Lawrence Livermore National Laboratory

Science & Technology REVIEW

January 2021

TEAM SCIENCE TAKES ON Lab Infrastructure

Also in this issue:

About the Cover

As Lawrence Livermore strives to support a growing workforce, rapid advances in information technology, and the challenge of two major stockpile modernization programs, it is marshaling its signature strengths and a $2 billion infrastructure investment plan to guide the transformation of its facilities, utilities, programmatic equipment, and workspaces over the next decade. To execute this major endeavor, as the article on page 4 details, the Laboratory is using an NNSA evaluation and planning methodology referred to as "science-based infrastructure stewardship," that has many hallmarks of the scientific method: It is computationally based, data-driven, transparent, and it adheres to a rigorous verification and validation process.

Cover design: Mary J. Gines

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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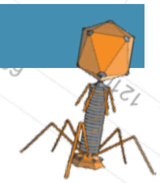

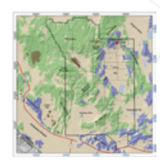

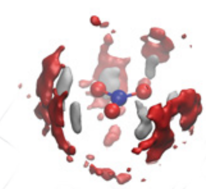

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Livermore Scientists Solve Molecular Transport Mystery

Determining how single-valence negatively charged ions or "monovalent anions," can squeeze through a carbon nanotube 20,000 times thinner than a human hair despite their similarity in size and lack of chemical reactivity was no easy feat, but a team of Lawrence Livermore scientists solved this molecular mystery. Their findings were published in the May 14, 2020, issue of *ACS Nano*.

With funding from the Department of Energy's Office of Science and the LLNL Grand Challenge Program, the team used fluorescence assays and stopped-flow spectrometry to uncover how four monovalent anions—chloride, bromide, iodide, and thiocynate—manage to travel through carbon nanotube porins (CNTPs) so narrow that just one water molecule or one ion can traverse the nanotube at a time. The measurements revealed unexpectedly strong differential ion selectivity with permeabilities of different ions varying by up to two orders of magnitude. "Seeing differential selectivity for diverse anions is important because of the need to design very selective membranes that could separate these ions," says Livermore scientist Alex Noy, lead author of the article. The team then applied first principles molecular dynamics simulations and determined that "In general, an ion with lower hydration energy permeates more readily than an ion with higher hydration," according to Tuan Anh Pham, co-author on the study and modeling director for the project.

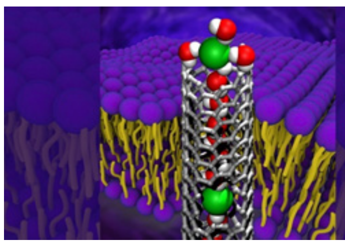

Image by Zhongwu Li, Fikret Aydin, Tuan Anh Pham and Alex Noy/LLNL

Understanding which anions permeate the nanotube pore could be critical to many separation processes, including desalination. "The observation of this strong differential selectivity is based on a mechanism unique to nanometer-scale pores and could pave the way for a new generation of custom-designed separation membranes," says Zhongwu Li, the first author of the paper.

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Quantum Simulations Reveal Missing Physics

Engineering models for shock initiation safety and explosive detonation performance rely on physics models that focus on hot spots of elevated temperatures which accelerate the chemical reactions governing explosions. Models for 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) explosions based on the hot spot paradigm, however, have been unable to describe both the initiation and detonation regimes, indicating missing physics in the fundamental understanding of what processes drive insensitive high-explosives detonations. Two Lawrence Livermore scientists discovered a new ignition mechanism that explains the unusual detonation properties of TATB. Their research appears in the May 22, 2020, online edition of *Physical Review Letters*.

To uncover the missing physics, the team used supercomputer simulations involving millions of atoms to examine the material response behind a detonation shock wave. They discovered the formation of networked shear bands, regions of highly disordered material produced under extreme stress. Illuminating the chemical reactivity of shear bands required deploying quantum-based molecular dynamics (QMD) simulations and high-performance computing. "The main challenge with QMD is that it can only be applied to small systems, so we developed a multiscale modeling technique to look at the chemistry of shear band and crystal regions," explains Matthew Kroonblawd, lead author of the study.

Through scale bridging with QMD, the team also discovered that disordered material in shear bands becomes chemically activated, forming in strongly shocked TATB, and reacting 200 times faster than the crystal. The scientists describe this newly discovered phenomena as "chemical activation through shear banding," which leads to enhanced reaction rates without the local heating typically evoked by hot spots.

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Iron Performance Under Pressure

The heaviest element produced by stellar nucleosynthesis, iron is also the most abundant heavy element in Earth's interior, and most studied for its socio-technological and planetary importance. Stable at ambient conditions in a body-centered cubic form, iron transforms to a nonmagnetic hexagonal close-packed structure as pressures rise above 13 gigapascals, 130,000 times the atmospheric pressure on Earth. To better understand this transition, Lawrence Livermore physicist Hyunchae Cynn and a team of international collaborators identified the sub-nanosecond phase transitions in laser-shocked iron, revealing all of iron's known structural types. Their research appears in the June 5, 2020, edition of *Science Advances*.

The team used a combination of a short-pulse optical laser and an ultrashort x-ray Free Electron Laser (XFEL) probe to observe the atomic structural evolution of shock-compressed iron at an unprecedented time resolution at 50 picosecond (ps) intervals. Team members also discovered the appearance of new phases after 650 ps with densities similar to or even lower than the ambient phase. This transition happens to be one of the fastest, occurring in less than 50 ps, with one of the highest strain rates recorded.

The research could further reveal the physics, chemistry, and magnetic properties of the Earth and other rocky planets by measuring time-resolved high-resolution x-ray diffractions for the entire duration of shock compression. "This is the first direct, complete observation of shock wave propagation associated with the crystal structural changes recorded by high-quality time series data," says Cynn, co-author of the paper.

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Commentary by Eric G. McKinzie

People Make the Mission **Possible**

OPERATING a national laboratory requires more than just state-of-the-art equipment. It requires a reliable infrastructure, modern systems, clear processes and procedures, proper tools, and most importantly, people. While the legacy of a laboratory may lie in its scientific breakthroughs, the heart of a laboratory lives in the people who do the work. Our scientists, engineers, administrators, expert communicators, craft workers, and others come together on the Laboratory's campus in support of our national security mission. Truly, our people make the mission possible.

To enable the mission, Laboratory employees are supported by a wide variety of infrastructure resources. Creating capabilities like the world's largest and highest-energy laser or the fastest supercomputer requires specialized systems and equipment, and the technology and infrastructure supporting those systems must be adaptable to mission needs. Exceptional buildings like the National Ignition Facility, the High Explosives Application Facility, and the Computing Facility are specifically designed to host some of our most advanced systems and technologies, which not only help scientists successfully conduct their research, but also attract and retain a world-class workforce.

While the Laboratory's scientists and engineers work on solving our nation's biggest problems, our service support employees act as partners, ensuring work gets done efficiently, safely, and cost-effectively. Our facilities personnel maintain clear roadways, walkways, and bike paths; our chefs provide healthy food options (and much-needed coffee breaks) in our cafeterias; and our custodial staff ensures our facilities remain sanitary and clutter-free—just to list a few examples. Our service employees are the unsung heroes of the workforce, working tirelessly to ensure all of us have a comfortable place to work.

The Laboratory's infrastructure also helps foster community. Organizations like the Lawrence Livermore Employee Services Association and the Laboratory's Employee Resource Groups help employees find a community of colleagues and friends, as well as provide lifestyle support such as childcare, a gym, and health services. To support group events and activities, the Laboratory invests in gathering areas and strategic landscaping—the community outside of the office is oftentimes as important as the one inside.

Further, operating a national security laboratory means Livermore's resources must be secure. The Laboratory's chief information officer and information technology teams make sure employees have the technology they need to get their jobs done safely and securely. The Laboratory also ensures its people and facilities are safe in the event of an emergency. With over 8,000 employees spread across 531 buildings and trailers, the Laboratory currently has a $20.2 billion replacement plant value. An onsite emergency management team and security force ensure a quick response to emergency situations. Lastly, organizations like Work Planning and Control, as well as Environment, Safety, and Health ensure the Laboratory is in compliance with federal standards that define how employees do work. All of these resources support our people, and when people are fully supported, they excel.

In a campus with so many moving parts, aging infrastructure is a challenge. The Laboratory was founded almost 70 years ago, and its age shows in some of the facilities and equipment. Luckily, we find ourselves at a historical crossroads with ample opportunity for growth and improvement. The Laboratory's demographics are changing, we are hiring at an unprecedented rate, and we're adding new equipment and facilities while modernizing others. To ensure our infrastructure keeps up with our growth, the Laboratory is investing in extensive infrastructure planning. Master infrastructure planning helps us shape what we want the Laboratory to look like a decade, or even two decades, from now. It helps us visualize our future and align our current steps with that vision. As the Laboratory grows, we also remain conscious of sustainability and responsible stewardship of taxpayer money. The Laboratory is leading efforts to conserve water, reduce energy and fuel, and implement electric vehicle stations. As beneficiaries of Earth's resources, we have a responsibility to protect and care for the planet.

The Laboratory faces its share of challenges in the coming decade, but the future is bright. We're scaling up our technology and resources, improving our processes and procedures, modernizing our infrastructure, and investing in the areas that will support our mission the most. Ultimately, investments in infrastructure will ensure the Laboratory meets mission needs and fosters the growth and success of our people, now and in the future.

■ Eric G. McKinzie is Deputy Principal Associate Director for Operations and Business.

TEAM SCIENCE TAKES

The Laboratory's new Emergency Operations Center will consolidate Livermore's emergency response functions and facilitate better collaboration with external emergency partners.

ON INFRASTRUCTURE

Using science-based infrastructure stewardship, the Laboratory tackles 10 years of infrastructure modernization as it anticipates several major projects and a rapidly growing workforce.

THE University of California Radiation Laboratory, now Lawrence Livermore National Laboratory, was opened on September 2, 1952, on the site of a decommissioned naval air station used to train pilots during World War II. Operating under the aegis of the U.S. Atomic Energy Commission, the Laboratory was tasked with the mission to advance nuclear weapons science and technology (S&T) to defend the nation at the height of the Cold War. As a "new ideas" laboratory guided by E.O. Lawrence's "team science" approach, in its first six years, the Laboratory produced rapid, innovative breakthroughs in nuclear weapons S&T. In six years, its workforce grew from 76 employees to more than 3,000, and its budget burgeoned from $3.5 to $45 million. Over the next 70 years, Lawrence Livermore continued to make significant advances in data-driven, computationally and experimentally based S&T, and established a reputation for its multidisciplinary approach, integrity, and commitment to excellence.

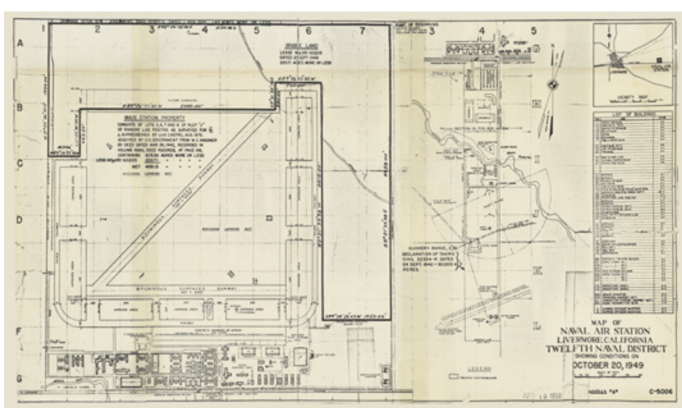
Today, with a workforce of more than 8,300 employees, contractors, postdoctoral fellows, and students, and an operating budget of $2.3 billion, the Laboratory's mission has evolved to stockpile stewardship, nuclear nonproliferation, and application of world-class S&T to strengthen the nation's security. The Laboratory's continued success draws from its ongoing commitment to its core S&T strengths and foundational values: team science and innovation. As Lawrence Livermore strives to support a growing workforce, rapid advances in information technology, and the challenge of pursuing two major National Nuclear Security Administration (NNSA) stockpile modernization programs, it is marshaling its signature strengths and a $2 billion infrastructure investment plan to guide the transformation of facilities, utilities, programmatic equipment, and workspaces over the next decade to fulfill its mission.

Mission Delivery Is Key

The Laboratory's Site Development Plan, Campus Capability Plan, and NNSA's Master Asset Plan outline the orchestration and execution of more than 500 infrastructure projects at Livermore ranging from the complete demolition and construction of entire buildings to the renovation of computing and data storage facilities, advanced manufacturing and materials labs, experimental glovebox rooms, and science enclaves that will impact and upgrade 80 percent of the Laboratory's workspace. When surveying infrastructure modernization needs, Lawrence Livermore and NNSA faced the complex question of where to begin and how to proceed. Seventy-six percent of the Laboratory's buildings are over 30 years old, and the sprawling campus has approximately 670 structural assets across 7 million gross square feet. Fortunately, the Laboratory's key mission drivers provided a good starting point.

The Laboratory's most important mission deliverables fall under the area of stockpile stewardship—maintaining and modernizing the United States nuclear weapons stockpile without conducting nuclear tests (*S&TR,* July/August 2015, pp. 6–14). Currently, Lawrence Livermore has two major stockpile projects directly supporting this mission: the W80-4 Life Extension Program and the W87-1 Modification Program (*S&TR,* October/November 2018, pp. 4–11). Stockpile modernization programs, major efforts to extend the service life of a warhead by as long as 30 years, typically draw on most, if not all, of the Laboratory's technical and scientific resources, as they constitute Lawrence Livermore's most significant weapons development effort since the Cold War. "To determine what areas to invest in, you have to look at what assets will have the greatest impact in supporting a stockpile modernization program," says Office of Laboratory Infrastructure director Cliff Shang, "Capabilities like hydrodynamic testing, high explosives testing, computing, high-energy-density physics, advanced manufacturing, and materials research are critical."

One of the broadest-impact areas of stockpile stewardship is radiochemistry, which has had four supportive laboratories and a glovebox facility renovated as part of the infrastructure investment plan. In one of the radiochemistry laboratories, scientists analyze aged post-detonation shot debris to characterize an explosion. One challenge radiochemistry scientists face is reducing ambiguity in their test results. "High-fidelity measurements help us refine our models, reduce uncertainty, and even measure and discover new things," explains Nuclear and Radiochemistry group leader Tim



(left) Members of the Naval Air Station, Livermore, stroll down Second Street in the 1940s. (right) A map depicts the Laboratory when it was acquired by the United States government in 1942.

Photos of the Laboratory's radiochemistry lab show recent renovations to the facility.

Rose. In addition to equipment, the team requires clean laboratory space. "Recent improvements in our laboratories have allowed us to handle the most sensitive materials and reduce the risk of cross-contamination." It has also allowed the Laboratory to take on more specialized ventures, like developing surrogate material debris for the Technical Nuclear Forensics mission. "Surrogate materials resemble the real thing, which people can process in different laboratories to compare results," says Rose. "These experiments help provide benchmarks for nuclear materials research." A modernized workspace is not only critical for the work itself, but for attracting and retaining scientific staff—updating lab space makes the Laboratory a more desirable place to work. For radiochemistry, that rings especially true. "New hires are important for sustaining our workforce. We need a modern facility for cutting-edge research and development."

Advanced Modeling Tools

Modernization of the radiochemistry laboratories serves as a successful example of Lawrence Livermore's extensive use of data to drive modernization decision-making processes (*S&TR,* September 2016, pp. 16–19). With a Laboratory and NNSA evaluation and planning methodology referred to as "science-based infrastructure stewardship," Livermore's infrastructure researchers use advanced computer modeling to predict and model infrastructure trends. Science-based infrastructure stewardship has many of the hallmarks that define stockpile stewardship and the scientific method: It is computationally based, data-driven, transparent, and there is a rigorous verification and validation process. "The budgetary constraints that come with being a government institution require us to maintain existing infrastructure much longer than in private industry, which puts Lawrence Livermore and NNSA at the forefront of facility modernization and innovation," says Jill Farrell, deputy for the Office of Laboratory Infrastructure. In fact, Farrell and two retired Livermore employees hold a U.S. patent for a maintenance recapitalization model that set a precedent for similar models used across NNSA.

Infrastructure enterprise-level modeling tools, including BUILDER, a specialized NNSA software program developed by the U.S. Army Corps of Engineers, and Move Management System (MMS), analyze equipment conditions, manage and prioritize facility improvements, track existing assets and ongoing maintenance costs, and even manage office and lab space utilization. Critical amongst these tools is Equipment Data Archive and Decision Support (EDADS). EDADS is a web-based information system

The Equipment Data Archive and Decision Support (EDADS) web-based information system helps the Laboratory manage programmatic equipment investments.

that allows the Laboratory to manage programmatic equipment investments, like the those needed in radiochemistry. Within EDADS, scientists and engineers can enter equipment replacement or purchase requests, which are reviewed by group leaders in their areas. EDADS generates a score based on the equipment's benefit, risk, and complexity, which stakeholders use to create a prioritized request list as well as to approve equipment acquisition. The full capability-based portfolio is provided to NNSA to inform decision making on a yearly basis. "Before EDADS, nobody gathered equipment requirements or understood strategic planning to give people the resources they needed at a systematic, Laboratory-enterprise scale," says Weapons Infrastructure deputy program director Katy Lu. "You really need to bring an enterprise-level view into the process early on to understand the needs required to support the mission."

In device testing, that early input has proved critical for meeting experimental test schedules supporting weapons engineering and research and development. "In the weapons program facilities, we fabricate, assemble, and test components and assemblies. Some parts are classified, some are radiological, but all of them require high-precision tools to fabricate," says Chris Adams, Livermore's associate program leader for NNSA's Capabilities-Based Investment Program. Computerized coordinate-measuring machines and transmission electron microscopes are examples of the unique equipment needed to facilitate the team's work. "Recently, we implemented a new hydraulic skid to control the doors of the firing tanks. That simple improvement reduces the firing tanks' risk," says Adams.

New equipment investments have also supported high explosives field tests at Site 300, the Laboratory's remote testing site (*S&TR,* July/August 2017, pp. 12–15). "When the Laboratory is ready to test explosives at scale, they go to Site 300. There, we have diagnostic equipment like cameras, oscilloscopes, and specialized recording devices to measure the characteristics of the explosives. Capability-based investments have allowed us to efficiently acquire and upgrade these critical equipment systems," says Adams. The EDADS tool has worked so effectively that it has been shared with sister laboratory Los Alamos, and other institutions have expressed interest in the program. "Our ultimate goal is an enterprise system for programmatic equipment. EDADs has helped us better understand and communicate our resource needs," says Lu.

Another critical piece in the Laboratory's infrastructure toolbox is CostLab—a facility maintenance and operations modeling tool that is the result of a decades-long collaboration between the Laboratory and commercial real estate services company, Coldwell Banker Richard Ellis (CBRE). CostLab helps the Laboratory predict budget requirements needed to sustain the Laboratory's current facility and utility asset portfolio, also known as "real property." The risk-based model can predict maintenance needs up to 10 years, allowing the Laboratory to plan for real property equipment and system replacement expenditures earlier in the budget planning cycle. Similarly, for the Laboratory's buildings, Lawrence Livermore has utilized an NNSA implementation of BUILDER to track facility condition and functionality. BUILDER aggregates data from other infrastructure tools like the Laboratory's Computerized Maintenance Management System (CMMS) to track overall building and trailer conditions.

Lawrence Livermore even has a tool for moving people's offices and tracking utilization of office space within the Laboratory. "On a one-square-mile campus with hundreds of buildings and trailers, it's important to be aware of what office spaces are available," says Farrell. The

The Contained Firing Facility at Site 300 supports the Laboratory's design and certification capabilities.

Laboratory's MMS solves that problem by cataloging each office space in real time, ensuring efficient, high-asset utilization of the nation's investments. As the Laboratory experiences unprecedented growth coupled with changes in how and where employees work, especially with new work controls established during the COVID-19 pandemic, the MMS is critical to office space planning. The tool includes features like floor plan maps, room reservations for new employees, and documentation of secondary offices, eliminating the need for yearly labor-intensive building walkarounds to survey the Laboratory's working spaces. The MMS has even been applied to other, more unique purposes—such as modeling a post-COVID-19 office repopulation scenario and locating people onsite for emergency planning purposes.

Innovation in Construction

"The last piece of infrastructure planning, and probably the most important, is execution. That's the Project Management Office," says Shang. The Project Management Office (PMO), an in-house construction management team, handles everything from design and budget estimation to engineering and construction. Under a "one team" approach that takes the Laboratory's model of team science and adapts it to construction, PMO collaborates with other programs and entities around the Laboratory to complete projects. Organizations like Environment, Safety, and Health; the Laboratory's financial office; and the Supply Chain Management organization all work with PMO to ensure federal regulations are followed and to procure the equipment, materials, and subcontractors needed to execute a facility construction project.

A key innovation developed by Lawrence Livermore and NNSA for construction is the use of "area plans." Many capital construction projects—projects costing more than $20 million—are expensive and can take years to complete, which does not always align with the delivery of major scientific research. The area plan essentially creates a time-phased approach to infrastructure investment, so programs can obtain the facilities and equipment they need more quickly at a more affordable price. A key example of an area plan applied to scientific research is in materials engineering. One of the most important aspects of stockpile stewardship is understanding the behavior of the materials placed in nuclear weapons. "Over the lifetime of a weapon there may be material incompatibility issues. Before putting nuclear material into a package, you need to exhaustively test and understand how it behaves over time," says Shang. The time and resources necessary to update the materials engineering facilities as a single capital project would take over a decade to complete, so Livermore and NNSA developed the Applied Materials Engineering (AME) area plan. "Rather than allocating a large amount of time and money into a single building, we will construct a limited set of smaller buildings and repurpose existing ones. There's a little bit of innovation on how you do that, and there's a lot of modeling and analysis by subject matter experts," says Shang. Not only is the AME facility getting renovated 15 years earlier, it is also consolidating and better utilizing available space, decreasing its environmental footprint, and improving sustainability. The materials engineering facility footprint will shrink from 150,000 to 80,000 square feet while maximizing the available workspace and equipment.

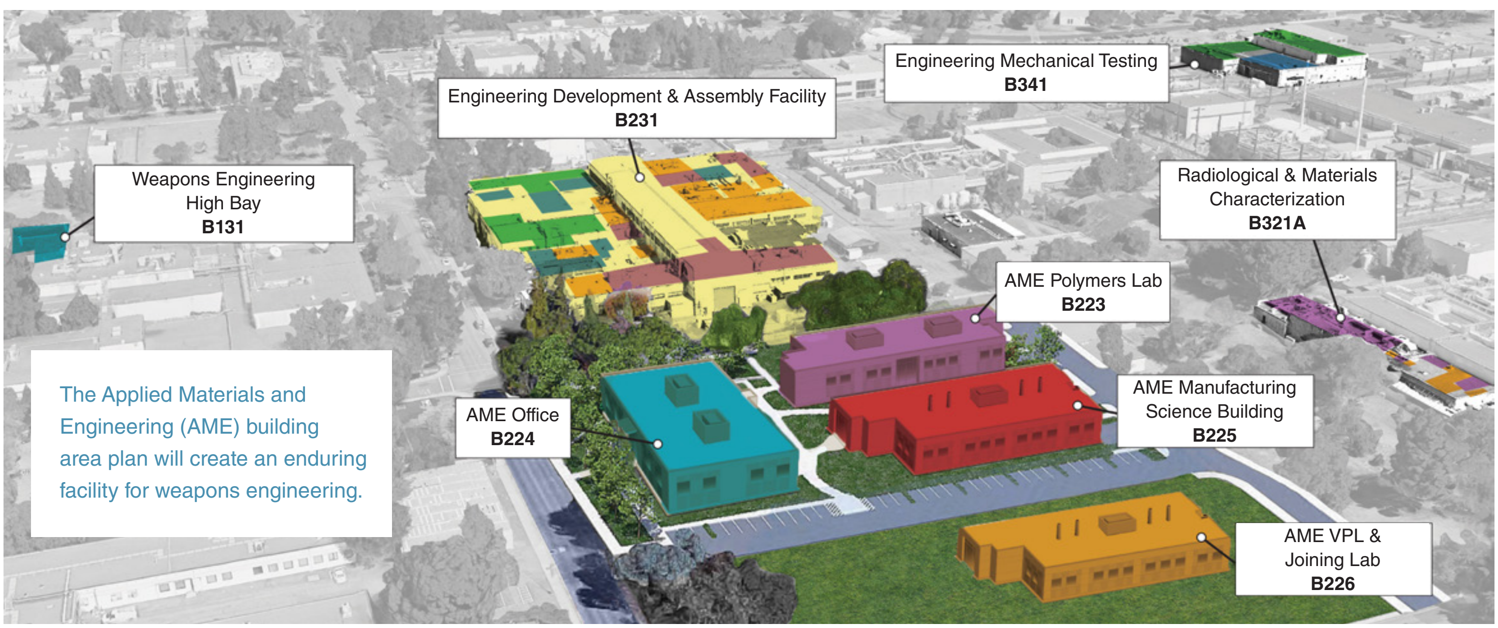
Lawrence Livermore's infrastructure team is applying area plans in other locations across the Laboratory such as the 3200 building block, where engineers and expert machinists manufacture experimental assemblies and parts. As demands for complex hardware not found commercially increase, the need grows for a modernized infrastructure to support the Laboratory's manufacturing capabilities. A revitalized infrastructure will allow the 3200 block to introduce new manufacturing techniques, augment capacity for increased demand for precision parts, and sustain activities on critical building systems' utilities and specialized equipment.

Out with the Old, In with the New

In tandem with new construction and renovation, the Laboratory decommissions and demolishes buildings too old to modernize or seismically retrofit without incurring exorbitant costs. The Laboratory's history as a naval air station has contributed to some of its contaminated and obsolete facilities. Lawrence Livermore's Transition and Disposition (T&D) program monitors these facilities and works to remove them to reduce risks and environmental impacts as well as lessen the Laboratory's footprint and make space for new, modern facilities.

"There's usually an economic breakpoint when deciding to demolish or refurbish a building," says Farrell, "For example, a roof might get replaced every 20 or 30 years. On a 70-year-old building you're probably replacing the roof for at least the second time, and now other parts of the infrastructure are failing. It becomes so expensive to maintain the facility that it makes more sense financially to demolish it and build a brand-new building." The Laboratory is currently completing several major T&D efforts, including demolishing its excessed Mars E-Beam facility and a long-vacant pool-type reactor with funding and support from the DOE. "This funding allows Livermore to remove some of the highest risk buildings from the site and clear the way for new construction. T&D efforts contribute in a significant way to site renewal," says T&D program manager Mark Costella.

This pool-type reactor at the Laboratory was contaminated by multiple elements, including beryllium and cobalt 60. The Laboratory has been authorized to receive funding for its demolition.



The Applied Materials and Engineering (AME) building area plan will create an enduring facility for weapons engineering.

(from left) Laboratory director Bill Goldstein, Weapons and Complex Integration principal associate director Kim Budil, former National Nuclear Security Administration administrator Lisa E. Gordon-Hagerty, and Livermore Field Office manager Pete Rodrik dedicated the new AME campus in September 2020, which will include a new polymer production development enclave.

The Next 10 Years and Beyond

The integration of the Laboratory's infrastructure planning efforts are represented in its Site Development Plan, Campus Capability Plan, and NNSA's Master Asset Plan—essentially blueprints for how each capability will be supported by infrastructure and equipment investments, so the Laboratory can continue to support its national security mission and its people. A modernized infrastructure enables scientists to not only support stockpile stewardship, but also conduct groundbreaking research in areas such cancer, traumatic brain injury, drug synthesis, and more. "We're essentially upgrading the entire Laboratory," says Lu.

The Laboratory recently completed construction of an advanced manufacturing laboratory, a new office building, and a materials laboratory. It is updating its computing complex to host a new exascale computer and recently broke ground on a state-of-the-art emergency operations center. A new polymer production development enclave is being built in partnership with Kansas City National Security Campus and NNSA, which will allow scientists and engineers an opportunity to reinvent how the Laboratory produces parts for the stockpile. All of these buildings will require specially dedicated utilities, power, and cooling, among other things, which all factor into infrastructure planning. "Our new slogan is 'Pardon Our Dust' because of all the construction going on," quips Farrell.

As the Laboratory launches into the 21st century, Laboratory veterans like Shang fondly remember its history. "I can say when I walked into the Laboratory as a new graduate, I was pretty amazed by this place. The infrastructure has degraded in the last 10 years, but that's what is really energizing about this. Right now, our staff in collaboration with NNSA have a direct hand at turning things around." Shang boils down infrastructure investments to its most important benefactors: "When you invest in infrastructure, it's actually an investment in our people."

—Lauren Casonhua

Key Words: advanced computer modeling, applied materials engineering, area plan, BUILDER, campus capability plan, CostLab, Equipment Data Archive and Decision Support (EDADS), high explosives, infrastructure planning, Move Management System (MMS), radiochemistry, science-based infrastructure stewardship, Site Development Plan, stockpile stewardship.

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Fighting Bacterial Infections with Machine Learning

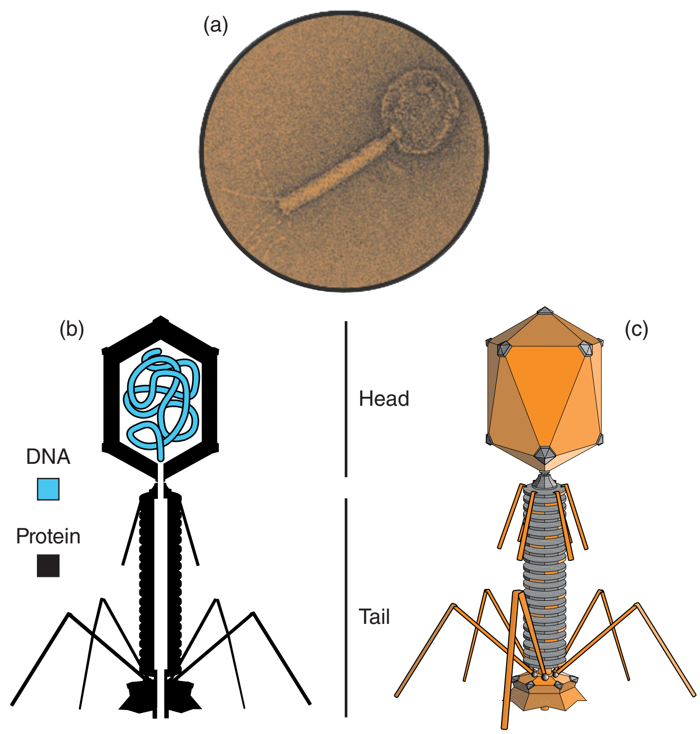
IN 2015 while vacationing in Egypt, Tom Patterson contracted a drug-resistant strain of *Acinetobacter baumannii*, a bacterium known to infect as many as 8,500 and kill 700 people in the United States every year. After a battery of antibiotic treatments, recurring bouts of septic shock, and slipping in and out of a coma over the course of several months in what his doctors called, "the worst infection on the planet," Patterson was transferred to the University of California, San Diego (UCSD) where clinicians are familiar with *Acinetobacter* infections brought home by U.S. forces returning from the Middle East. Running out of options and seeing her husband's condition continue to deteriorate, Patterson's wife, Steffanie Strathdee, an infectious disease epidemiologist at UCSD, proposed an unconventional treatment: bacteriophage therapy. Discovered in the early 1900s, bacteriophage therapy was an emergent, yet controversial means of treating bacterial infections before penicillin took the world by storm. Patterson's treatment would involve an experimental cocktail of microbial viruses to attack the bacteria infecting his body. Within a few days of intravenous administration, Patterson awoke from his coma and began to recover.

Patterson was the first person in North America to receive intravenous bacteriophage therapy to treat a systemic bacterial infection, and his dramatic recovery from what appeared to be an inevitable death sentence helped spark a renewed interest in a potential treatment, which had largely been eschewed by the medical community in the United States and Europe.

To successfully combat increasing antibiotic resistance and treat challenging bacterial infections like Patterson's, scientists in the Forensic Science Center (FSC) at Lawrence Livermore have partnered with San Diego State University and UCSD to advance bacteriophage therapy. Using Livermore's high-performance computing resources and a novel computational algorithm called "PHANOTATE," scientists are predicting the protein structures and functions of bacteriophage genes so they can help researchers develop targeted therapeutics to treat bacterial infections.

The World's Most Abundant Predators

Sometimes referred to as microbial viruses, bacteriophages, literally meaning "bacteria eaters," are more abundant than any other living organism on Earth. Typical microbial viruses are composed of a protein capsid (DNA-filled head), an elgongated body with a collar, and a tail. These viruses have a penchant for a specific victim: bacteria. Unlike antibiotics, bacteriophages target specific bacteria species, and they evolve over time to keep up with their bacterial counterparts' mutations. "Bacteriophages have recognition molecules on their tails that help them identify their preferred bacterial host. They attach to the host and inject their DNA into the bacterial cell, turning the cell into a virus parts factory," explains Brian Souza, group leader for Biosecurity and Bioforensics

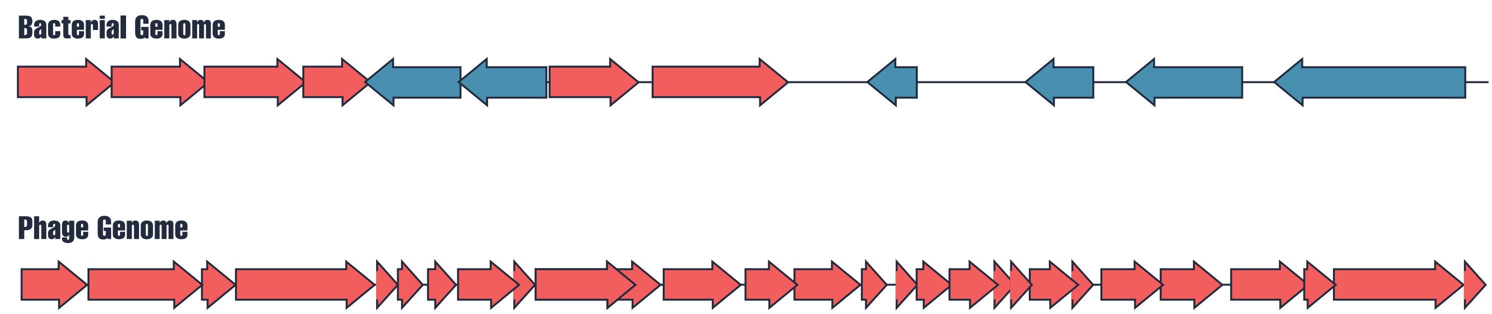


A bacteriophage, also known as a microbial virus, (a) magnified by a transmission electron microscope, (b) in 2D cross-section, consists of a DNA-containing head and a tail made up of protein, and (c) in 3D.

at Lawrence Livermore. Near the end of their reproductive cycle, bacteriophages produce holin, a protein that creates holes in a bacterium's cell wall. The bacteriophages then produce another protein called endolysin, which "lyses" or breaks the cell apart to release the newly generated bacteriophages so they can go on to infect other bacterial cells.

Genetic Testing for Bacteriophages

One of the first, biggest obstacles researchers faced in setting the groundwork for effective bacteriophage therapy was matching the particular bacterium infecting a person's body with the bacteriophage that would neutralize it. This matchmaking required characterization of various bacteriophages, particularly identification and annotation of their genes. "Before we began this project, a gene finder specifically for bacteriophages didn't exist. We had to use bacterial gene finders, which don't account for phage-specific characteristics," explains Carol Zhou, a computational biologist working on the PHANOTATE algorithm. "Phage genes are shorter, they're usually transcribed unidirectionally, and they're more compact than bacterial genes," says Zhou.



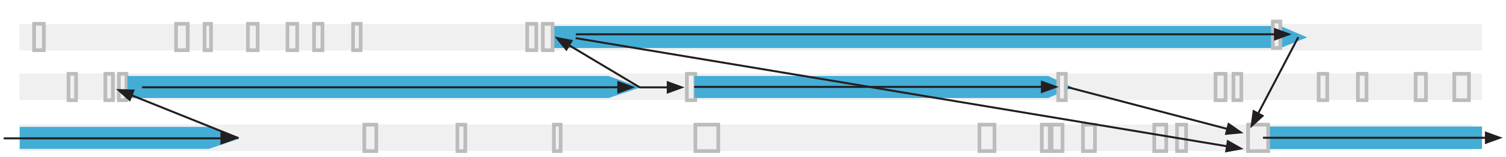
Compared to the bacterial genome, the phage genome is much more compact and is usually transcribed in one direction.

Phages also frequently exhibit unusual characteristics like gene overlap and nested genes within genes.

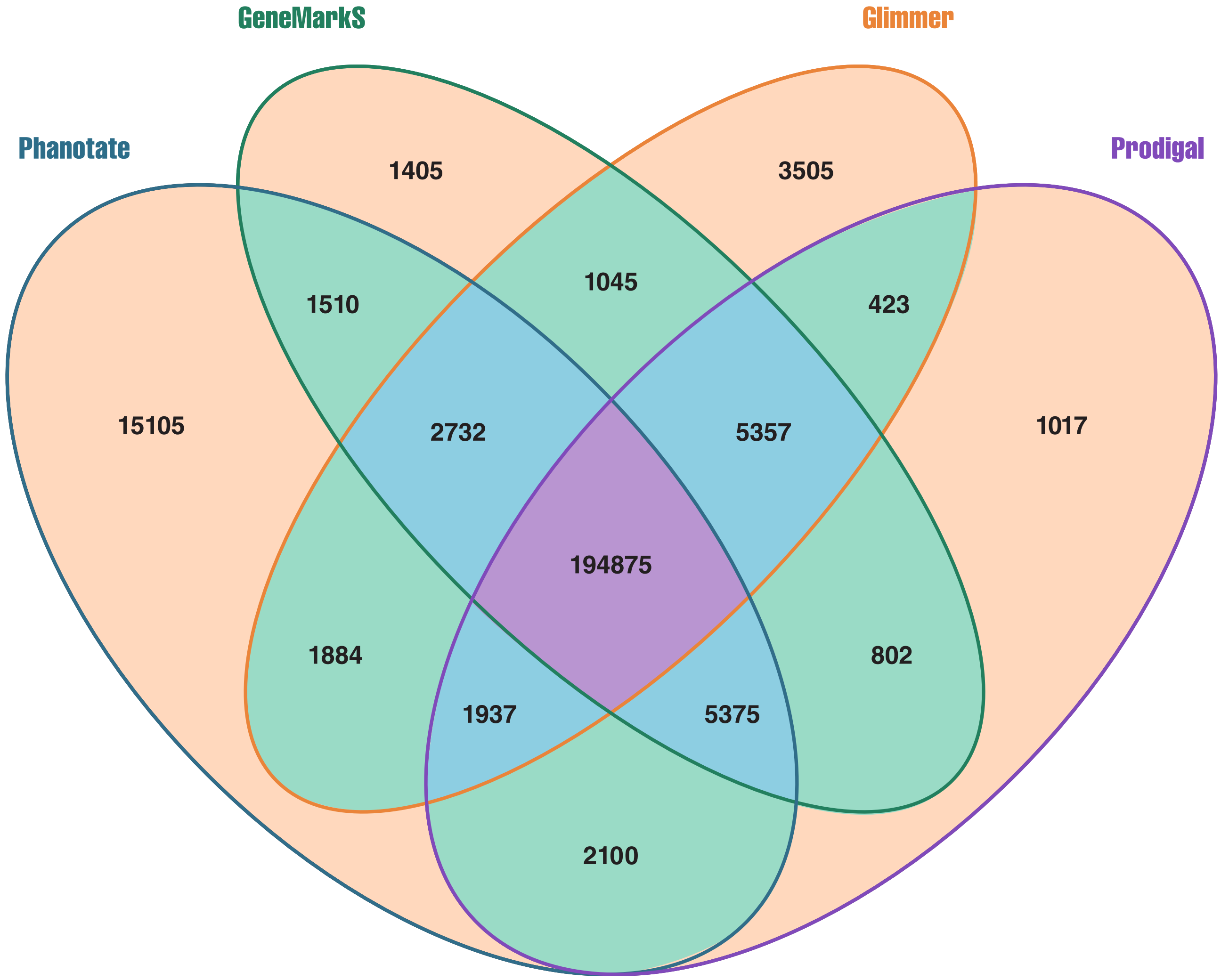
To develop a way to identify bacteriophage genes, the team created PHANOTATE, a gene caller machine learning algorithm specifically designed to identify phages. Given bacteriophages' diversity, unusual characteristics, and an abundance estimated to be 10^{31} (a number that translates into approximately one trillion phages for every grain of sand in the world), the computational burden necessary to curate massive datasets of phage genes made Lawrence Livermore particularly suited for the effort. "We decided our algorithm would model bacteriophage genomes with a weighted graph that has nodes and edges," says Zhou. "The nodes represent start and stop codons—sequences of three nucleotides which form a unit of genetic code—while the edges represent their translatable parts or open reading frames (ORFs), gaps, and strand switches. There's a weight penalty for anomalies, which the algorithm detects and works into the statistical likelihood of occurrence," explains Zhou.

The team implements the algorithm using the Bellman–Ford method, which treats the phage genome as a network of paths, with ORFs as the most favorable, and overlaps and gaps as less favorable. The network of connections portrayed by the weighted graph allows scientists to find the optimal gene path for picking the right bacteriophage to neutralize a particular bacterium. These paths are then compared to the results of established, bacteria-focused gene annotation tools to ensure PHANOTATE predicts accurate pathogen genomes. "Out of the four bacteria gene-calling codes we compare PHANOTATE against, our algorithm actually produces the largest total set of genes, including smaller genes that the other gene callers can't find," says Lawrence Livermore biomedical scientist Stephanie Malfatti. To ensure PHANOTATE does not produce false positives, the team leverages large databases like the National Center for Biotechnology Information (NCBI) Sequence Read Archive. "When we analyzed PHANOTATE's smaller genes, we found a number of good sequence matches and determined that not only can PHANOTATE find smaller genes than other gene callers, but it's also identifying them accurately," says Malfatti.

To locate and identify or "annotate" genes, the Livermore team also developed an automated throughput pipeline: the multiple-genome Phage Annotation Toolkit and Evaluator, or "multiPhATE." multiPhATE provides a scalable pipeline into which phage genomes can be entered, so their protein structures and predicted functions can be accessed by the biomedical research community. "The PHANOTATE algorithm results are put into the multiPhATE system and processed by annotation tools against a number of databases, several of which are specific to viruses," says Zhou. The combination of these two programs helps researchers identify the genes that, when translated into proteins, play a role in the infection and destruction process of a host cell. The team shares their codes on the open-source software platform GitHub, where the public has already identified potential enhancements. "One of the benefits of this platform is that other people can use and improve it," says Zhou.



A Bellman–Ford algorithm finds the optimal gene path for a phage.



Number of genes predicted by the four primary bacterial gene prediction algorithms: GeneMarkS, Glimmer, Prodigal, and PHANOTATE and combinations thereof, with PHANOTATE identifying the largest total set of genes. Orange background: predicted by a single algorithm; green background: predicted by two algorithms; blue background: predicted by three algorithms; purple background: predicted by all four algorithms.

Implementing Bacteriophage Therapy

Phages can be either lytic or temperate, so the team is focused on identifying lytic phages because they will quickly corrode and kill bacteria. Malfatti explains, "Gene annotation gives us the ability to look at specific suites of proteins and identify the genes that will enhance a phage's effectiveness, as well as the phages that will be most effective against a particular bacterium after comparative analyses."

With renewed funding, Souza's team of collaborative, multidisciplinary experts is working on refining and further enhancing the PHANOTATE algorithm even further, so it can identify additional gene overlaps and nested genes. Ultimately, the team anticipates that bacteriophage therapy will one day be used in a wide range of areas, including infectious diseases, skin grafting, tissue repair, and gut health. Says Zhou, "For us, success is defined in stages. Reaching deployment and use of the code by other scientists or publishing another paper about our findings are hallmarks of success."

—Lauren Casonhua

Key Words: bacteriophage therapy, Forensic Science Center, gene annotation, microbial viruses, multiPhATE, National Center for Biotechnology Information (NCBI), pathogen, PHANOTATE.

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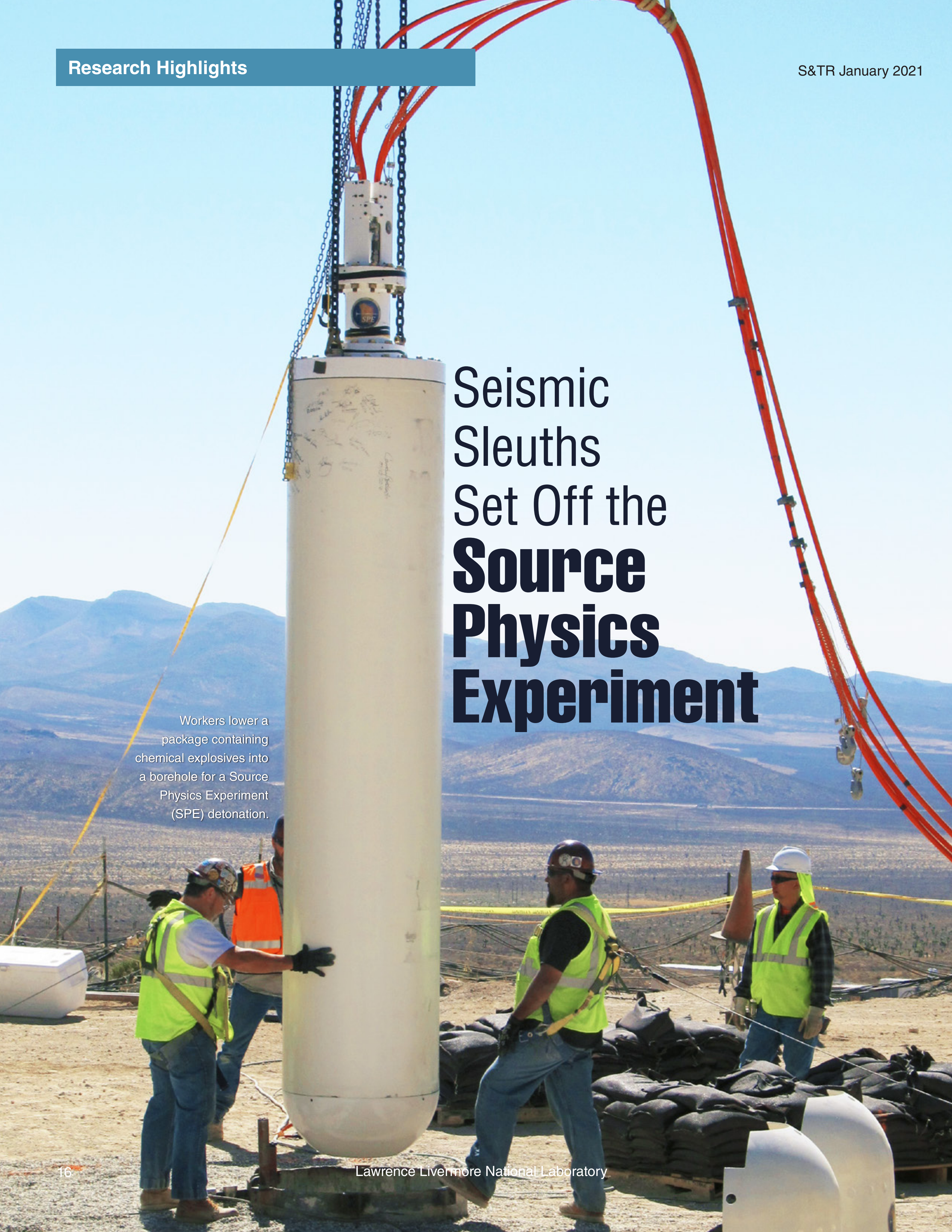
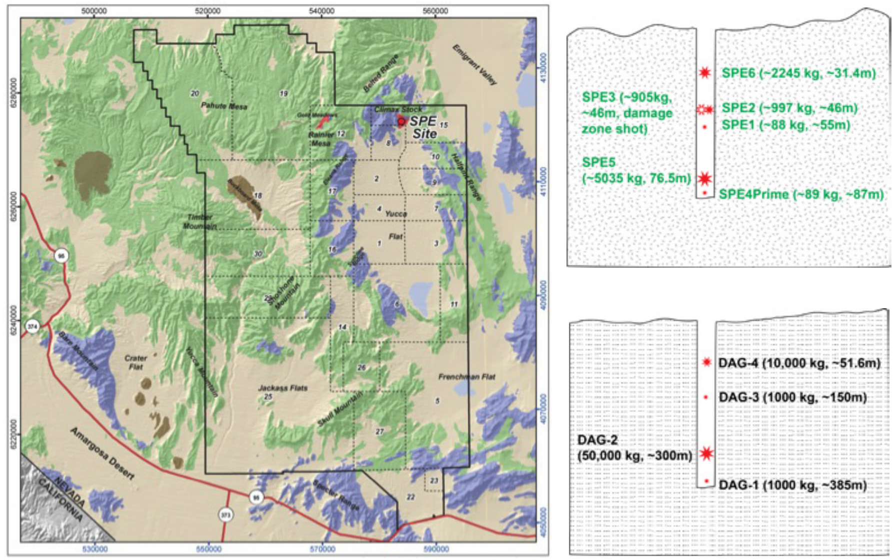
Seismic Sleuths Set Off the **Source Physics Experiment**



Workers lower a package containing chemical explosives into a borehole for a Source Physics Experiment (SPE) detonation.



The locations of the SPE experiments at the Nevada National Security Site (NNSS). The insets show the depth and explosive yields of each detonation of SPE Phase I in granite, and SPE Phase II DAG (Dry Alluvium Geology).

THE ground rumbles and seismic waves radiate away from an underground chemical explosion less than 100 meters below the Earth's surface in southwestern Nevada. The waves travel through granite at speeds of two to eight kilometers per second depending on the type of wave. Above ground, more than 100 seismic instruments record every nuance of the waves' frequencies, travel times, and amplitudes, while additional instruments record acoustic, electromagnetic, and visual data. Planning for this test took months, but the results, which will yield vast amounts of data in a matter of seconds, will provide important, new insights.

The data will help the scientists of the Source Physics Experiment (SPE) discriminate among the seismic fingerprints of a small, illicit nuclear explosion, an earthquake, a mine disaster, or any of the other noises, squeaks, and geophysical undulations that a variety of human activities and natural phenomena generate. The results of the SPE will make a difference half a world away—or anywhere throughout the world—where adversaries try to surreptitiously develop nuclear weapons. The SPE data will also help characterize the yields of declared underground nuclear tests—the most recent of which were conducted by the Democratic People's Republic of Korea (North Korea). "The purpose of the Source Physics Experiment," says William R. Walter, Lawrence Livermore geophysicist and chief scientist for several of the SPE series experiments, "is to provide the data to develop, test, and validate software codes used to monitor for nuclear explosions and characterize any that are detected. Now that nuclear testing is no longer performed, we need physics-based methodologies to perform validation."

Massive Undertaking of Many Partners

A considerable endeavor involving Lawrence Livermore, Los Alamos, and Sandia national laboratories; the Nevada National Security Site (NNSS) and its operator, Mission Support and Test Services; the University of Nevada, Reno; the Air Force Technical Applications Center; the Defense Threat Reduction Agency; and the National Nuclear Security Administration (NNSA), SPE improves the identification of nuclear events, and the ability to tell them apart from non-nuclear occurrences, as well as bolsters the ability to estimate the yields of nuclear explosions in different types of rock and to model underground detonations.

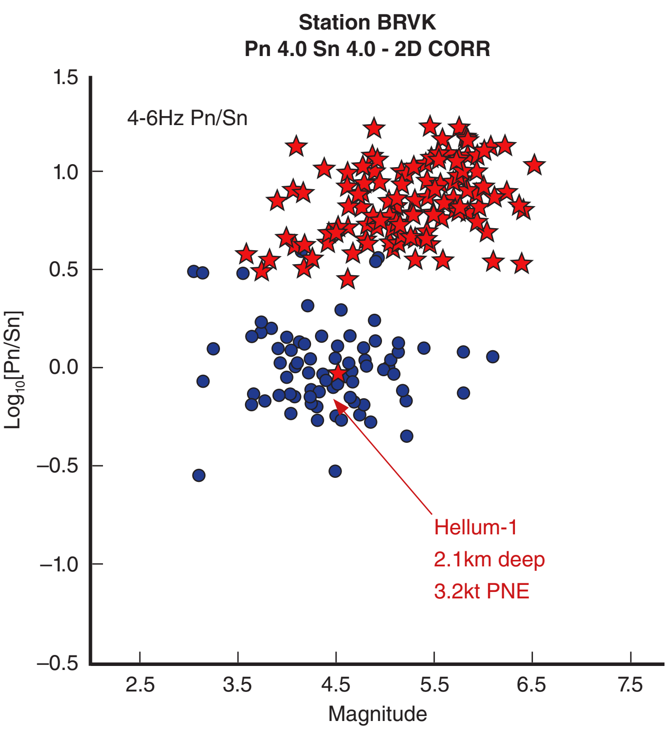
Phase I of SPE occurred between 2010 and 2016 as a series of detonations at the NNSS, formerly called the Nevada Test Site, where many U.S. nuclear tests were performed before the cessation of testing in September 1992. SPE Phase I consisted of six detonations at varying depths between 31 meters and 87 meters in a borehole drilled into the area's granite "basement" rock. The chemical explosions' yields ranged from an equivalent of 80 kilograms to 5,000 kilograms of trinitrotoluene (TNT).

The SPE team carried out Phase II, the Dry Alluvium Geology (DAG), between 2017 and 2019. These four explosions were emplaced in a hole drilled into sandy, rocky, and boulder-filled sediments in another area of the NNSS. The geologic opposite of Phase I, the Phase II DAG shots ranged at depths from 50 to almost 400 m, with two explosion yields of 1,000 kg, one at 10,000 kg, and one at 50,000 kg. The Phase II blasts were designed to be 10 times larger than those of SPE Phase I to produce the same degree of shaking in alluvium as in granite. More than 1,000 seismometers recorded seismic data from the surface and from underground boreholes near the detonation, while other instruments collected surface and airborne acoustic data of sound waves above the site, as well as low-frequency infrasound waves generated by the quakes, electromagnetic measurements, and video footage.

Geology Matters

Correctly estimating the yield of shots and modeling them with high-performance computers requires understanding how seismic waves propagate in different geologies. "The geology of the detonation site matters a lot," says Walter, "The geology in Nevada is very different from the Russian test site and the former Soviet test site in Kazakhstan." As a result, seismic recordings of U.S. and Soviet tests from the nuclear testing era are not directly comparable, so back in 1988, the U.S. and Soviet Union agreed to monitor each other's underground tests to assist treaty verification.

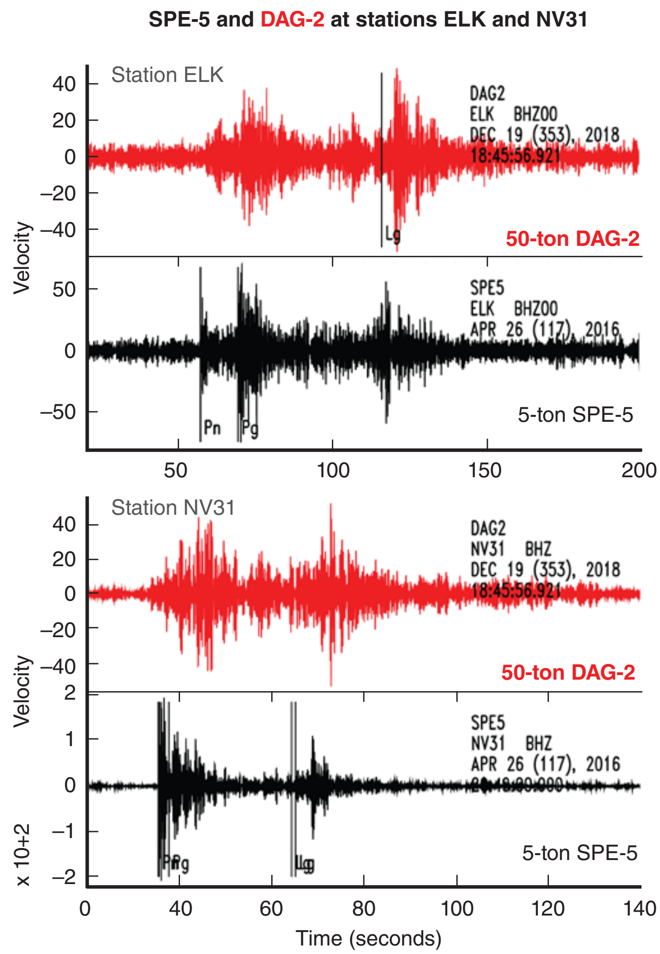
Earthquakes produce several types of waves, including primary or pressure (P) and secondary or shear (S) waves. P-waves are similar to sound waves, and the medium through which they travel compresses and expands in the same direction the wave travels. P-waves travel faster than S-waves, which are produced as the medium oscillates perpendicularly to the wave's direction of travel, producing a shear force. The ratio of the heights, or amplitudes, of P-waves to S-waves (P/S ratio) varies between explosions and earthquakes at high frequencies, providing a generally reliable way of differentiating the two. In explosions, measured P/S wave ratios are usually greater than one, but earthquakes produce higher-amplitude S-waves, resulting in very low P/S ratios. Sometimes, however, this method produces inconsistent results. For example, researchers do not understand why the P/S ratio of one recorded, unusually deep nuclear detonation was more like an earthquake rather than a nuclear test. Anomalies like this, and the lack of seismic models for explosions in dry alluvium, have motivated the SPE program to gather data from different types of geology.



A nuclear explosion usually generates a ratio of P-waves to S-waves amplitudes (red stars) greater than one (Note that 0.0 = Log (1), 0.5 ~ Log (3) and 1.0 = Log (10)), while earthquakes generate far more powerful S-waves than P-waves (blue circles), resulting in lower P/S ratios. But the P/S ratio of one unusually deep nuclear test, Hellum-1, looks like an earthquake. Explaining anomalies like these motivated the SPE's research program.

With the SPE Phase I and II shots complete, the team is now analyzing the voluminous amounts of data they have collected. Already, the data have revealed discoveries. The DAG shots display distinct differences from explosions in granite, including major differences in the size and frequency content of the seismic amplitudes that will provide helpful methods for evaluating yields in different geologies.

Although earthquakes generate both types of waves, explosions theoretically should not generate S-waves as the energy emanates radially. In fact, explosions often create S-waves, but how they are generated has been poorly understood. "No one had a good model for how chemical explosions in the alluvium generate S-waves, but the DAG



Examples of data collected during an SPE 5-ton shot in granite (black waveform) vs. a 50-ton DAG shot in alluvium (red) show similar amplitudes despite their large yield difference and more subtle difference in their relative P- and S-wave amplitudes. These differences will help the SPE team develop better methods to model detonations in different types of geology.

data shows in great detail how they do," says Walter. "Now there will be a push to revise the monitoring models used for these explosions to correctly predict S-wave generation and propagation." The SPE team also saw evidence that S-waves were generated very close to the explosion, indicating that multiple mechanisms appear to contribute to what previously could only be monitored from a distance.

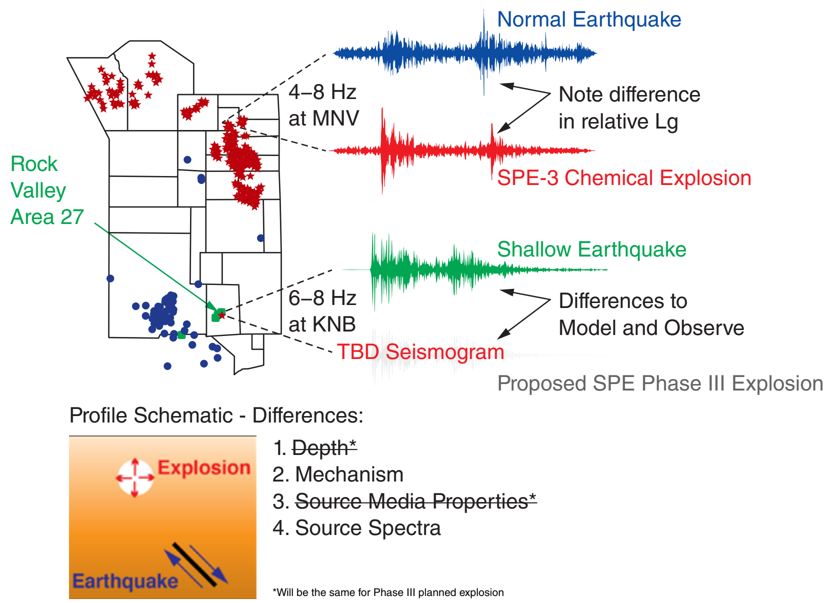
Wave Transformations

Another effect revealed in the DAG data was the conversion of P- and surface waves into S-waves as they travel. The transformation happens quickly, within about one or two km from the explosion. The SPE data led to significant improvements and validation of the modeling codes. Two wave modeling codes are used: GeoDyn-L, which models the nonlinear hydrodynamic behavior of rocks under strong shock, and SW4 (Seismic Waves 4th Order), which models seismic wave propagation in three-dimensions. Both codes leveraged institutional Laboratory Directed Research and Development investments, and together they represent the state of the art in modeling seismic wave generation and propagation in complex earth structures.

A third surprise in the data was the presence of aftershocks in the alluvium shots. Aftershocks were observed following some nuclear tests, but were fewer than typically observed after earthquakes. As a result, the number of aftershocks measured after an unknown event could help determine whether it was an explosion or an earthquake. The team recorded few aftershocks after the SPE shots in granite, but to their astonishment, they saw many tiny aftershocks in the alluvium shots following the largest 50-ton DAG-2 test. The mechanisms behind the generation of these aftershocks is still being studied, but the answer could help explain why induced earthquakes sometimes occur where fracking for oil and gas in porous or sandy rock formations takes place. One explanation is that an explosion gradually drives pressurized gases through the sediment to the surface, causing tiny tremors.

Releasing Data to All Users

Since the SPE began, the multi-institutional team has produced more than 40 peer-reviewed publications and in January 2021, the SPE Phase II DAG team received the Department of Energy's Secretary of Energy Achievement Award. In addition, all of the data from SPE Phase I shots are publicly available now, and the Phase II DAG shot data will eventually be made accessible on the Incorporated Research Institutions for Seismology website: www.iris.edu. SPE data and results provide valuable resources to the world's nuclear nonproliferation community. For the United States, the SPE data and scientific results equip experts with better tools, such as high-performance computer modeling of explosions



SPE Phase III will directly compare the relative P/S wave amplitudes of a new chemical explosion with earthquakes in the same media and at the same depth in a region of the NNSS where unusually shallow (1–3 km depth) earthquakes (green) have occurred. This will improve understanding of the P/S differences observed between normal depth (5–15 km) earthquakes (blue) and SPE-3 chemical explosions (red).

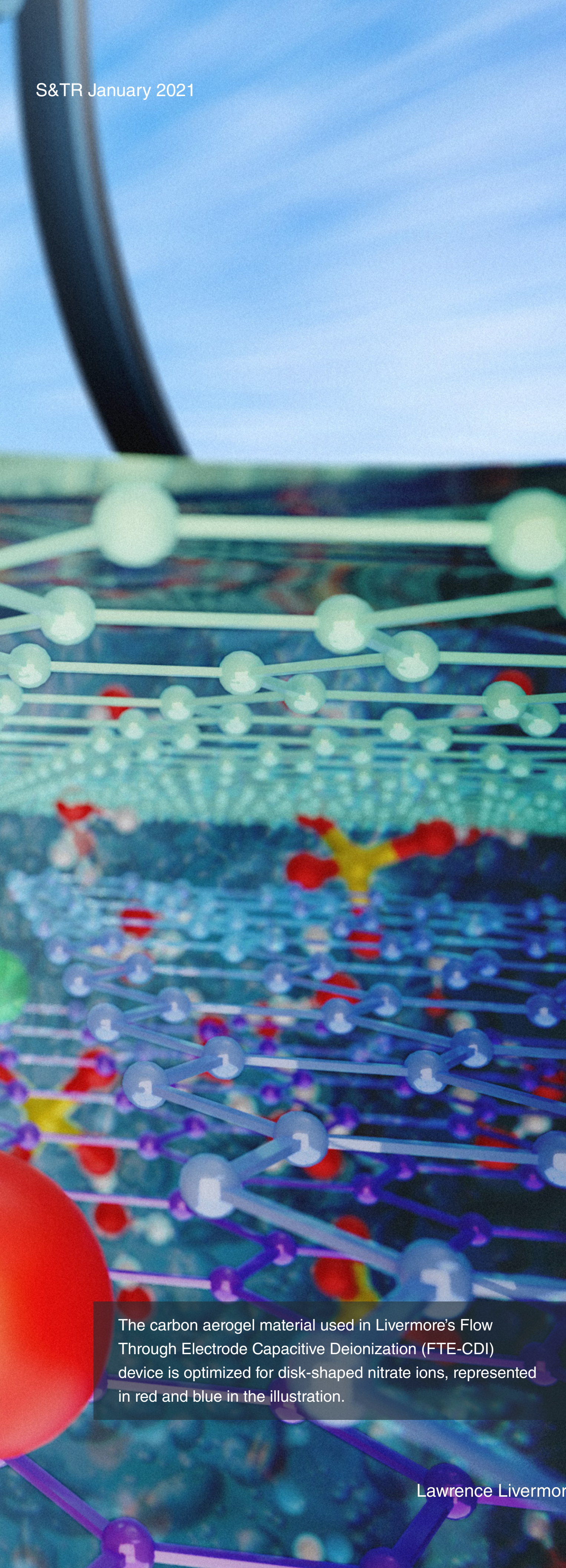
to discern the signals of actual illicit nuclear tests from other natural geophysical phenomena. Yet some uncertainties remain between deciphering explosion and earthquake signatures, which SPE scientists hope to resolve in SPE Phase III. For this next phase, the team is exploring ways to obtain a direct comparison of the two kinds of seismic waves in the exact same media at the same depth by drilling into the location of a previously recorded earthquake, setting off explosions, and recording the explosive test data at the same stations that recorded the naturally occurring earthquake. "Explosion monitoring is a nice problem in geophysics," says Walter. "You get to use every tool in the toolbox, including many types of field data, algorithms, and lab experiments. And there is satisfaction in knowing that the work helps make the world a safer place."

—Allan Chen

Key Words: The Defense Threat Reduction Agency, Dry Alluvium Geology (DAG), GeoDyn-L, granite, Incorporated Research Institutions for Seismology, National Nuclear Security Administration (NNSA), Nevada National Security Site (NNSS), pressure (P) waves, shear (S) waves, Source Physics Experiment (SPE), SW4.

For further information contact Bill Walter (925) 423-8777 (walter5@llnl.gov).

Tailored Water Treatment **Ready to Clean Up**



The carbon aerogel material used in Livermore's Flow Through Electrode Capacitive Deionization (FTE-CDI) device is optimized for disk-shaped nitrate ions, represented in red and blue in the illustration.

A homeowner would not brick up her patio door, eliminating a natural light source and access to her garden, just to eliminate an ant infestation. Nor would she select furnace filters that required daily replacement to ensure clean air. Yet many water purification technologies on the market operate in similar all-or-nothing terms. To guarantee that treated water is free of targeted contaminants, reverse osmosis devices nonselectively remove almost all ions and other constituents from a water stream, even the calcium, magnesium, and fluoride ions desirable for taste and health. Ion-selective membranes and resins that bind specific ions for removal also require frequent disposal and replacement and can unintentionally remove beneficial ions as well.

Livermore scientists working alongside Stanford University researchers have made headway toward a new generation of tailored, reversible water treatment. The research team used an electrode of ultramicroporous carbon aerogel, an ultralight, high-surface-area material, for capacitive deionization (CDI), in which ions adsorb to the charged electrode surface, to selectively remove nitrate from water containing a mixture of contaminants. Device-scale modeling and atomistic-scale simulations indicated that Livermore's Flow Through Electrode CDI (FTE-CDI) device can be tailored by tuning the electrode's pore-size distribution to be selective for particular ions. The process is completely reversible, ending when electrodes are no longer charged.

Tuning for Environment and Industry

Selecting the contaminants a water purification system removes could simplify environmental cleanup and enable reuse of industry wastewater, saving operational costs and resources. Tuning a device to eliminate arsenic in well water or nitrate from agricultural water, for example, could be a scalable solution to boost availability of drinking water, particularly in disadvantaged areas of the world. Rare-earth elements could be extracted from geothermal water sources to provide new channels of materials needed in consumer electronics, health care equipment, and automotive catalysts. "We can tune this material to address a variety of selective removal applications," says Patrick Campbell, a Livermore climate and security materials synthesis researcher.

Selectivity in Livermore's FTE-CDI platform was first observed during a 2012 research project in which a porous carbon aerogel electrode used for CDI yielded faster, more efficient desalination than reverse osmosis. A remarkable feature struck the lead scientist, Michael Stadermann. "We observed selective removal of nitrate not only over ions of equal valence or charge, but also over divalent ions, which was unexpected," says Stadermann. "Even in well water containing 10 times the sulfate and chloride of the nitrate portion, nitrate removal exceeded the other removal rates: 65% nitrate removal compared to 12% for chloride and 16% for sulfate."

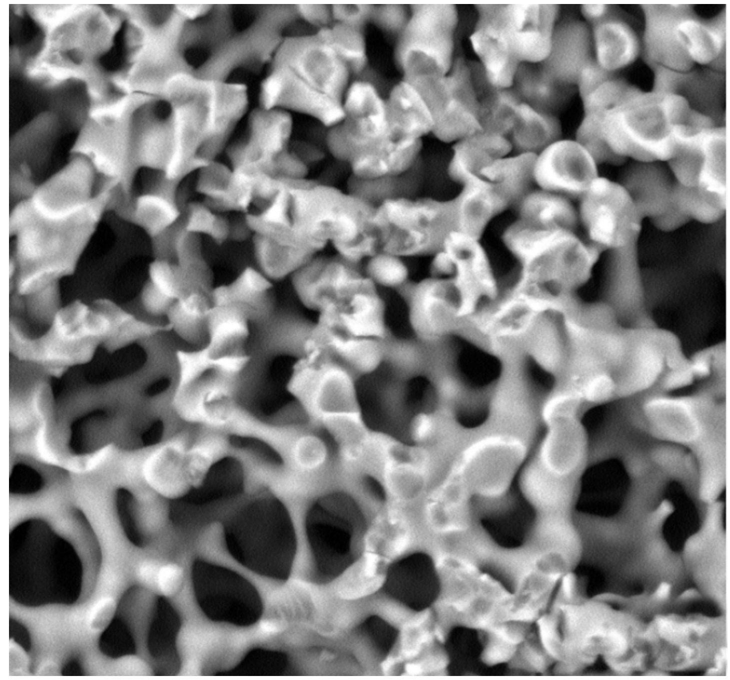
Stadermann and his team could not explain the preference for nitrates at the time. The opportunity to revisit selective ion removal, however, arose with the award of Laboratory Directed Research and Development funding to a new project led by Campbell. The project, which kicked off in 2017, zeroed in on nitrate removal using the same carbon aerogel electrode material Stadermann had studied earlier. The research team continued the focus on nitrates, observing that the concentration of nitrate in groundwater has increased in recent years due to industrial agricultural practices. Nitrate limits, regulated by the U.S. Environmental Protection Agency (EPA), gave researchers a clear target to measure success, with the goal of branching out to other ions in future studies.

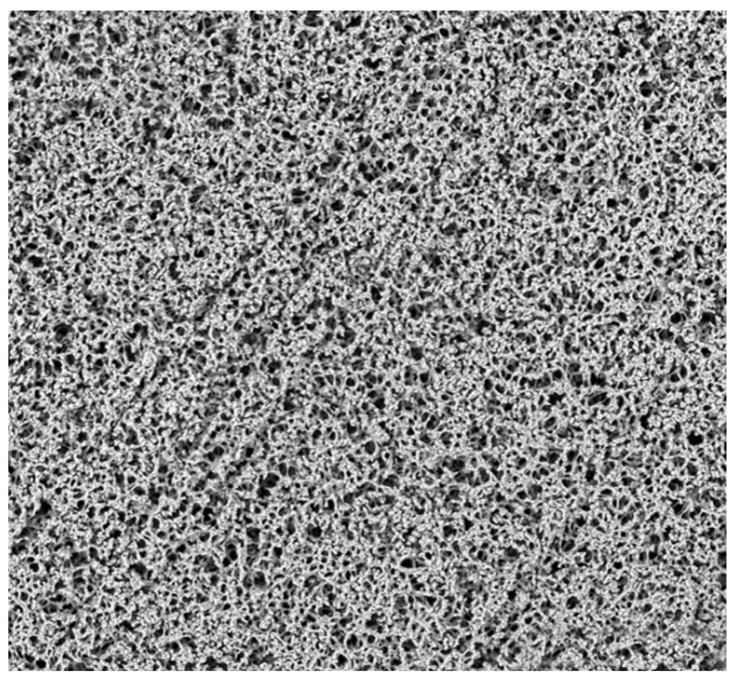
The How and Why of Selective Removal

Properties of ions such as size, charge, mass, and mobility are factors in all ion separation options, and sometimes combine to make a technology ineffective. For example, a filtration material that excludes an ion based on membrane pore size may not differentiate between differently charged ions of similar size. The researchers set out to define characteristics that affect adsorption on the FTE-CDI material.

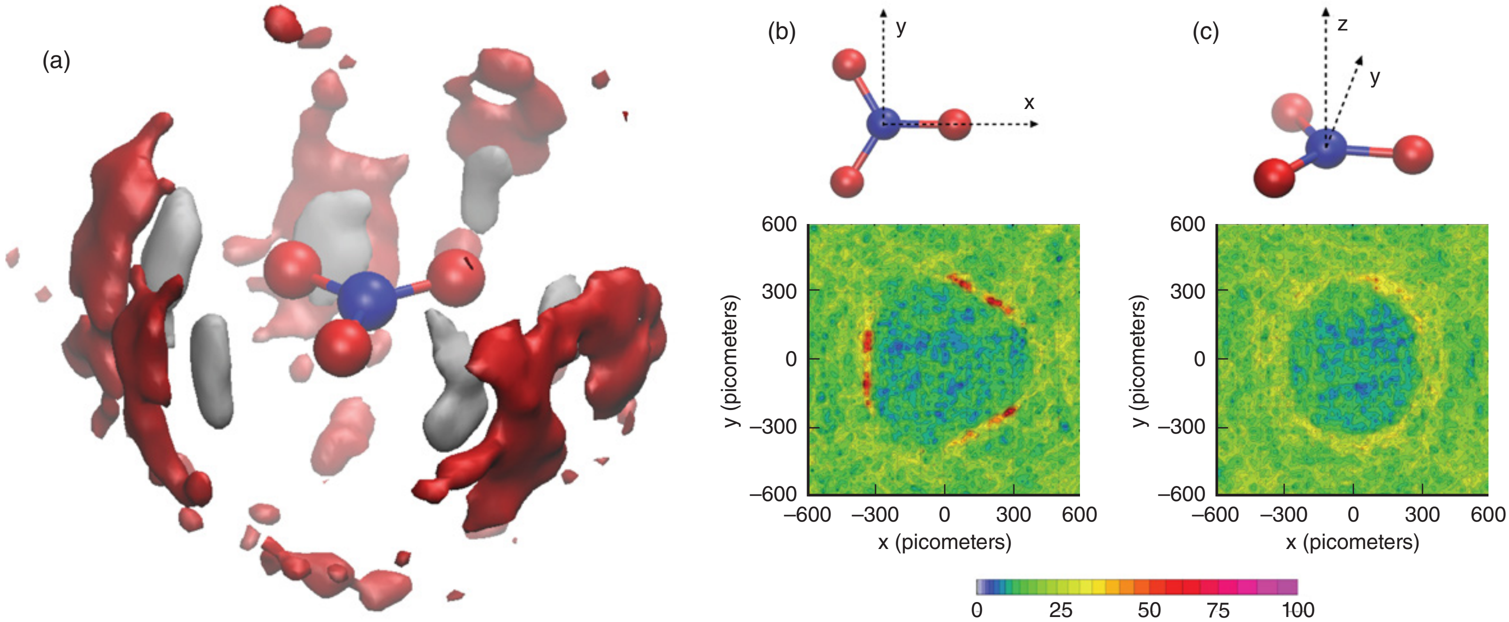
In the first phase, they validated an existing "continuum" operational model capable of computing the flow-through device's performance with variable ion mixtures, flow rates, current, pH, and other factors by changing one characteristic at a time. Selectivities that the operational model could not predict were marked for evaluation in the next phase, calling on high-resolution, quantum-scale computer simulations. "The continuum model represents how the device performs, how it should be removing ions in an engineering sense," says Campbell. "The quantum simulations in the next phase helped explain why the device performs this way, so we can deliberately tune the operation and optimize the electrode material."

The second stage of the project called on Livermore's strength in simulations of electrochemical interfaces, powered by high-performance computing, to investigate specific interactions of the ions and solvent with the carbon aerogel electrode. To accurately model how ion characteristics influence selectivity, the team combined *ab initio* or first-principles techniques and high-performance computing resources to perform quantum mechanical simulations. Quantum simulations determined the relationship of interfacial (electrode surface) capacitance, specific adsorption, and charge transfer on factors that determine selectivity, such as surface chemistry, confinement, and composition of the solution to be treated. "The quantum simulations leveraged Livermore's high-performance computing resources and novel algorithms to describe the electrochemical operating environment with unprecedented realism and fidelity," says Campbell. Livermore's Brandon Wood and Tuan Anh Pham,





Ultramicroporous carbon aerogel is the electrode material in Livermore's FTE-DCI. The material, shown at high (top) and low (bottom) magnification, can be activated to achieve pore distribution suited to adsorbing specific ions.



The weakly hydrated axial region around the nitrate molecule enables it to fit in the narrow, slit-shaped pores of the carbon aerogel electrode (a). Projection distributions indicate the asymmetrical solvation of nitrate in planes parallel (b) and perpendicular (c) to the plane of the anion. The color scale represents the spatial distribution factor—from low (0 - blue) to high (100 - magenta)—an indication of the relative density of the surrounding water.

both two-time participants in Livermore's Computing Grand Challenge Program, supported the FTE-CDI team.

Modeling Makes the Difference

Information from the quantum mechanical simulations was incorporated into the bulk operational model to re-evaluate ion selectivity, this time considering more complicated ion mixtures. The combined approach created a multiscale modeling framework that integrated the strength of quantum methods with the scalability and flexibility of a classic physics model to simulate device operations.

In the case of nitrate, the team found that the solvated (acted on by solvents) ion takes on a flattened disk shape, which is a perfect fit for the aerogel's natural pore structure. For this reason, nitrate adsorption is preferred when compared to other spherically shaped contaminants. "This was only revealed in the quantum simulations," says Steven Hawks, a Livermore staff scientist on Campbell's team, "The simple view of ion size would not predict selectivity, but the detailed simulation did. The modeling made the difference." In CDI, selectivity can be achieved through a combination of the ion's characteristics and the electrode's pore-size distribution and chemical functionality. In follow-on research, the Livermore researchers demonstrated fully tunable monovalent/divalent ion selectivity based on pore-size distribution control. These results verified the team's analysis and examination of nitrate selectivity and established that the research can be expanded for a range of results.

Seeking the First Customer

Campbell and Hawks were accepted into Cohort 10 of Energy I-Corps, a Department of Energy entrepreneurial training program helping researchers build a business case for their emerging technologies through customer discovery interviews. The team believes that the technology is expandable to several water purity concerns beyond nitrates such as mineral buildup or scaling, water hardness, and industrial wastewater and recirculated process water treatment.

"We're looking for the best application to enter the market," says Campbell, "Answering the question, 'Who is the first customer?' tells us what ions we will target." Stadermann, a past Energy I-Corps participant, understands the entrepreneurial challenge. "The team must match perceived need and willingness to purchase," says Stadermann, "The problem of high nitrate concentration is widespread, yet the technology's first customer is somewhat unclear at this time. The driver for commercialization may lie in another application, another ion."

—Suzanne Storar

Key Words: aerogel, arsenic, capacitive deionization (CDI), Department of Energy, Energy I-Corps, entrepreneurial training, flow through electrode, groundwater, quantum computing simulation, nitrate, rare-earth elements, water treatment.

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (uspto.gov).

Patents

Laser-Driven Hydrothermal Processing
Raymond P. Mariella, Jr., Alexander M. Rubenchik, Mary A. Norton
U.S. Patent 10,583,526 B2
March 10, 2020

Symmetric Out-of-Plane Configurations of Diffractive Gratings and Method
Emily F. Link, David A. Alessi, Leon C. Haefner, Jerald A. Britten
U.S. Patent 10,594,106 B2
March 17, 2020

Personal Electronic Device for Performing Multimodal Imaging for Non-Contact Identification of Multiple Biometric Traits
Stavros Demos
U.S. Patent 10,599,932 B2
March 24, 2020

Shape Memory Polymer Foams for Endovascular Therapies
Thomas S. Wilson, Duncan J. Maitland
U.S. Patent 10,610,230 B2
April 7, 2020

Awards

The **National Nuclear Security Administration's** (NNSA's) Office of Safety, Infrastructure, and Operations (NA-50) awarded Laboratory teams with the following nine **NA-50 Excellence Awards** (the most the Laboratory has ever received in a year). The annual award program was established to recognize teams and individuals for exceptional accomplishments made in support of NA-50 efforts to achieve the NNSA mission.

The **Office of Laboratory infrastructure within the Director's Office** was recognized for Excellence in Integration of NNSA and Site Asset Planning Systems to Support Real Property Asset Management Planning. This team was recognized for best-in-class integration of facility data, models, and analyses supporting NNSA's science-based infrastructure stewardship using data-driven, risk-informed, performance-based information to communicate the health of NNSA's infrastructure.

The **Expand Electrical Distribution System (EEDS) Project Team** was recognized for the successful execution of Lawrence Livermore's and NA-50's EEDS Project. The team delivered the project safely, on time, and under budget with no lost time or recordable accidents.

The **LLNL Computerized Move Management System for Optimized Space Utilization of NNSA Assets Team** was recognized for skillful and creative innovation in the development and deployment of a computerized Move Management System that allows NNSA, for the first time, to have real-time understanding of office asset utilization at the lab-enterprise scale.

The **BUILDER Innovation: Improving Science-Based Modeling and System Integration Team** was recognized for innovation, creativity, and rigor in developing and applying science-based projection models for real property building systems. The BUILDER project tracks asset inventory and inventory condition and helps NNSA understand the infrastructure needs of the Laboratory and the NNSA enterprise.

The **No FY19 reportable Injuries in WCI High Hazard Facilities in an Increased Operations Tempo Team** received an award in recognition of Laboratory and Livermore Field Office personnel working in Weapons and Complex Integration's high-hazard facilities for their dedication and commitment to meeting mission goals, completing critical upgrades, and maintaining safe programmatic and facility operations with zero reportable injuries in fiscal year 2019, culminating in a contiguous two-year safety record.

The **Lawrence Livermore SAFER Data Integration Prototype Team** was recognized for rapid development of a prototype dashboard and database for displaying and interpreting enterprise safety risk data.

Martin Martino, real property administrator, was recognized for **Improved LLNL Real Estate Program and Increased Cost Savings to the Federal Government,** which leveraged solutions to utilize existing assets, resulting in significant cost savings to the federal government.

The **Design and Implementation of Enduring Transuranic Waste (TRU) Characterization and Certification Program** was recognized for excellence in the implementation of new TRU characterization and certification processes and programs at Lawrence Livermore to support TRU shipment.

The **NIF Facility and Infrastructure Systems Section** was recognized for excellence in early implementation of predictive maintenance best practices.

Abstract

Investing in the Laboratory's Future

Lawrence Livermore was founded in 1952 on the site of a decommissioned naval air station. Nearly 70 years later, much of the original infrastructure remains, with naval barracks and trailers continuing to house office spaces. As the Laboratory takes on two major weapons revitalization projects and experiences unprecedented employee growth, it finds itself facing aging infrastructure that requires updating to support mission needs. Armed with a 10-year, $2 billion infrastructure portfolio and a suite of advanced modeling tools and data, Lawrence Livermore's infrastructure teams seek to bring its one-square-mile campus into the modern age.

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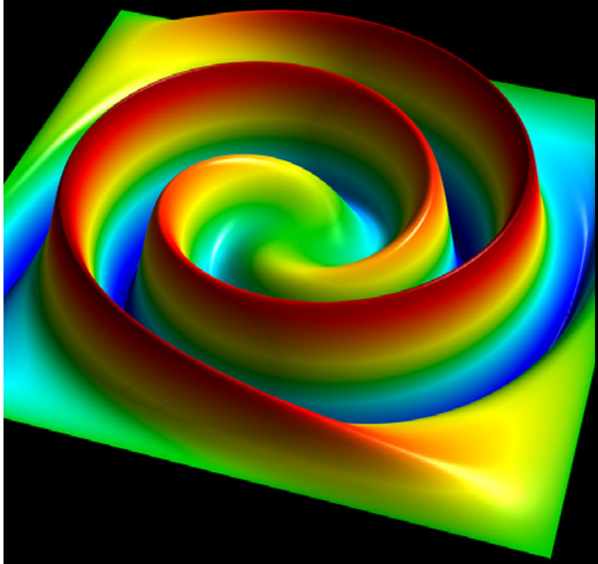
Coming Next Issue

Advancing Software for the Exascale Era



The Exascale Computing Project and a new Livermore initiative drive innovative software research and development for next-generation supercomputers.

Also in this upcoming issue...

- *For nearly half a century, the Laboratory has created unique one-page charts that diagram the nation's energy use and consumption in an easy-to-understand format.*
- *In collaboration with Las Positas College, Livermore scientists and engineers share their research with students, faculty, and the Tri-Valley community through outreach seminars.*
- *A technology once rejected for fusion power plants now supports a promising new flash neutron-imaging capability.*

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