited in his classic quantum mechanics paradox that a cat that may or may not have been poisoned after being placed inside a closed box is, until the box is opened, both dead and alive. Schrödinger's famous cat illustrates a concept called quantum superposition—the ability of two states to exist together. Superposition is one of the things that gives quantum computing the potential to be much faster than classical computing for specific types of problems. Instead of the traditional ones and zeros of classical computers, qubits (quantum bits, made of subatomic particles) are able to be the equivalent of one, zero, and everything in between.

Another way quantum computers are able to produce extremely fast operations is through entanglement. Entanglement describes two quantum particles that are so intrinsically connected that their states, and changes in those states, are correlated. How and why entanglement exists is still a mystery, but the phenomenon is very useful when utilized for quantum computing.

Superposition and entanglement can lead to interesting and powerful computing properties that are not possible with classical computers. Quantum computers won't be useful for most things—they aren't going to make websites load faster or help us with most calculations—but, for a very specific subset of problems, they have the potential to move from the beginning to the end of operations at almostunbelievable speeds—millions of times faster than their classical counterparts. Because of this, quantum computers cannot replace classical computers, but they do have exciting potential for some specific problems, especially large mathematical calculations.

Cryptography (the computerized encoding and decoding of information) is one of the most promising fields for quantum computing, as it involves patterns in numerical systems. The race to develop superior quantum computing capabilities in codebreaking is of particular importance for national security. If another country gains the ability to use quantum computers to break codes, and the United States does not yet possess that ability, all of our digital security measures could be rendered useless in the blink of an eye. The type of codebreaking that takes classical computers a very long time could be much faster on a quantum computer.

Advancement in quantum computing is tricky and arduous. Right now, most quantum computers struggle to add two plus two. Some of the most significant obstacles to quantum computing are in the infrastructure required to run the machines. Many require extreme cooling (temperatures near absolute zero), they are incredibly expensive (at least tens of millions of dollars per system), and they aren't particularly useful—yet. So quantum computers and the scientists who work on them are rare.

There are also myriad problems inherent in machines that use subatomic particles and physical processes that are difficult to understand, much less control. Qubits are prone to decoherence, a decaying and falling-apart that prevents them from finishing their jobs. One of the biggest causes of decoherence is noise. This means not that the computers are loud, but that they produce a great deal of energy—noise—that interferes with the qubits, preventing operations from being correctly performed. A team at Los Alamos led by physicist Patrick Coles has recently developed a method to make theoretical earplugs for qubits. "Our method is analogous to how a vaccine makes you immune to a virus," Coles says, "in that we produce circuits that are immune to a given device's noise."

Challenges aside, Los Alamos "is one of the strongest national labs when it comes to quantum computing theory," says Rolando Somma, a physicist in T Division, who is active in the Laboratory's quantum computing summer school. The participants, a combination of graduate students and upper-level undergraduates, come to Los Alamos each summer to be mentored by scientists working on quantum computing theory. In 2020, the school was conducted virtually but with the same number of lectures and projects as previous years. The school "typically results in new collaborations and papers," Somma says.

And while the Laboratory is busy collaborating with students, it's also collaborating with other research institutions. In August, Los Alamos joined the Quantum Science Center (QSC), a new Department of Energy initiative based at Oak Ridge National Laboratory to develop research in quantum computing. Los Alamos will lead one of the QSC's three major research thrusts—quantum simulations and algorithms—and will contribute to the other two (quantum materials discovery and design, and quantum devices and sensors for discovery science).

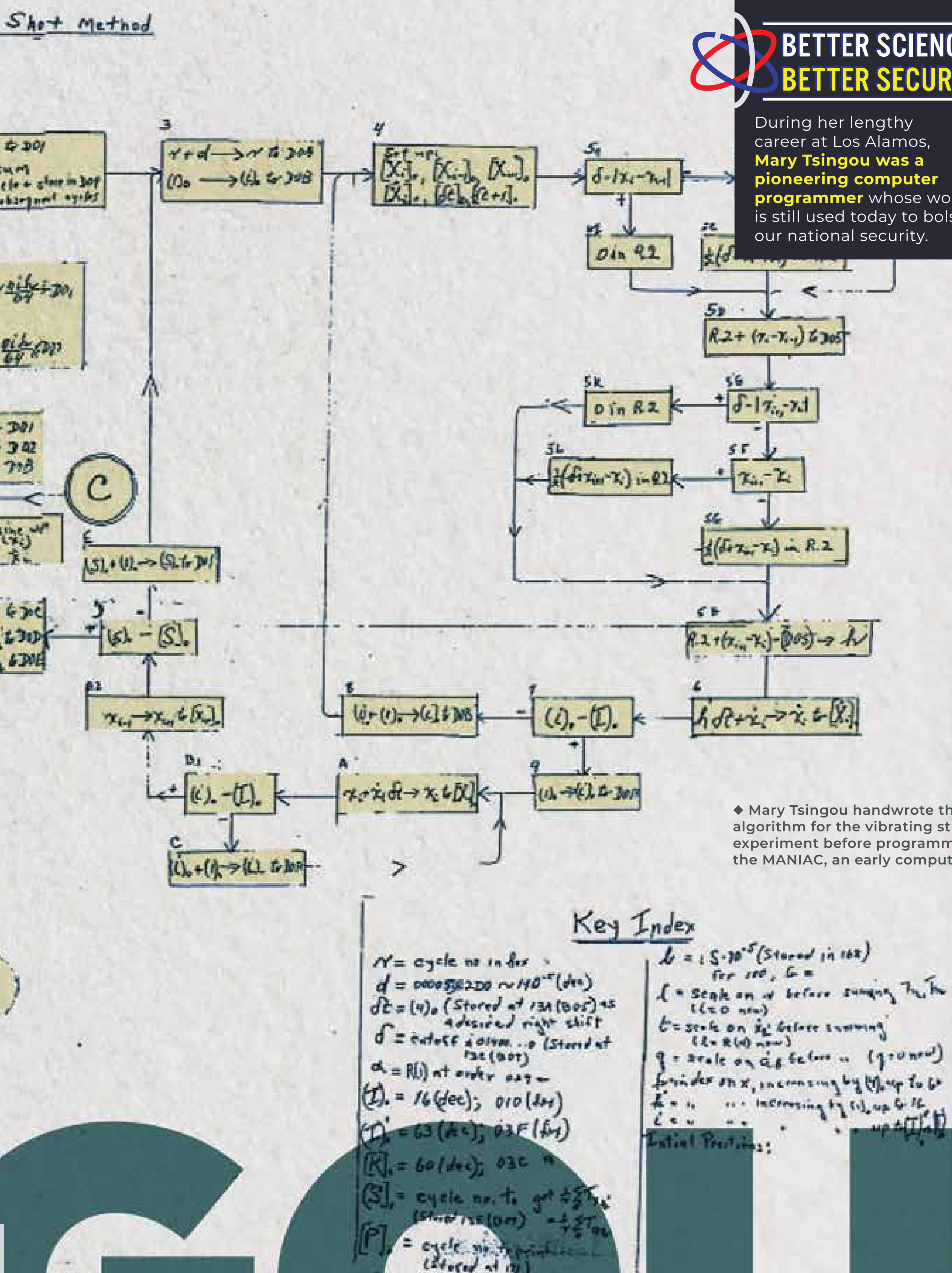
"Quantum simulation is expected to exponentially transform our ability to predict quantum phenomena," says Andrew Sornborger, a scientist in the Computer, Computational, and Statistical Sciences Division who will lead Los Alamos' quantum algorithm efforts in QSC. "Being at the front of this research will extend our scientific computing capabilities well beyond the state of the art." ★

◆ Schrödinger's cat, alive in this iteration, represents a fundamental paradox in quantum physics that is used in the theory and development of quantum computing.
Photo: Dreamstime photograph 121112695 © Sonsedskaya

“WE THANK MISS MARY TSING

A half-century after being mentioned in the footnote of a seminal physics paper, one of the Laboratory’s first computer programmers gets the recognition she deserves.

BY VIRGINIA GRANT

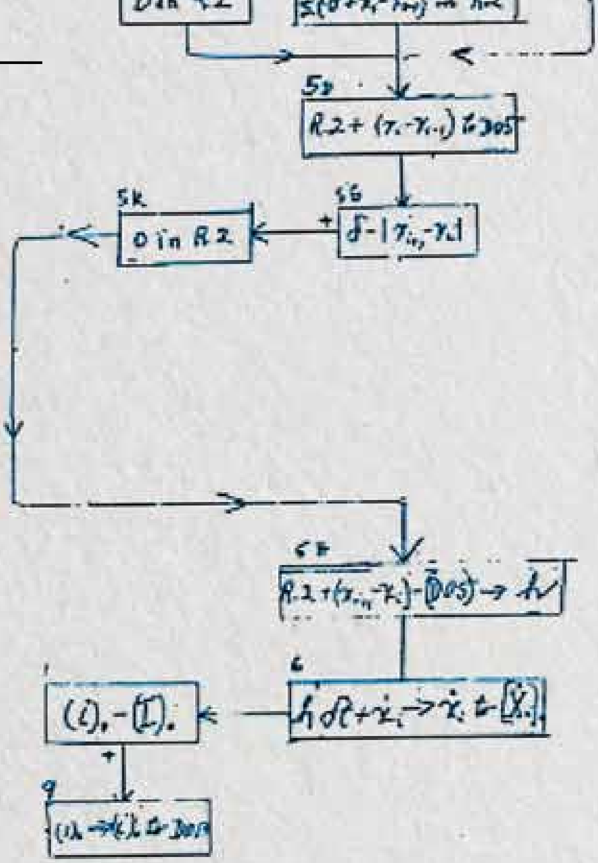


BETTER SCIENCE = BETTER SECURITY

During her lengthy career at Los Alamos, **Mary Tsingou was a pioneering computer programmer** whose work is still used today to bolster our national security.

◆ Mary Tsingou handwrote the algorithm for the vibrating string experiment before programming it into the MANIAC, an early computer.

GOU”



◆ Mary Tsingou in 1955.

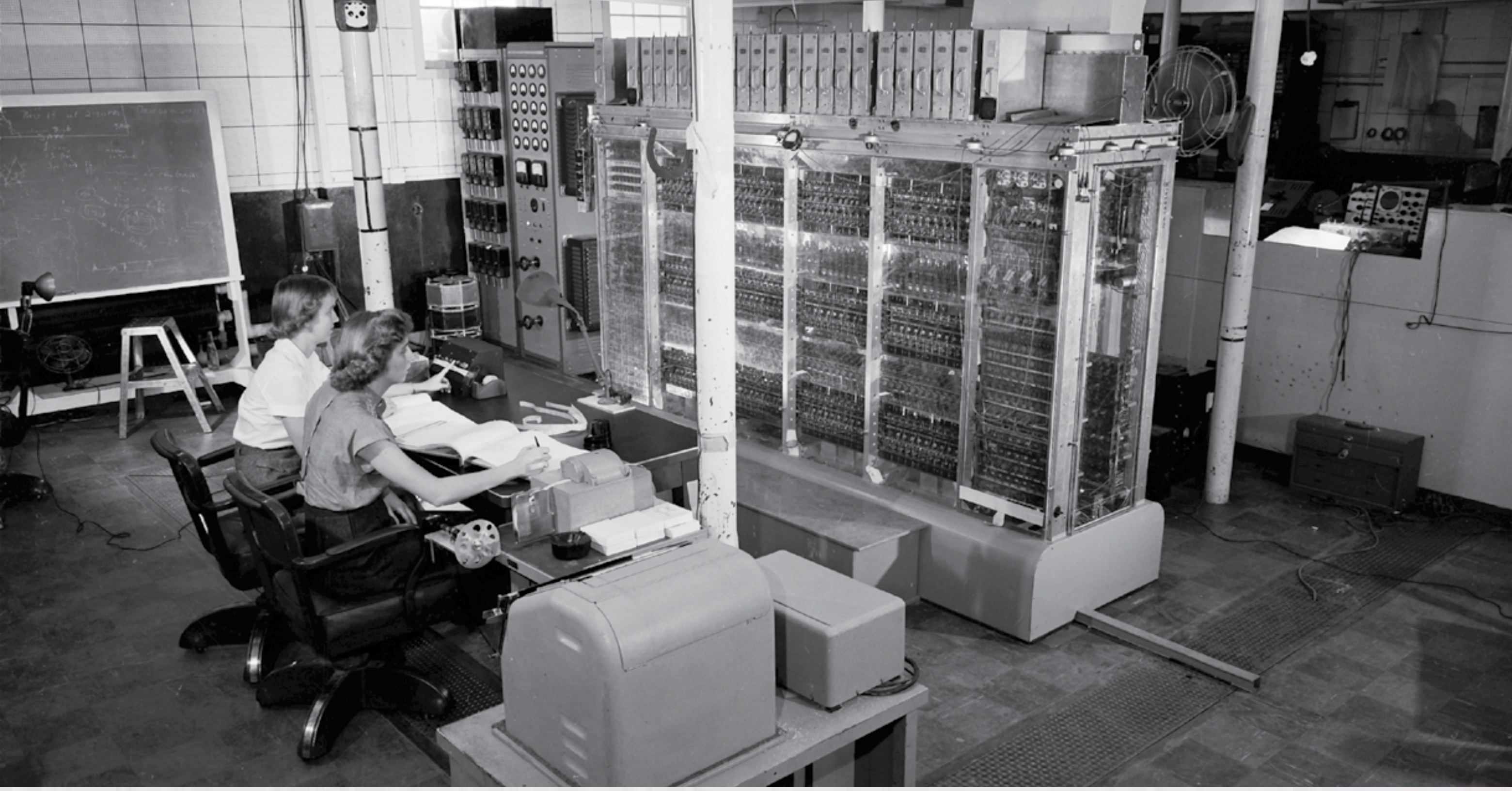
IN 1955, Los Alamos Scientific Laboratory published the paper "Studies of Nonlinear Problems," which detailed the methods and results of a mathematical physics simulation run on the MANIAC, the Laboratory's first electronic computer. The scientists who wrote the paper—Enrico Fermi, John Pasta, and Stanislaw Ulam—were quickly recognized for the remarkable simulation, which came to be called the Fermi-Pasta-Ulam (FPU) problem. In a footnote, the authors wrote, "We thank Miss Mary Tsingou for efficient coding of the problems and for running the computations on the Los Alamos MANIAC machine."

It would be decades before that footnote would gain attention from the global scientific community, but Mary Tsingou Menzel (her name since getting married in 1958) was well-known among her colleagues throughout her 40-year career as a mathematician and computer programmer at Los Alamos. Today, she sees that early simulation as only a blip in a career that included the development of the first hydrogen bomb and work on the proposed missile-defense program known as Star Wars (the Strategic Defense Initiative). Though she retired almost 30 years ago, some of her coding work is used to this day, and her legacy remains in the monumental work she performed as one of the first computer programmers of the 20th century.

Human calculators

In 1951, Mary Tsingou was an undergraduate studying mathematics and education at the University of Wisconsin when an instructor told her, "They're looking for women mathematicians at Los Alamos." The Korean War was on, and the Lab had found that hiring and training men as mathematicians was mostly futile because they were so often drafted. Faced with a job market that was particularly tough for female math teachers, Tsingou decided to apply. She landed the job, and on January 7, 1952, she moved to Los Alamos.

Upon being hired, Tsingou was flatly informed that she and the other young



▲ Operators work on the MANIAC in the 1950s.

women would be paid less than men with the same skills and qualifications because "men were breadwinners and women were just supplementary." Still, Tsingou was excited about work at Los Alamos; she had chosen the job over others at companies such as General Electric because "the salary was twice as much" and because she had never been out West. She also felt pride in her position, working at a national security science laboratory during the Cold War. "We were doing this in the same way young men went into the military," she says of herself and her colleagues. "We knew it was something that was important for the country."

Tsingou's first job was in Theoretical (T) Division, and she worked in the T-1 group on calculations used in preparation for testing the design of the hydrogen bomb, which uses fusion (in addition to fission) to create an explosion even larger than the one an atomic bomb produces. Los Alamos was racing against the Soviets to develop the hydrogen bomb, and the calculations performed in T-1 were of vital importance in determining if and how such a device could be detonated.

Almost all the mathematicians who worked as human calculators at Los Alamos were women, most in their early 20s and just out of college. Using Marchant calculators—early machines that could add, subtract, multiply, and divide—they solved specific problems. Tsingou was surprised on her first day of work to discover that she wasn't using her math degree—she was just using a calculator to add and subtract. "I was sort of disappointed," she remembers. "When we get out of college, we say we're going to set the world on fire," but instead she was assigned what she calls "mundane types of jobs."

Becoming a coder

Tsingou was soon recruited to work as one of the first programmers, or coders, of the MANIAC (Mathematical Analyzer, Numerical Integrator, and Computer). When the MANIAC was up and running, Tsingou says, the Lab didn't have anyone to program it, so Jack Jackson, a Los Alamos programmer who later ran the aerospace division at IBM, gave a class on programming. "I was very interested in learning programming," Tsingou says, "because it was pretty boring sitting there doing addition and subtraction."

Tsingou's job as a programmer was to tell the machine what calculations to perform, which required that she

* We thank Miss Mary Tsingou for efficient coding of the problems and for running the computations on the Los Alamos MANIAC machine.

▲ Scientists Enrico Fermi, Stanislaw Ulam, and John Pasta authored "Studies of Nonlinear Problems," the paper on the vibrating string experiment, which was programmed by Mary Tsingou.

know binary (two-symbol) coding language. "It was a very rudimentary machine language," Tsingou says. "It was nothing like what we have now." The programming was extremely laborious. "You had to use what the machine recognized, which was only ones and zeros. We typed the directions on a tape and put it in the machine."

While learning to work on the MANIAC, Tsingou was given the task of programming the computer to compute the sine of an angle (in a right triangle, the length of an angle's opposite side divided by the length of the hypotenuse, which is the longest side). She checked and rechecked her work many times before running it through the machine. The first time she programmed her work into the MANIAC, her computation came out correct. She says, however, that this was the first and last time in her long career that she ever got a calculation to run correctly on the first try.

Tsingou soon moved to T-7, the MANIAC group, where she worked mostly with theoretical physicists Stanislaw Ulam and John Pasta. While much of their work was in weapons development, the physicists of T Division were also interested in fundamental science—that is, science that is developed purely for scientific advancement, often without a specific endgame. The MANIAC opened new avenues for such inquiry, and Pasta and Ulam were among those quick to explore them.

The Fermi-Pasta-Ulam-Tsingou Problem

Once the MANIAC was operational, physicists began trying to think of problems that could not be solved with hand calculations but that could be simulated on the computer. Simulations, now widely used but then in their earliest stages, use math to create models of how systems will interact or develop; simulations can tell us what would happen if something created theoretically were to happen in real life.

"I remember sitting there one day with Pasta and Ulam," Tsingou says, as they brainstormed "some problems we could do on the computer, some really mathematical problems." They tried several things, but, eventually, she remembers, "they came up with this vibrating string."

The vibrating string was a theoretical experiment involving "a finite number of points" along a string "with ends fixed and [energy] acting on the elements of the string," according to the resulting paper. Under the assumption that the string could move in all directions—not just back and forth—Tsingou programmed the MANIAC to simulate how energy would move between points on the string.

The scientists thought that the energy would eventually reach equilibrium, spreading out in an equal distribution along the string and settling that way. The result of the simulation was completely unexpected. "Let us say here that the results of our computations show features which were, from the beginning, surprising to us," the authors wrote. The energy moved periodically between different points on the string, never spreading out and never coming to rest.

The Fermi-Pasta-Ulam problem was a game changer for mathematics and science, and it was a seminal development in computational physics. The problem launched the field of nonlinear science and a number of other scientific concepts, including chaos theory, which posits that patterns exist even in seemingly random, complex systems.

The experiment proved that there were ways to simulate problems that could not be studied with literal experiments or solved with traditional theoretical methods of numerical analysis. According to Cynthia Reichhardt, a scientist in the current T-1 group, Physics and Chemistry of Materials, that revelation "combined with improvements in computer technology, led to the flowering of simulations as a third research approach, complementary to both experiments and traditional analytic theory."

And in a 2009 American Scientist article, scholars Mason Porter, Norman Zabusky, Bambi Hu, and David Campbell claimed that the problem "rocked the scientific world" and "sparked a revolution in modern science."

Fermi, Pasta, and Ulam developed the theory; Tsingou made it work. "They didn't know anything about programming," she remembers. "They set up the equations, and I did all the programming." Tsingou is quick to mention that she was given credit in the paper as a programmer. But today, many scientists think she deserves more. In 2008, French physicist Thierry Dauxois argued in a *Physics Today* article, "Fermi, Pasta, Ulam, and a Mysterious Lady," that Tsingou had not been given the credit she was due. "It is time for a proper recognition of her contribution," he wrote. "Let us refer from now on to the Fermi-Pasta-Ulam-Tsingou problem." As a result, some scientists now refer to the simulation as the FPUT rather than the FPU.

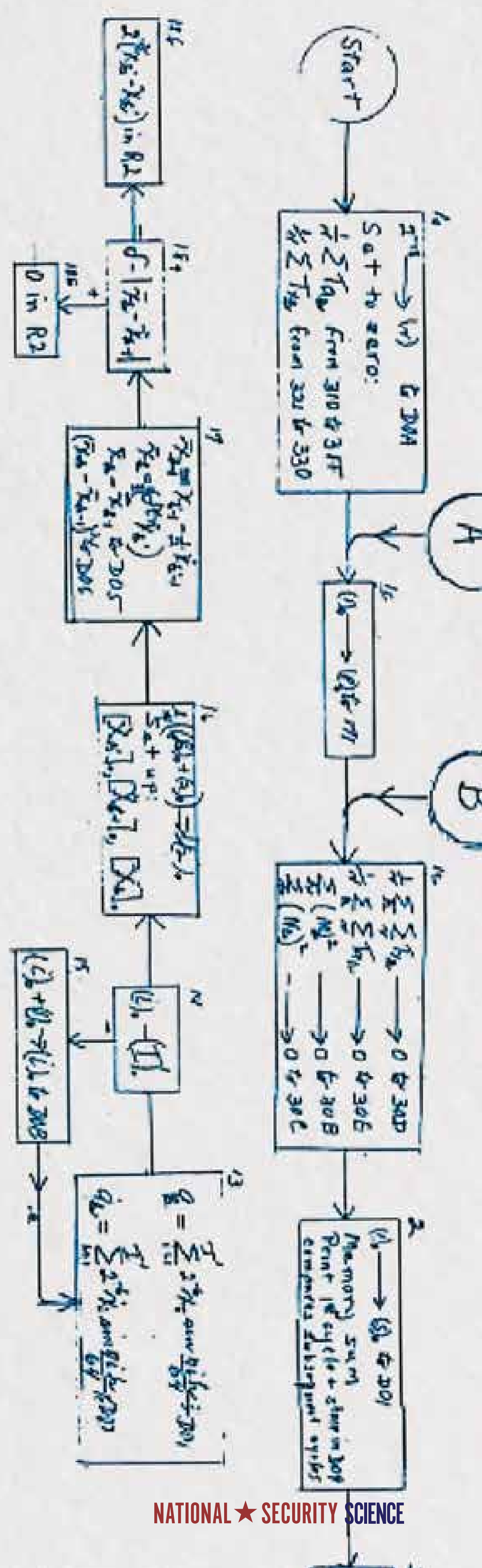
The first time Tsingou programmed her work into the MANIAC, her computation came out correct.

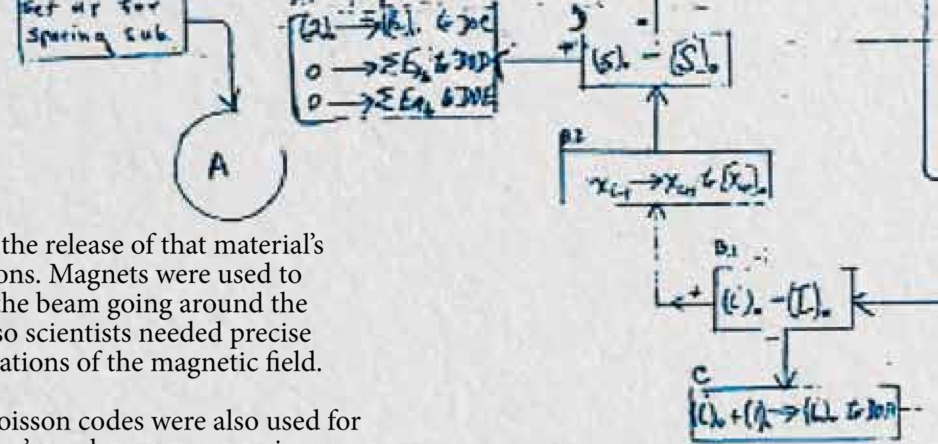
By today's standards in the scientific community, Mary Tsingou would have been an author on the paper—she might have even been the first author, the person who contributed the most to the project. Among those who agree with the renaming of the problem is David Campbell, Professor of Physics, Electrical and Computer Engineering, and Materials Science and Engineering at Boston University and former director of the Center for Nonlinear Studies at Los Alamos. "Certainly," he says, "today she would have been listed as co-author, which is why the current practice is to refer to the FPUT problem."

The experiment set in motion the field of nonlinear science, currently studied worldwide, including at Los Alamos, where the Lab houses an entire Center for Nonlinear Studies. Nonlinear science, broadly defined, is the study of complex systems that are typically very difficult to solve because they can't be broken down into smaller, simpler systems. The central ideas of the field, Campbell says, "have spread over essentially all scientific disciplines and also moved into the social sciences, altering the way we look at the world."

Tsingou was asked to re-create and expand the simulation at times during her career. "I'm surprised that it got so much notice, even from the beginning," Tsingou says. "Even when I was still working, people would call me up about it." Researchers have picked up Tsingou's work and continue it to this day, pushing the parameters further to see if the energy on the string will ever settle. So far, it has not.

Despite the experiment's profound influence on modern science, Tsingou remains very humble about her work on the problem. Its name, she says, "didn't matter to me. I was just doing the job. I was glad to get paid."





A Fortran "paradise"

Though she initially agreed only to a six-month assignment on the MANIAC, Tsingou ended up working on the MANIAC until she temporarily left the Lab in 1954 to get her master's degree in mathematics from the University of Michigan.

After returning in 1955, she worked on various computers and projects, gaining particular notice for her expertise in an early programming language called Fortran.

"When Fortran came, it was almost like paradise," she says. The new programming language was much less laborious than the language used for programming the MANIAC, and it was capable of commands that were impossible before, so programming the calculations was much easier and much faster.

As an early Fortran expert, Tsingou went on to many more career accomplishments, including editing and manipulating the Poisson Group codes. These codes were used on a number of Los Alamos projects, including a proton storage ring used to facilitate the acceleration of a beam of electrons so the beam could travel fast enough to, upon striking another material, cause the release of that material's neutrons. Magnets were used to keep the beam going around the ring, so scientists needed precise calculations of the magnetic field.

Simulations can tell us what would happen if something created theoretically were to happen in real life.

The Poisson codes were also used for Tsingou's work on programming a system for Star Wars that could pick out a nuclear weapon from a group of weapons, some nonnuclear. "The idea at the Laboratory," Tsingou says, "was that the Soviets might send a nuclear warhead toward the United States that would be surrounded by missiles carrying nonnuclear warheads, leaving the United States unsure which one to take out in defense." Tsingou worked with groups that "created simulations to detect which incoming objects were carrying nuclear weapons."

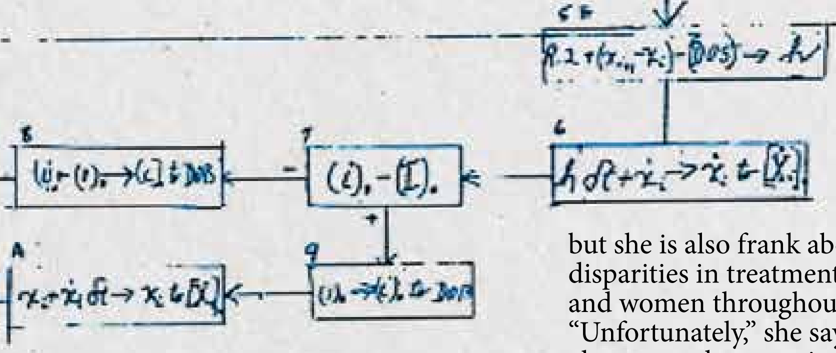
People called from all over the country with questions for Tsingou about the Poisson Group codes. Frank Krawczyk, an Accelerators and Electrodynamics group scientist who currently manages the Poisson codes at Los Alamos, explains that the users of the codes are still widespread. "All U.S. national laboratories that use accelerators or electromagnetics in general are using the codes," he says. Poisson is a teaching tool at universities and is included in the curriculum of the U.S. Particle Accelerator School. Tsingou's team "helped develop software tools that changed the way scientists developed subsystems for accelerators," Krawczyk says, and these same tools, "are still relevant in the 2020s."

Before Tsingou retired in 1991, she was one of the main writers of the codes' user manual. Although the manual has been revised over the years, sections of the current version are "mostly identical to the earlier versions," according to Krawczyk.

Women in mathematics

Mary Tsingou lauds Los Alamos as a wonderful place to work,

▼ An example of MANIAC output data (not from the FPUT experiment).



but she is also frank about the disparities in treatment of men and women throughout her career. "Unfortunately," she says, "the men always got the more interesting problems, and the women were always relegated to the mundane—keeping the machine going and stuff like that."

An anecdote told by Mary Kircher, another mathematician who started working at Los Alamos around the same time that Tsingou did, highlights the gender inequalities that were prevalent in the mid-20th century. "Back in the MANIAC days," Kircher told an interviewer in 2002, "the first sign that it was really not going to be a woman's job anymore was when Jack Jackson got some of the young men together—none of the women" for an important MANIAC project. "We were not invited.…And there was some bitterness about it, of course.…I know Mary [Tsingou] was upset."

"We as women were expected to be second rate," Tsingou says. She was repeatedly told by supervisors that they were trying to raise her salary to equal that of a man with her skills and experience; she never understood, she says, why they couldn't just do it. Not long before she retired, Tsingou received a settlement from a gender inequity lawsuit filed against the Laboratory by Janet Wing, a fellow computer programmer; Tsingou used the money to buy a video camera for her then-pregnant daughter.

Tsingou still lives in Los Alamos with her husband, Joseph Menzel, whom she met in Los Alamos when he worked in protective forces. They live in the home they were assigned based on the Laboratory's early point system, determined by salaries, how long they had worked at the Laboratory, and the size of their family. "At that time," Tsingou says, "when you were married, you were only eligible for apartments, and then when you were at least three months pregnant, you were eligible to apply for a house." The Menzels moved into their home when Tsingou was pregnant with their first daughter. Their two daughters now live in Texas and Pennsylvania, "but this is our place," Tsingou says. "This is our home."

Looking back on her career, Tsingou expresses fondness for the projects she worked on and marvels at the ways in which the world is different from what scientists of the mid-20th century thought it would be. "They thought nuclear energy was going to change the world," she says, "but it's the computers that have changed the world." ★

▲ In 2019, Mary Tsingou Menzel and her husband, Joe Menzel, were photographed in their Los Alamos home during an interview for the American Institute of Physics. Photo: David Campbell

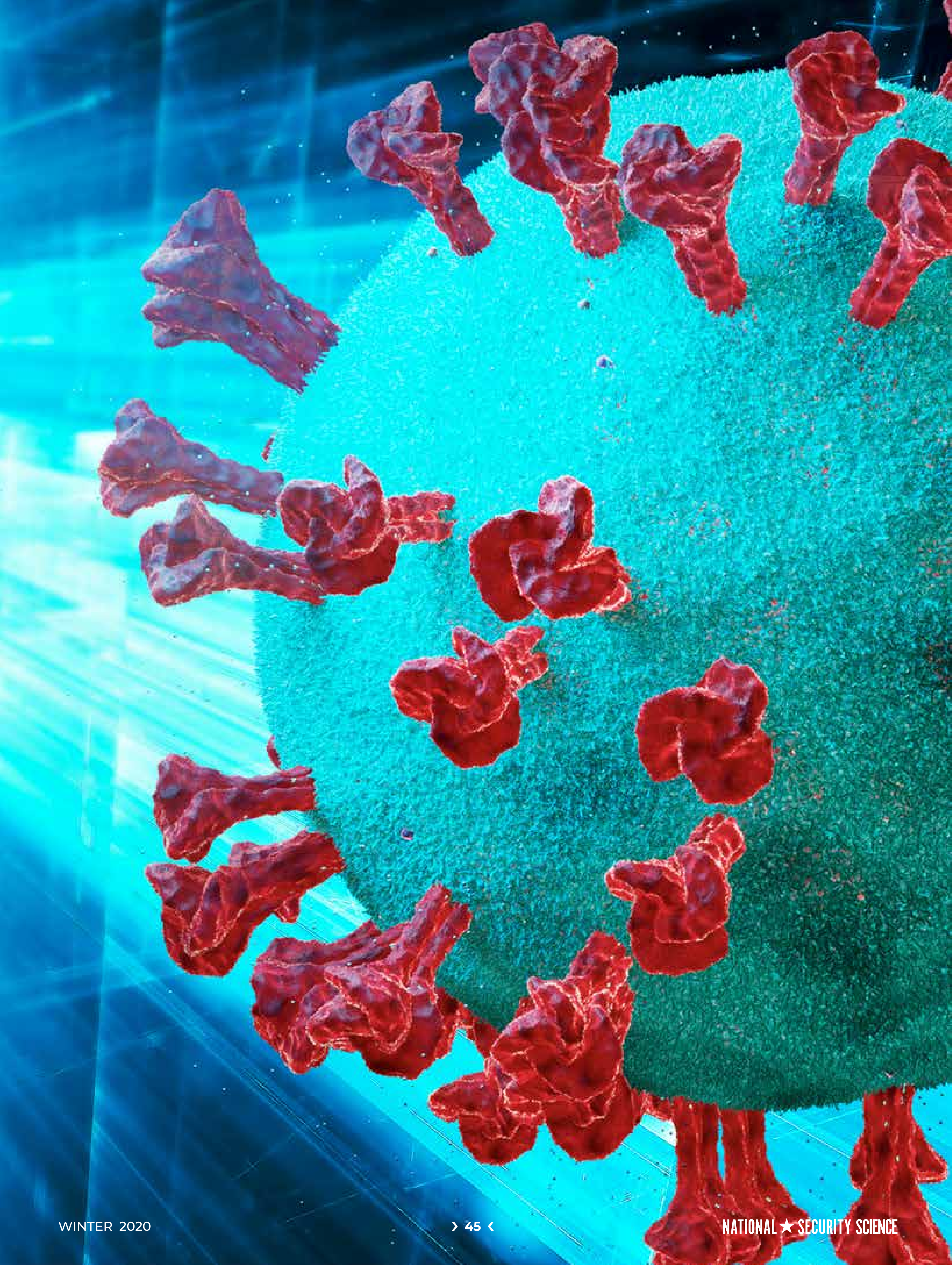
BETTER SCIENCE =
BETTER SECURITY

Drawing on past epidemiological work, Lab scientists are using vast computing resources **to model and fight the spread of COVID-19.**

COMPUTING FOR A CURE

BY J. WESTON PHIPPEN

COVID-19 poses an unprecedented threat to national security. But scientists at Los Alamos National Laboratory are fighting back by harnessing the power of computers.



The first confirmed case of COVID-19 in the United States was discovered in Seattle, Washington, on January 21, 2020. By the time the World Health Organization declared the coronavirus-induced illness a global pandemic 10 days later, Wuhan, China, where COVID-19 originated, was already on full lockdown. In February, the virus spread to the United Kingdom and parts of Africa and Europe. By March, global cases reached 86,000.

COVID-19 reached New Mexico, home to Los Alamos National Laboratory, on March 11. But some six weeks before that, Lab scientists had already set aside their usual research to help tackle the worst virus outbreak in the world since the Spanish flu of 1918. By early summer, the Lab was hard at work on more than 40 projects focused on COVID-19.

"With our history in epidemiological modeling and research, it was a natural pivot for us," says associate Laboratory director J. Patrick Fitch, who leads the Lab's coronavirus response. "From an impact point of view, the modeling we're doing with computers has changed our country's understanding of this pandemic."

Scientists at the Lab are harnessing computing power to help return life to normal. Some have used models to simulate how the virus spreads around the globe and how social media misinformation helps it spread. Others have created virtual communities, then infected their virtual communities with SARS-CoV-2, the coronavirus that causes the COVID-19 illness. And as the world races to develop a vaccine, Lab supercomputers are helping to discern if a vaccine will really spell the end of the virus, or if SARS-CoV-2 is here for good.

FORECASTING THE FLU—AND COVID-19

A virus' indiscriminate attack on a country's people can disable its economy and have national security implications. So, as part of its mission to study national security threats,

each week for the duration of flu season, with a more accurate forecast each time new data is incorporated. “Submitting each week of the season,” he explains, “allows forecasters to update their forecasts in light of current data—similar to how, for instance, hurricane forecasts are updated as the hurricane is unfolding.”

Compared with other, more complicated forecasting models, Osthus jokes, “if I were listening to me describe our system, even I wouldn’t trust it. But thankfully we have the CDC prize to prove that it’s one of the best in the country.”

This year, for the 2019–2020 season, Osthus again submitted two models, including an updated Dante that includes “internet-based nowcasting,” which “develops and uses a model that maps Google search traffic for flu-related terms onto official flu activity data.” But before the competition could conclude, the coronavirus pandemic hit. The FluSight challenge was abruptly ended as, Osthus says, “the whole flu forecasting community turned its attention to COVID-19 modeling.” Now, Los Alamos’ winning flu-modeling team is hard at work modeling the novel coronavirus.

The flu and COVID-19 are similar in that they’re both spread through microscopic droplets of water in a person’s breath. They’re also similar in that an infected person can spread the virus to others before showing symptoms. So pulling Dante into the COVID-19 effort was natural, but the modeling required for COVID-19 is different in some ways from that used to model the flu. Dante was very good at using the past to predict the future; the model used “20 years of historical flu data to make

> **“The modeling we’re doing with computers has changed our country’s understanding of this pandemic.”**
>
> —J. PATRICK FITCH

Los Alamos has invested significant time into understanding viruses, including dengue fever, Zika, malaria, HIV, and even the flu.

Since the fall of 2013, the Centers for Disease Control and Prevention (CDC) has hosted an annual flu forecasting competition, the FluSight challenge, which asks researchers to forecast—to predict the timing, peak, and short-term intensity of—the unfolding flu season. The winner of the challenge for 2018–2019 was Dave Osthus, a statistician in the Lab’s Computer, Computational, and Statistical Sciences Division. The team also included Kelly Moran, Reid Priedhorsky, Ashlynn Daughton, Sara Del Valle, and Jim Gattiker. Osthus submitted two models; they won first and second place. The first-place model, named Dante, most accurately predicted the 2018–2019 flu season at the national, regional, and state levels.

Flu models generally collect a large variety of data inputs—weather, the mobility of a state’s population, a state’s vaccination rate, even internet keyword searches for flu symptoms. But as inputs increase, the forecasts can actually become less predictable. So, for Dante, Osthus and his team did away with as many inputs as possible. Instead, they focused almost entirely on the confirmed flu cases that are reported each week by hospitals and then passed to the CDC.

“When the flu season starts, we observe the first week of flu activity data,” Osthus explains. “That data point constrains what our predictions look like. As the flu season unfolds, each week we get another data point.” Dante makes a new prediction forecasts for the new flu season," Osthus says. But "there is no historical COVID-19 data," so the new model is built "basically from the ground up," using a great deal of knowledge gained from years of flu forecasting.

At first, the team thought it could compensate for this lack of past data by increasing inputs. They accounted for rate of transmission, the time it took for a person to show symptoms, and how many people an infected person might come into contact with beforehand—about a dozen inputs in all. But as the team members wrestled with all the variables, they slowly cut the number of inputs, finally reverting to a much simpler method.

> **It will be interesting to see whether living in a place where online misinformation about COVID-19 is widespread makes you more likely to buy into that misinformation and put yourself at risk."**
>
> —ASHLYNN DAUGHTON

"The model that's now running on our site is the seventh iteration," Osthus says. It's much like the original Dante. Each week, the COVID-19 model of Dante analyzes data published by Johns Hopkins University and, similar to the flu version, it uses only confirmed data of infections, confirmed deaths, and also factors in the population size of the forecasted area. Then the model constantly reanalyzes its prediction with each new reported dataset, growing more accurate each week. But whereas the original Dante could run on a laptop, the COVID-19 version requires the Lab's Darwin supercomputer because not only is Dante crunching data for every U.S. state, it's doing the same for 250 countries around the world.

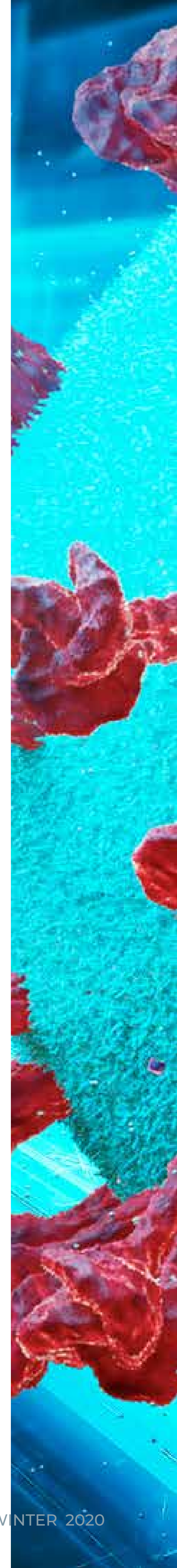
"As of now," Osthus says, "our system is one of only a handful of models being used by the CDC that has consistently outperformed the baseline models."

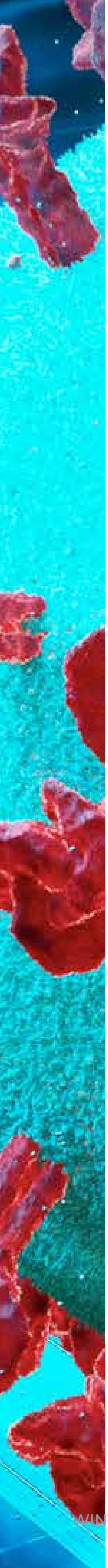
SIMULATING A SICKNESS

Unlike the flu, the spread of COVID-19 hinges on many factors that scientists are only beginning to understand. Human behavior, including opting to wear masks, social distance, and quarantine—or not—has presented new situations that past models never needed to consider.

Accounting for people's actions during the coronavirus pandemic requires a much different type of model, one that the Lab has already developed.

Over the past 15 years, Timothy Germann, a computational scientist, has helped develop EpiCast, one of the most accurate agent-based virus models in the country. An agent-based model can simulate the actions and interactions of individual or collective agents to see how those actions and interactions affect an entire





system. The way EpiCast works is kind of like Sims, the life-simulation video game. EpiCast can create a virtual city populated with virtual citizens who can be assigned ages, incomes, children who attend school, and jobs that take them through the community—all of it based on information pulled from sources such as the U.S. Census Bureau's decennial census.

EpiCast can be used to model a pandemic spreading through areas as diverse as New York City or the state of Georgia. And although EpiCast was originally built to study smallpox, and later the avian flu, it's flexible enough to allow researchers to swap in the characteristics of almost any virus. As the coronavirus pandemic reached New Mexico in March, Germann along with mathematical and computational epidemiologist Sara Del Valle and applied mathematician Carrie Manore, put this powerful modeling tool to work in their home state.

Each week, Del Valle and Manore met with the New Mexico Department of Health to discuss how COVID-19 might spread through different counties and what the best policies might be to prevent infections. The health department then consulted with the governor, Michelle Lujan Grisham, whose actions would impact the lives of the state's 2.1 million residents.

Lujan Grisham, formerly New Mexico's secretary of health, declared one of the first statewide health emergencies in the nation. New Mexico hospitals offered free COVID-19 testing. Businesses deemed nonessential were closed and slowly allowed to reopen once the infection curve had mellowed. By late summer, New Mexico, a state with one of the lowest hospital and physician rates per capita in the country, had fared much better during the pandemic than neighboring states.

By August, the debate about whether to open schools was in full swing. "We were able to put our model to use analyzing a few different options for New Mexico," says Del Valle, explaining that she, Manore, and Germann used EpiCast to test three scenarios (students attend in-person school five days a week, students attend virtual school from home, and students do a combination of in-person and virtual school). Based in part on the results of EpiCast simulations and other Lab modeling efforts, New Mexico's decision has been a hybrid of these options. Counties with less than a 5 percent COVID-19 positivity rate opened schools to partial capacity, with students doing a combination of in-person and virtual learning, with one day reserved for thorough cleaning of schools.

Later, Del Valle and Germann ran similar simulations for the nation. "At that point, we were not only working with the state, we were also informing the CDC," Del Valle says.

STUDYING SOCIAL MEDIA

The tough part about models, even one as advanced as EpiCast, is that human behavior is hard to predict. Humans don't always act rationally or lawfully. For example, despite municipal or state laws requiring masks, some people refuse to wear them. This could simply be because these people find masks inconvenient or uncomfortable. But Lab information scientist Ashlynn Daughton also wondered if this behavior could be traced to a larger influence.

Daughton's past work used an algorithm to study public social media posts to understand how seriously people considered the Zika virus to be a threat. To do this, the algorithm looked for signs on social media that indicated people had canceled travel plans to areas with Zika. Daughton hoped to do something similar with COVID-19.

She began by building an algorithm that helps her study public social media posts on Twitter and Redditt. The algorithm looks for posts that express feelings for or against safe behavioral practices, such as adhering to social distancing, washing hands, or wearing masks.

In all, the algorithm looks for 30 virus-related behaviors posted on social media. The algorithm uses the words in a post to identify what behavior is being discussed, and it recognizes if the post is a personal

DAVE OSTHUS

SARA DEL VALLE

THOMAS LEITNER

ASHLYNN DAUGHTON

J. PATRICK FITCH

observation ("I am wearing a mask") or a general observation ("here is an article about mask wearing"). The observation is then analyzed to decide if it reflects safe or risky practices, and its geolocation is crossed with COVID-19 outbreaks.

"In the long term, it will be interesting to see whether living in a place where online misinformation about COVID-19 is widespread makes you more likely to buy into that misinformation and put yourself at risk," Daughton explains.

If it can be proven that there is a correlation between outbreaks and social media influence, the data could also feed into larger modeling systems, such as EpiCast, to create even more-accurate simulations of how the virus can spread.

LOOKING INTO THE LUNGS

Similar to the way EpiCast creates a digital representation of a community, mathematical biologist Ruy Ribeiro and his team have created a model to understand how SARS-CoV-2 interacts with the human respiratory and immune systems. They hope their work will enable physicians to develop better treatments to save lives.

One of the main interests of Ribeiro's team is how SARS-CoV-2 migrates from the upper respiratory tract (the nose and mouth) to the lower one (the lungs). A virus like the flu tends to linger in the upper tract, but SARS-CoV-2 can move fairly quickly to the lower tract, where it can do serious and sometimes fatal damage. Typically, the virus infects cells to make more (tens of millions of) copies of itself, and the body uses its immune system to fight back. This immune system response usually starts with the production of proteins that protect cells against infection and prevent the virus from replicating. Often, specialized B and T defense cells join the fight. But in some COVID-19-positive patients, the communication between the first responder

CARRIE MANORE

TIMOTHY GERMANN

BETTE KORBER

RUY RIBEIRO

cells and the reinforcement T and B cells becomes garbled.

With its model, Ribeiro's team analyzes viral replication and the virus' interaction with the body's defenses. The team found that people are most infectious when their viral load (the amount of virus present in a person) is above 10,000 copies of the virus per test swab.

From there, Ribeiro's team can introduce different treatments into the model to see if any of the treatments help the body's immune system fight the virus. Remdesivir, for example, is an antiviral medication that slows virus reproduction and has been shown to shorten patient recovery time. Ribeiro's model showed that remdesivir can in fact help patients with mild symptoms recover more quickly, but only if the treatment is started very early in the process, almost on day one of infection. Beyond day three, they found little-to-no benefit for treating patients with remdesivir.

Another question the team wanted to understand is how SARS-CoV-2 mutates once it's inside the body. Using a handful of available studies in which infected patients were repeatedly tested for up to 20 days, Ribeiro and his team are running thousands of simulations that show how the virus can replicate itself and how rapidly it can mutate.

"This is like the holy grail of the research being done now," Ribeiro says, "because it will tell us not only how quickly the virus is evolving in the human body, it will also tell us how it's evolving."

Understanding this progression is of the utmost importance as a vaccine against the virus is developed. If the SARS-CoV-2 mutates rapidly enough, it might evolve beyond the vaccines currently being developed, rendering them ineffective. Creating a vaccine is like aiming at a moving target: you can't just shoot where it is, you have to aim where it will be.

VARIATIONS OF THE VIRUS

Theoretical biologist Bette Korber—a Laboratory Fellow renowned for her HIV work—is also studying how SARS-CoV-2 mutates. In July, she and 20 co-authors published a paper in the journal *Cell* that stated a variation of the virus, called D614G, has become the most prevalent form of the virus globally.

"The D614G variant first came to our attention in early April, as we had observed a strikingly repetitive pattern," Korber says. "All over the world, even when local epidemics had many cases of the original form circulating, soon after the D614G variant was introduced into a region it became the prevalent form."

Geographic information from samples from GISAID, a global science initiative that provides open-access to genomic data of viruses, enabled tracking of D614G, which occurred at every geographic level: country, subcountry, county, and city.

"It is possible to track SARS-CoV-2 evolution globally because researchers worldwide are rapidly making their viral sequence data available through the GISAID viral sequence database," Korber says. GISAID was originally established to encourage collaboration among influenza researchers, but early in the coronavirus pandemic, the consortium established a SARS-CoV-2 database, which soon became the de facto standard for sharing outbreak sequences among researchers worldwide. Currently, tens of thousands of sequences are available through this project, and this enabled Korber and colleagues to identify the emergence of the D614G variant.

"There are fewer atoms in the universe than the number of topologies I can create with 49,000 genetic variations of this virus."

—THOMAS LEITNER

The SARS-CoV-2 virus has a low mutation rate overall (much lower than the viruses that cause influenza and HIV-AIDS). The D614G variant appears as part of a set of four linked mutations that appear to have arisen once and then moved together around the world as a consistent set of variations.

"These findings suggest that the newer form of the virus may be even more readily transmitted than the original form," Korber says. "Whether or not that conclusion is ultimately confirmed, it highlights the value of what were already good ideas: to wear masks and to maintain social distancing."

MAPPING THE SPREAD

Computational biologist Thomas Leitner is trying to understanding how SARS-CoV-2 has evolved on a global scale as it has spread across cities, regions, and countries. "At the moment, SARS-CoV-2 has spread through communities quickly," Leitner says. "But viruses like this tend to evolve faster when they have time to settle for longer periods in a host community, so we're just beginning to understand the nature of how it's changing."

To understand that question, Leitner is developing a genetic tree for COVID-19, not unlike the family trees schoolchildren fill out. Leitner's tree traces the most current genetic variants of the virus back to their beginning in China, where the virus is believed to have originated in horseshoe bats.

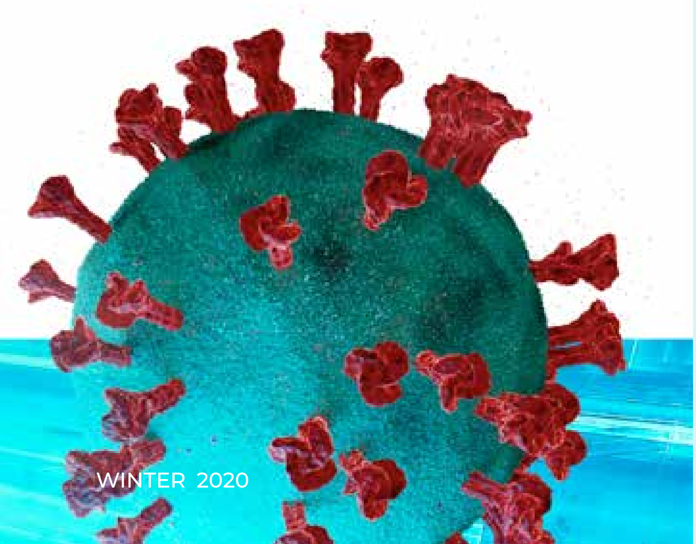
Every week, Leitner downloads the latest information released by GISAID, where there are currently more than 49,000 logged genetic sequences of the novel coronavirus. Slowly, Leitner is building topologies—related configurations—that reveal how the virus has spread across the world in human populations.

"There are fewer atoms in the universe than the number of topologies I can create with 49,000 genetic variations of this virus." Leitner says. "I've definitely got my work cut out for me."

Once Leitner models the SARS-CoV-2 genetic tree, he'll be able to understand how the virus evolves as it's passed around the world. Leitner's work could also prove crucial to creating a vaccine because after a prolonged time the virus' genetic code may evolve to look very different in one region of the globe than it does in another. If, for example, SARS-CoV-2 in America differs dramatically from the variant in Brazil, this might require specialized vaccines for each region.

"The ultimate goal for this work is to then couple it with the other research being done that looks at how SARS-CoV-2 evolves inside the body," Leitner says. When that time comes, the Laboratory's computing power will be instrumental in linking various research together.

"Over the decades, we've built a robust computing capability," Fitch says, "and it is perfectly suited for fighting the COVID-19 outbreak." ★



VIABLE VENTILATORS

When a ventilator shortage worried the nation, the Lab stepped up with a couple inventive solutions.

In February, a surge of COVID-19 patients at hospitals across the country led to the realization that the United States might not have enough ventilators—machines that help people breathe—to keep severely ill patients alive. This problem prompted some innovative responses from the Laboratory.

Two groups of engineers wondered if they could build their own ventilators using locally sourced supplies. One group purchased parts from hardware and car supply stores in Los Alamos, took them back to someone's garage, and fashioned them into a ventilator. Another team partnered with health experts from Presbyterian Health Services to build a ventilator using plumbing from a hardware store. As the projects progressed, the engineers made improvements as they assessed how well the ventilators worked on simulated lungs.

Typical ventilators deliver to patients regularly timed spurts of oxygen, which can be unnatural for someone whose breathing is labored or erratic. So, Lab engineers modified one of their ventilators to deliver oxygen in response to a patient's natural pace of breath. Then they added pulsed aerosols into the oxygen delivery system in hopes that the aerosols would break down mucus in the lungs of infected patients.

"What we're doing is essentially transforming a machine meant to keep people alive into a potential treatment," says associate Laboratory director J. Patrick Fitch, who's leading the Lab's coronavirus response. The new ventilator is now a joint project with Idaho National Laboratory.

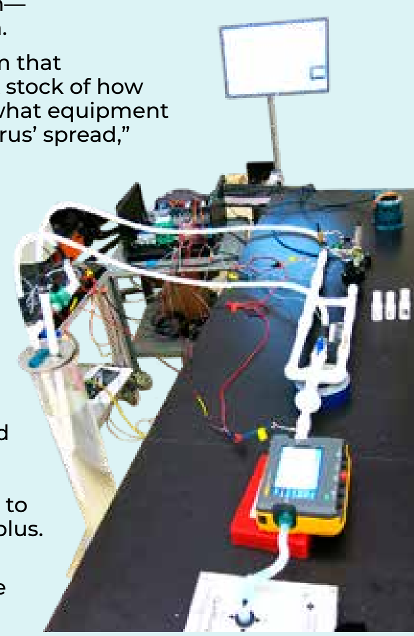
Predicting the need for ventilators

Data analyst Paolo Patelli and computational scientist Nidhi Parikh viewed the ventilator shortage as a supply and demand problem—one for which they had a solution.

"Our idea was to create a program that policymakers could use that took stock of how much equipment they had and what equipment they would need, based on the virus' spread," Parikh says.

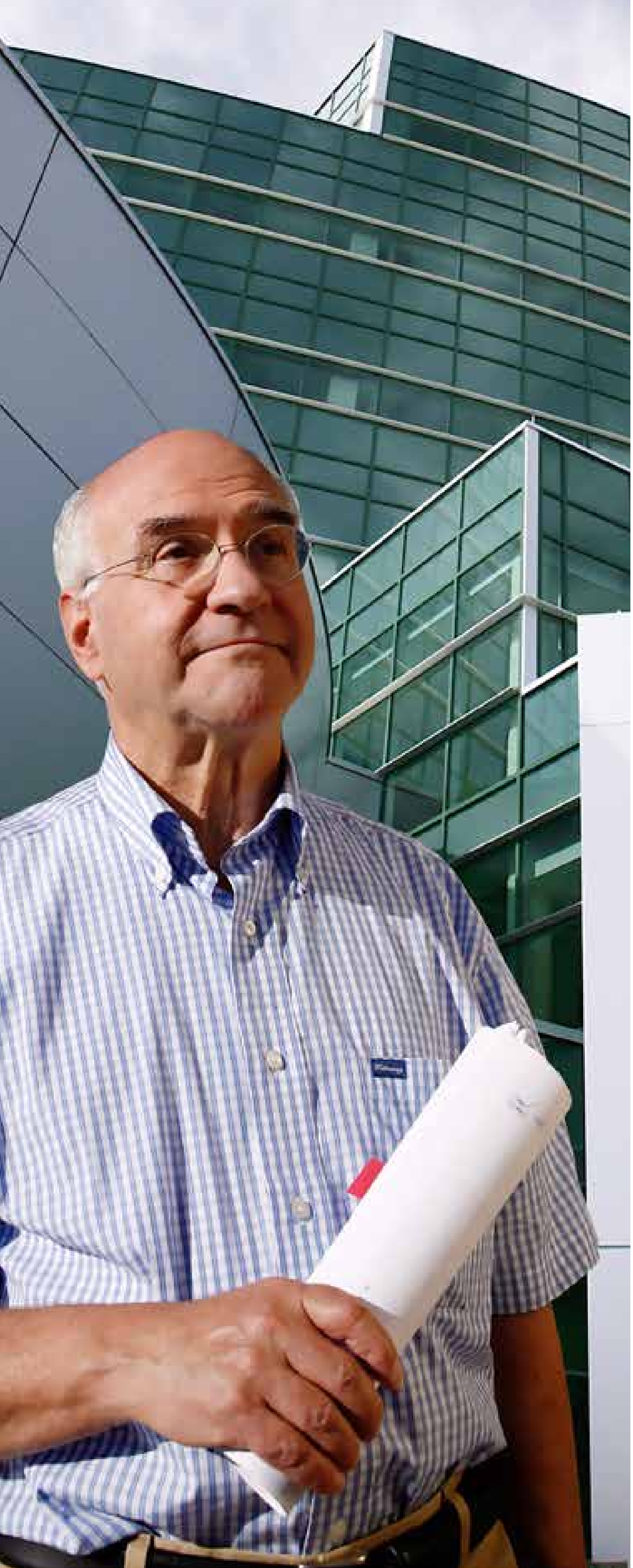
The program they developed accounts for a state's supply of ventilators, as well as the supply of neighboring states. It uses a model that predicts the future infection rate of that state, and then measures how many infected people will potentially end up in a hospital with need of a ventilator. If there aren't enough ventilators on hand during the projected COVID-19 outbreak in one location, the program can direct policymakers to regions of the country with a surplus.

"Since then," Parikh says, "we've expanded the program to include personal protective equipment, medications, and almost anything a hospital needs to help COVID-19 patients." ★



▲ A ventilator made from hardware store parts.

▼ Reis, pictured here in front of the Laboratory's National Security Sciences Building, spoke at Los Alamos during the Lab's 70th anniversary celebration in 2013.



THE ARCHITECT OF STOCKPILE STEWARDSHIP

Victor Reis shares his experiences at the intersection of policy and science.

AS TOLD TO WHITNEY SPIVEY

TRANSCRIBED BY ELIZABETH BRUG AND J. WESTON PHIPPEN

The United States stopped testing nuclear weapons in 1992. In August 1993, Victor Reis became assistant secretary for Defense Programs in the Department of Energy (DOE) and was responsible for developing a new way for the United States to maintain its aging nuclear stockpile. Reis was instrumental in creating a science-based stockpile stewardship program, which uses computer simulations and nonnuclear experiments to evaluate the health and extend the lifetimes of America's nuclear weapons. The program, which relies heavily on computing modeling and simulation, has spurred the growth of several generations of supercomputers.

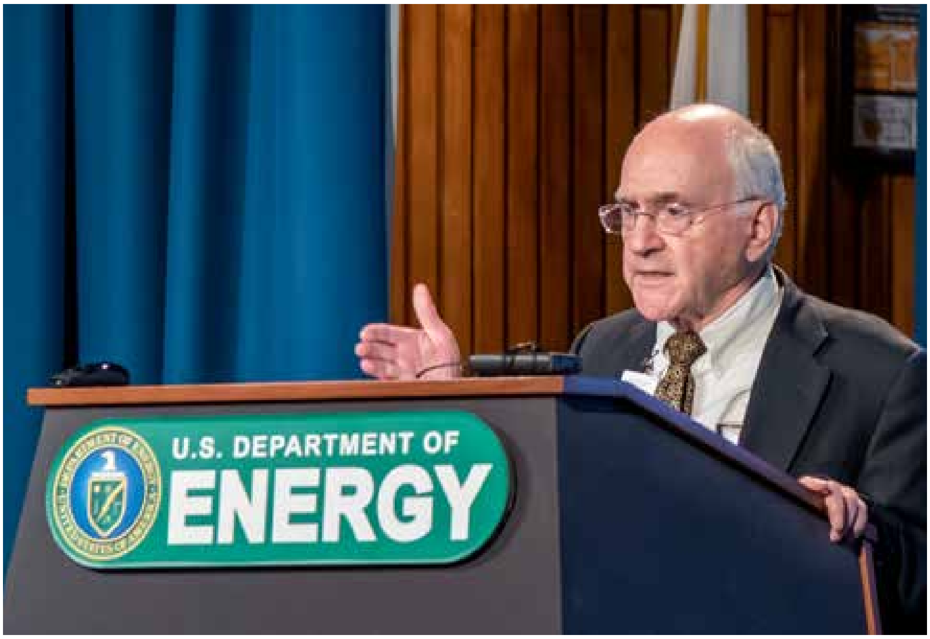
Reis sat down with NSS to talk about the creation of stockpile stewardship, specifically how he was able to bridge the gap between scientists and policymakers.

How do policymakers learn to trust the scientific community? How do they trust that scientists don't have a hidden agenda or that scientific data isn't skewed by funding sources? And how do scientists deal with that lack of trust by policymakers?

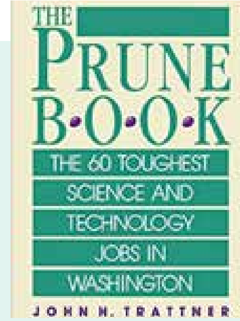
A good deal of my career has been based on getting scientists and policymakers to trust each other, particularly during my service in each one of the "prune positions"—what diplomat and author John Trattner called the toughest, presidentially appointed science and technology jobs in Washington, D.C.

In August 1993, I was confirmed in my fourth "prune position"—assistant secretary of energy for Defense Programs. President Clinton had just announced that the United States would maintain a moratorium on nuclear testing while seeking a Comprehensive Nuclear-Test-Ban Treaty (CTBT). Because nuclear testing had been an essential and dominant element of the DOE weapons program, the DOE weapons labs (Los Alamos, Livermore, and Sandia) had traditionally opposed a comprehensive nuclear-test-ban treaty. I found myself stuck in the middle: a member of what President Eisenhower in his famous farewell address called the dangerous "scientific-technological elite" and in a position of being able to affect national policy.

The important thing was to bring the national laboratories together to help them look toward a future in which they wouldn't be designing new weapons but rather maintaining old ones. I had to find a sweet spot between science, technology, and policy so the president's CTBT objective and the Department of Defense's deterrence mission could work together.



▲ Reis speaks about stockpile stewardship to NNSA employees in June 2019. Photo: NNSA



In 1992, John Trattner wrote *The Prune Book: The 60 Toughest Science and Technology Jobs in Washington.* Reis held four of those jobs throughout his career:

- Assistant Director for National Security and Space in the Office of Science and Technology Policy
- Director of Defense Advanced Research Projects Agency
- Director of Defense Research and Engineering for the Department of Defense
- Assistant Secretary for Defense Programs for the Department of Energy

The solution was a science-based stockpile stewardship program that would maintain the effectiveness and safety of the current nuclear weapons without testing. It was a challenging scientific problem, so the laboratories really couldn't help themselves because that's what scientists love to do.

To start, I asked each of the three nuclear weapons laboratory directors to send me a senior weapons designer and a senior scientist, for an offsite, "truth-be-told" meeting. John Immele and John Browne were the Los Alamos participants. The laboratories had been created to compete with one another—not for money but to design and build the next nuclear weapon. I told them, well, we're not likely to build any more weapons, and we're not likely to do any more testing. Our new strategy will be based upon new experiments and computer simulations that can validate the health of our aging weapons. At that time the necessary computing power was not available—not by a long shot—so the weapons programs had to strengthen their own computing groups, working with IBM and other major computing companies to develop a new class of high-performance computer. The weapons labs became the U.S. computing companies' biggest customers and subsequently drove the whole high-performance-computing industry.

Science-based stockpile stewardship put the laboratories in a powerful policy position because the responsibility of determining the health of the stockpile was theirs. If they ever believed that we had to go back to testing, they would have to say so. This is where scientific integrity comes in: you have to be able to say, no matter what the policy is, "This is what the science tells us." You can't be complacent. You can't say, "We've done this already." You need people saying, "Do we really understand?" You have to be able to criticize yourself all the time.

I think the laboratories were originally skeptical about stockpile stewardship, but they were willing to give it their best shot if resources were available.

The Department of Defense, on the other hand, said "What do you mean you're not going to test? That just doesn't make any sense. We always test our airplanes before we fly them!" I went to the chairman of the Joint Chiefs of Staff, General John Shalikashvili, and suggested he look the laboratory directors in the eye and ask them directly, "Do you think you can maintain the stockpile without testing?" And he did that. In fact, he said that question should be asked every year as the weapons age and as we learn more. This became an official annual procedure; every year the labs assess the health of the stockpile.

This annual assessment process has been very important; it puts the laboratories' scientific reputations on the line. The laboratories have to give their view, even if it goes against policy. And you have to ensure that the policymakers trust the scientists to give them the right technical answer, even if it's not what they want to hear.

At the time, we had not really demonstrated that stockpile stewardship—maintaining effective and safe nuclear weapons using science and computing in the absence of nuclear testing—would work. Some thought we wouldn't have enough data to be confident that our weapons are safe, secure, and effective. Some thought our confidence would erode over time. Maybe the continual questioning would cause potential adversaries to doubt our commitment to deterrence.

On the other hand, the policy risk must also be considered. If the United States resumes testing, then the Russians are going to test, and the Chinese are going to test. If that happens, would a return to testing improve our strategic posture? At what point do policy issues override the scientific uncertainty? The challenge is finding a balance.

Nearly 30 years later, science-based stockpile stewardship has actually evolved better than we expected. Many in the weapons community believe that the stockpile is more robust now than when we stopped testing—it's more reliable, and additional safety and security features have been added over the years. The 2018 Nuclear Posture Review reported that continuing to effectively extend the lifetimes of our nuclear weapons means that there's no need to resume testing.

Nonetheless, the system is configured so that if the laboratories say we have to return to testing, they will be trusted by the policymakers. Maintaining trust in the laboratories is—and will continue to be—the key to the future of the stockpile. ★

MATH AND MUSIC RUN IN THIS FAMILY

When not working on computers, siblings Joel and Candace Vargas write and record songs.

BY OCTAVIO RAMOS

Joel Vargas Jr. of the Los Alamos National Laboratory's Institutional Systems Services group sits in his recording studio, a music keyboard at the ready. In front of Joel are a computer and several high-fidelity speakers. Behind him stands his sister Candace of the Lab's Performance Assurance group. Although both have been creating, recording, and producing music from young ages, the siblings for the first time are intimately collaborating on a new music project that mines the past while pushing the boundaries of the future.

"We've sung and worked together before, but not like this," Joel says. "This new side project with my sister will showcase both our talents. It's an opportunity to craft a new, more progressive and electronic sound, one that will separate us from the pack."

"We've been trying different styles to incorporate my experience with Spanish and Tejano music with his electronic and more experimental music," Candace adds. "I'm helping him with lyrics and vocals."

CAREERS IN MATH AND COMPUTERS

With the Vargas family intimately involved with music, it comes as no surprise that mathematics and computing also run in this family. Candace's interest has been in mathematics and statistics (having received a bachelor's in applied mathematics from Northern New Mexico College), whereas Joel is currently working on a master's degree in software-driven systems and design at New Mexico Highlands University.

"I use math and statistics to assess issues management and risk assessment," Candace explains. "My group helps Laboratory management set priorities, identify and mitigate risks and issues, monitor performance, and identify and act on lessons learned. I feel like I make a difference, not only in my group but for the Lab in general. I'm very proud of what I do."

"I've always been fascinated by what computers are capable of," Joel says. "The skills I have in programmatic languages and hardware really help with my job at the Laboratory. I provide technical support for Weapons Facilities Operations and the Los Alamos Neutron Science Center (LANSCE)—and now I also provide support to LANSCE Facility Operations. My role is to ensure that Lab standards are met by empowering my customers with the knowledge needed to work in a secure environment."

A LOVE OF MUSIC

Both Joel and Candace attribute their love of creating music to their parents. Their father, Joel Vargas Sr., for many years has played rhythm guitar and tackled lead vocals for the band NortherN 505. Based in Española, New Mexico, the band plays a variety of music, from New Mexican rancheras and cumbias to American country and classic rock and roll. Their mother, Ruth Ann Vargas, manages the band.

Of the two siblings, Candace took to her father's love of traditional Spanish music. "When I was three years old, I was listening to my dad practicing a song on his guitar," Candace says. "Out of nowhere, I just started singing. My dad noticed that I had a little vibrato in my voice, and he said, 'Hey, we can do something with this.'"

Candace started recording music at nine years old and has since released nine full-length studio albums, the latest of which is titled *A Mi Modo* (*My Way*). Candace has received 22 Hispano Music Awards and a Quince Grandes Award for her music. Her principal genres are rooted in Tex-Mex and American country music.

An accomplished vocalist himself, Joel started to explore electronic music when he was in college. "What got me started was me analyzing my favorite songs and asking how certain parts of the song were made," Joel explains. "I am inspired by artists like Hans Zimmer and Danny Elfman—they both create very cinematic music."

✦ Joel and Candace Vargas perform at the Tejano Music Awards Fan Fair in San Antonio, Texas.

Joel has released his first piece of music titled "Guardians of the Gate." "With cinematic music in mind, I wrote my own song of an epic battle scene," he explains. "The guardians serve as the last line of defense against a horde that wants to destroy their stronghold. Throughout the song, classical elements dance with high-energy synthetic saws, with drums punctuating the intensity of the fight, with the guardians coming out victorious."

MUSIC IS MATH, AND MATH IS MUSIC

Both Candace and Joel believe that music contributes to every facet of their lives, including how well they execute their work at the Laboratory.

"Music is intertwined in my being—I'm always listening to music," Joel says. "Music keeps me creative, and I feel that being creative in a technical position at the Laboratory gives me an edge when it comes to the problem solving and troubleshooting that my day-to-day job requires."

"I found that my experience in performing in front of different audiences has really helped me do my job," Candace says. "I am equally at home presenting a training session to a Laboratory audience and performing on stage for cheering fans of my style of music." ★

Joel and Candace Vargas work on a new music project that for the first time will combine their talents.

Candace Vargas performs the national anthem at the Laboratory's Los Alamos Medal Ceremony.

Joel Vargas at the 2019 Tejano Music Awards.

BETTER SCIENCE = BETTER SECURITY

Hardworking people—the Laboratory's most important asset—**enable Los Alamos to perform its national security mission.**

THE DISTINGUISHED ACHIEVEMENTS OF LOS ALAMOS EMPLOYEES

John Benner is the new executive officer for Weapons programs. In his 25-plus years at the Laboratory, Benner has served as the project director for the W76-1 Life Extension Program, division leader for Weapon Systems Engineering, associate director for Weapon Engineering and Experiments, and acting executive officer for Weapons Programs. According to Bob Webster, deputy Laboratory director for Weapons, Benner's "most recent assignments at the Nevada National Security Site have provided [him with] broad insight across the nuclear weapons complex and make him exceptionally well qualified for this critical senior management position."

Deniece Korzekwa, of the Laboratory's Sigma Division, was named the 2020 Senior Laboratory Fellow for outstanding leadership and seminal contributions to nuclear weapons manufacturing science, global security initiatives, and international scientific exchanges involving plutonium and uranium. Korzekwa is an expert in actinide casting, with significant technical contributions across the entire Weapons program.

Carol Burns, executive officer for the deputy director for Science, Technology, and Engineering, was selected as the recipient of the 2021 American Chemical Society's Francis P. Garvan–John M. Olin Medal. This national award recognizes distinguished service in the field of chemistry by female chemists.

John Bernardin is a new Fellow in the American Society of Mechanical Engineers. Bernardin received the honor for challenging his workforce; promoting mechanical engineering ingenuity in our nation's nuclear weapons program; developing and sustaining research collaborations with academic institutions; advocating professional society activities; and championing new technology to prototype complicated ideas with additive manufacturing techniques.

Peter Lyons, an American Nuclear Society (ANS) Fellow and a society member since 2003, received the Dwight D. Eisenhower Medal in a virtual award ceremony during the 2020 ANS Virtual Annual Meeting. The Eisenhower Medal is awarded to individuals in recognition of outstanding leadership in public policy for nuclear science and technology or outstanding contributions to the field of nuclear nonproliferation.

Matthew Hoffman, of the Fluid Dynamics and Solid Mechanics group, received an Early Career Research Program funding award from the U.S. Department of Energy's (DOE's) Office of Science. Hoffman's winning proposal, "Creating a Sea-Level-Enabled E3SM: A Critical Capability for Predicting Coastal Impacts," creates a regional sea level modeling capability within the Energy Exascale Earth System Model (E3SM).

James Ahrens was selected as director of the Information Science and Technology Institute, one of six strategic centers within the National Security Education Center at Los Alamos. The institute provides outreach to the international community and serves as a mechanism for attracting students, postdocs, visiting scientists, and visiting faculty in information science and technology relevant to the national security missions of the Laboratory.

Michael Furlanetto is the new director of the Los Alamos Neutron Science Center (LANSCE) and senior director of the Associate Laboratory Directorate for Physical Sciences. LANSCE is a premier accelerator-based user facility for research underpinning Laboratory missions in national security, energy security, and fundamental science.

Ning Xu of the Actinide Analytical Chemistry group was selected as a member of the 2020 class of Fellows of the American Chemical Society (ACS). Xu is recognized for her sustained contributions to actinide analytical chemistry in support of national nuclear defense, technical nuclear forensics, nuclear material safeguards, and deep space exploration.

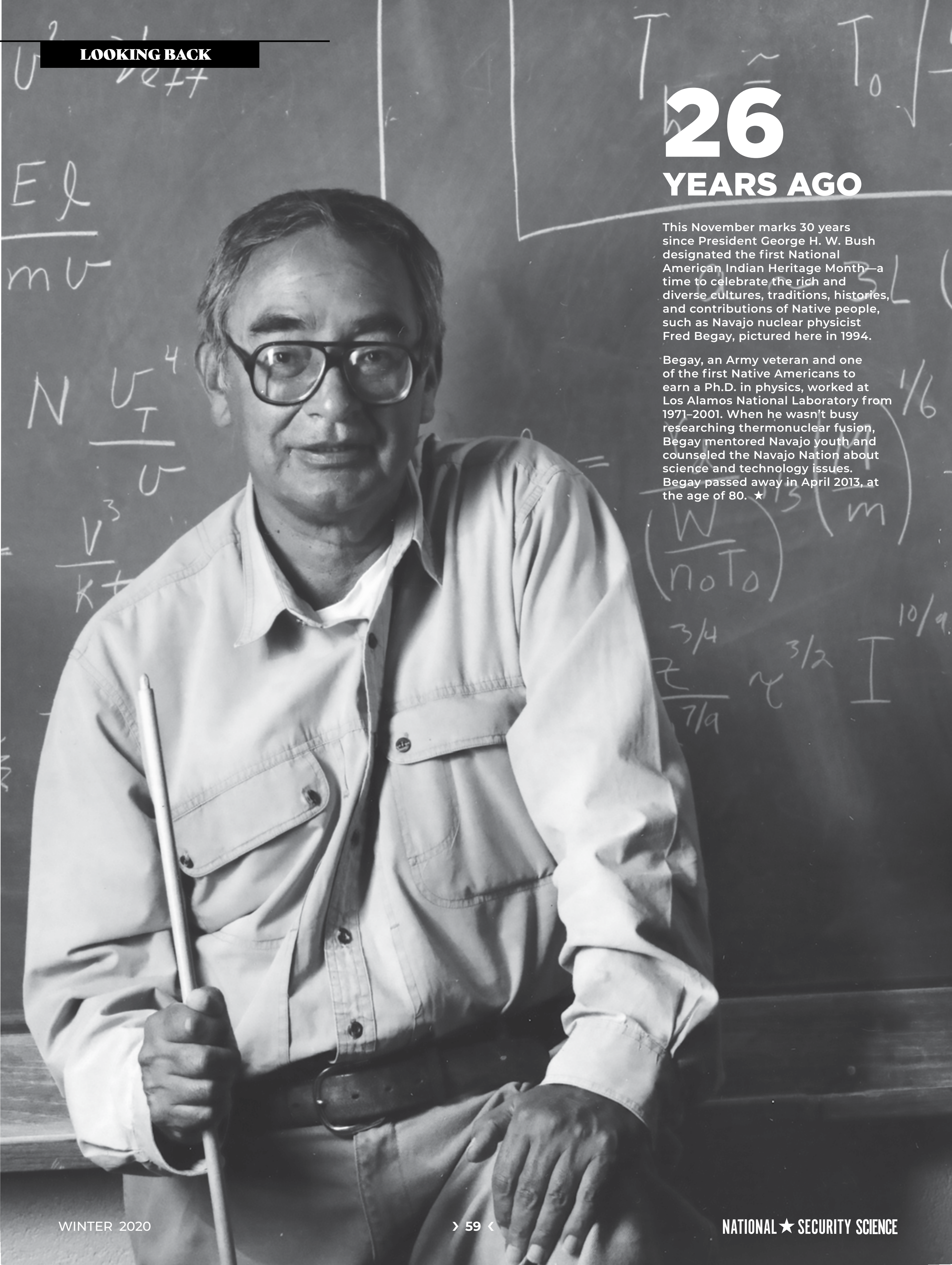
Rod Borup, of the Lab's Materials Synthesis and Integrated Devices group, has been named a 2020 Electrochemical Society (ECS) Fellow. The distinction recognizes advanced individual technological contributions in electrochemical and solid-state science and technology, along with service to the society.

Over the past several years, the Laboratory's weapons work at the Nevada National Security Site (NNSS) has increased considerably. To help manage and coordinate this growth, **Don Haynes** is leading the newly formed Nevada Programs Office. Haynes coordinates and negotiates with external and internal customers to determine what work will be done to meet program needs, establishes milestones, and determines funding requirements. ★

IN MEMORIAM

Kurt Nielsen

In 1997, Kurt Nielsen joined the Lab's Physics Division as a pulsed-power engineer. He was instrumental in the design of Atlas—the largest pulsed-power machine in the world at the time. After the assembly of Atlas was completed, Kurt went to work in the Dynamic Experimentation Division, where he worked on the pulsed-power components of the second axis of the Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility, which is the largest radiographic linear induction accelerator in the world. ★



26 YEARS AGO

This November marks 30 years since President George H. W. Bush designated the first National American Indian Heritage Month—a time to celebrate the rich and diverse cultures, traditions, histories, and contributions of Native people, such as Navajo nuclear physicist Fred Begay, pictured here in 1994.

Begay, an Army veteran and one of the first Native Americans to earn a Ph.D. in physics, worked at Los Alamos National Laboratory from 1971–2001. When he wasn't busy researching thermonuclear fusion, Begay mentored Navajo youth and counseled the Navajo Nation about science and technology issues. Begay passed away in April 2013, at the age of 80. ★

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THEN + NOW

Built in 1951 (and pictured here in 1959), Omega Bridge created a more direct route between the town of Los Alamos and Los Alamos National Laboratory. The steel arch bridge spans 820 feet across Los Alamos Canyon and sits more than 100 feet above the canyon floor. The bridge was listed on the National Register of Historic Places in 1997.

Omega Bridge is inspected annually to make sure it's safe for drivers and pedestrians. Because of the bridge's size and location, taking accurate measurements of things like cracks and corrosion can be difficult and time consuming. But by using augmented reality technology being developed by David Mascareñas (pictured) of Los Alamos National Laboratory's Engineering Institute, an inspector will be able to quickly take accurate three-dimensional measurements of the bridge using a headset or smartphone. As the bridge nears the end of its predicted life span, augmented reality technology will become crucial to determining when and where upgrades are needed. ★