

December 2018

Science & Technology REVIEW

Quantum Computing IS HERE

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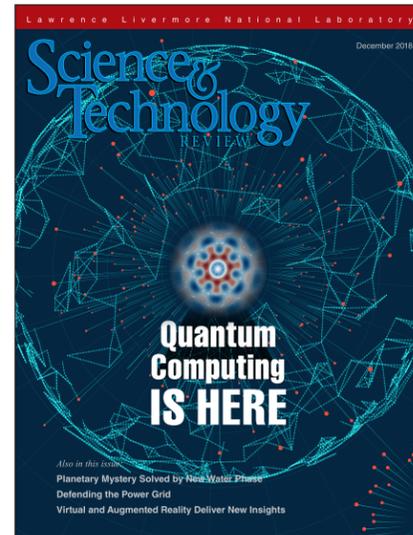
Planetary Mystery Solved by New Water Phase

Defending the Power Grid

Virtual and Augmented Reality Deliver New Insights

About the Cover

Quantum computing, which uses qubits instead of the bits of classical computing, is no longer mere theory but is being implemented with actual working quantum computers. These machines have the potential to exponentially transform processing speeds and so represent the next frontier of high-performance computing. As the article beginning on p. 4 describes, Lawrence Livermore is pursuing a diverse research portfolio that includes demonstrating a fully programmable quantum computing system and improving superconducting materials and devices. The cover image incorporates actual shapes from Wigner tomography, which geometrically represents quantum states. A classical bit in a state of 0 or 1 would only appear blue, whereas a quantum superposition of 0 and 1 appears as blue and red.



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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Please address any correspondence (including name and address changes) to S&TR, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3893. Our e-mail address is str-mail@llnl.gov. S&TR is available on the Web at str.llnl.gov.

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PRINT COORDINATOR
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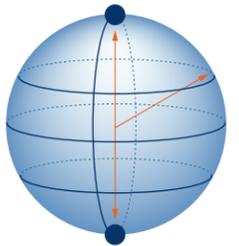
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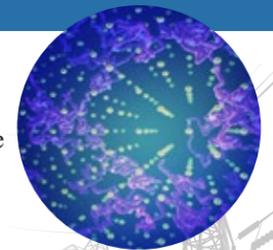
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Researchers Study Protein Filaments

To advance understanding of diseases such as Alzheimer's and Parkinson's, scientists have studied small protein filaments called amyloids, which can form fibrous clusters in the brain. Until now, even the best tools for studying amyloids have yielded only limited views of the filaments. However, an international research team including Livermore scientists Matthias Frank and Matt Coleman has developed a new method with the potential for revealing the detailed structure of individual amyloid fibrils using powerful beams of x-ray laser light. The method is described in a report published May 9, 2018, in *Nature Communications*.

Experiments were conducted at the Linac Coherent Light Source (LCLS). Although the team did not uncover the complete fibril structure, their innovative method opens a promising path for amyloid studies using x-ray free-electron lasers such as LCLS. The method leverages work by Frank and Coleman on novel sample supports. Previously, the team had developed sample supports based on small silicon chips with large numbers of small-area windows covered by ultrathin silicon nitride membranes to hold biological samples. For the LCLS work, the pair replaced the thin membranes on the chips with graphene, which is even thinner. Graphene is almost transparent to x rays, allowing the team to probe the delicate fibrils without significant extraneous signals from the graphene layer.

This new approach provided the solution to hold the fibril samples while supporting the graphene and scanning the material through the x-ray beam. Results at LCLS suggest that this technique may even be used in the future to determine the structure of individual amyloid fibrils.

Contact: Matthias Frank (925) 423-5068 (frank1@llnl.gov).

A Warm Look at Water's Structure

Boiling water traditionally involves adding energy to the molecules by conduction, convection, or thermal radiation. Now Livermore scientists and collaborators have developed a way to use an x-ray free-electron laser (XFEL) to heat water to temperatures above 100,000 kelvins (179,540°F) and pressures above 100 gigapascals (1 million times Earth's atmospheric pressure), where the liquid transitions into warm dense matter. The research appears online in the May 14, 2018, edition of the *Proceedings of the National Academy of Sciences*.

XFELs have opened the door to a new era in structural biology, enabling the imaging of biomolecules and dynamics that were impossible to access with conventional methods. Understanding the dynamics of warm dense matter benefits imaging in structural biology and can also provide insight into various fields such as inertial confinement fusion, planetary cores, shockwaves in dense material, and radiation damage in biological matter.

"This exotic ionic and disordered state of liquid density is structurally different from heating water the traditional way," says

Stefan Hau-Riege, Livermore physicist and coauthor of the paper. The ultrafast phase transition observed in water provides evidence that any biological structure exposed to these x-ray pulses is destroyed during x-ray exposure. This finding is significant because many imaging techniques for determining molecular structure use water or another liquid to deliver the sample into the x-ray interaction region.

Contact: Stefan Hau-Riege (925) 422-5892 (hauriege1@llnl.gov).

Prospecting for Antineutrinos

The Precision Reactor Oscillation and Spectrum Experiment (PROSPECT) has completed installation of a novel antineutrino detector that will probe the possible existence of a new form of matter—sterile neutrinos. (See image below.) PROSPECT, located at Oak Ridge National Laboratory, has begun taking data to study electron antineutrinos that are emitted from nuclear decays in a reactor to search for sterile neutrinos, and to learn about the underlying nuclear reactions that power fission reactors.



(Photo by Mara Lavitt)

"The successful operation of PROSPECT will allow us to gain insight into one of the fundamental puzzles in neutrino physics and develop a better understanding of reactor fuel, while also providing a new tool for nuclear safeguards," said spokesperson Nathaniel Bowden, a Livermore scientist and expert in nuclear nonproliferation technology. The installation of PROSPECT follows four years of intensive research and development by a collaboration of more than 60 participants from 10 universities and 4 national laboratories.

The experiment uses a novel antineutrino detector system based on a segmented liquid scintillator technology. The combination of segmentation and a unique, lithium-doped liquid scintillator formulation allows PROSPECT to identify particle types and interaction points. These design features—along with extensive, tailored shielding—will enable PROSPECT to make a precise measurement of neutrinos in the high-background environment of a nuclear reactor. PROSPECT's detector technology may therefore have applications in the monitoring of nuclear reactors for nonproliferation applications.

Contact: Nathaniel Bowden (925) 422-4923 (bowden20@llnl.gov).



From Bits to Qubits: Pursuing the Quantum Frontier

QUANTUM computing has been characterized as the next frontier in high-performance computing (HPC) ever since the first models were published in the 1980s. Packaging data in qubits instead of the bits of classical computing, quantum computing uses the principles of quantum physics to encode data in multiple states at once, thus opening the door to exponential increases in computing power. The technology changes how we view computational architectures, and the field is in a critical phase of moving from theory into experimentation. The article beginning on p. 4 is *S&TR*'s first cover story on quantum computing.

Lawrence Livermore is pursuing quantum computing and related technologies for myriad reasons. Most importantly, the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program (SSP) relies on scientific computing—particularly the large multiphysics codes that model material behavior and fluid dynamics—as a substitute for nuclear testing. As an NNSA national security laboratory, Livermore must continually advance computing technologies to achieve more accurate simulations with faster processors.

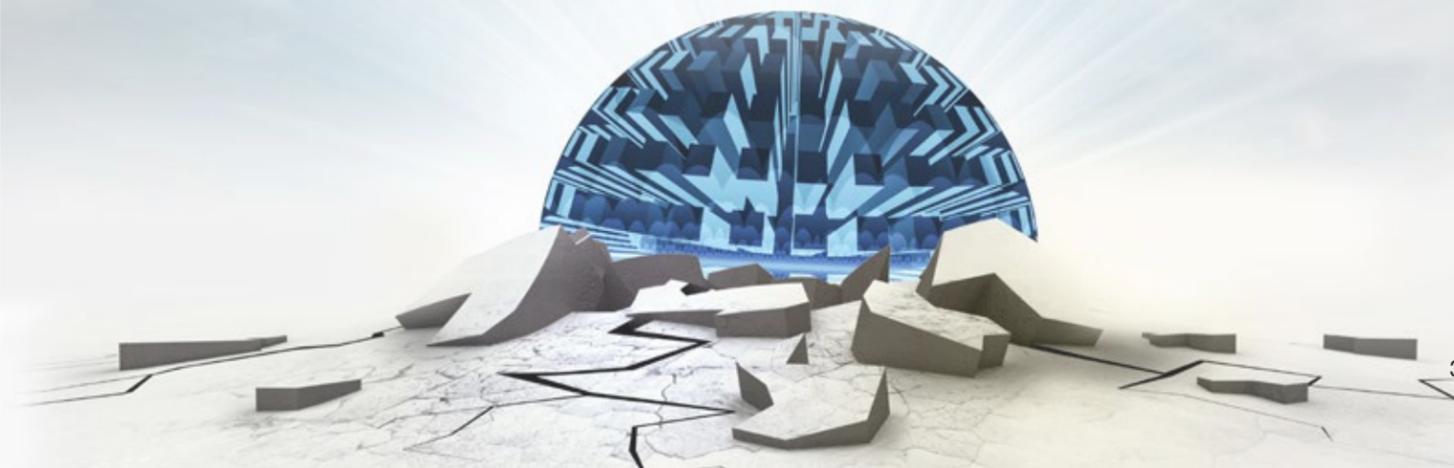
The SSP mission presents computational challenges in calculating partial differential equations, equations of state (such as the motion of atoms under extreme conditions), and predictions of physical and chemical processes (such as energy transport and nuclear reaction rates). The catch is that Moore's Law, which holds that classical computer performance doubles every 18 to 24 months, seems to be expiring: As power requirements increase with finer scale simulations, eventually classical computers will be unable to provide significant performance improvements. Quantum computers, however, are expected to perform such calculations faster, with higher fidelity and lower power consumption. Given trends in academia and industry, we may start to realize the potential of quantum computing in solving the above problems in the near future.

At the Laboratory, we are tackling quantum computing on several fronts, including hardware design, programming paradigms, and superconductive applications. Livermore has a history of driving science and technology forward through bold projects—and quantum computing is no exception. Indeed, we bring the best qualities of the Laboratory to bear on this growing field by developing unique technological capabilities and engaging multidisciplinary teams in physics, engineering, computer science, materials science, and more.

This work also creates mission-motivated opportunities across the programs. For example, the extremely low-energy environment necessary to sustain quantum coherence has applications in microwave detection, remote sensing, and other areas dependent on ultrahigh resolution. We can learn more about material properties in low-energy regimes, driving the development of novel materials. We can gain new physical insights by simulating quantum dynamics and augmenting classical models. We see possibilities for integration with HPC systems and collaborations with other institutions on next-generation computing platforms. Our research partners could benefit greatly from our quantum computing systems as direct end users.

Quantum computing and related quantum technologies represent an exciting research area for the Laboratory, one that will capture the imagination and harness the ingenuity of our scientists and engineers for years to come. This work is an opportunity for Livermore researchers to contribute on multiple fronts as we have done so often before—by advancing fundamental science and translating that science into practical solutions for our programs and missions. The future holds great promise, as in all fields of Laboratory involvement.

■ Glenn A. Fox is associate director for Physical and Life Sciences.



Livermore Leaps into Quantum Computing

Harnessing the elusive properties of quantum physics ushers in a new era of computational power.

AS high-performance computing (HPC) systems evolve, the rate of progress is slowed by the physical limitations and power demands of conventional microchips. To overcome these obstacles, HPC experts currently pursue advances in parallel processing to increase overall performance and reduce energy consumption. (See *S&TR*, September 2016, pp. 4–11; March 2017, pp. 4–11; and July/August 2018, pp. 20–23.) The next step is exascale systems, which are slated to come online soon. Beyond exascale, the next frontier of the HPC continuum is quantum computing. For some computing problems—such as linear solvers and quantum simulations—the advances possible with quantum computing could be unprecedented. According to Livermore physicist Jonathan DuBois, “With HPC being central to the Laboratory’s national

security mission, we are obligated to understand and advance the state of the art in computation, and the potential impact of quantum physics is enormous.”

Livermore scientists have been researching and developing quantum systems for approximately a decade, and today’s portfolio of projects reflects a multifaceted growth strategy. Funding sources include the Department of Energy’s Advanced Simulation and Computing (ASC) and Advanced Scientific Computing Research (ASCR) programs, as well as the Laboratory Directed Research and Development Program. DuBois leads the Laboratory’s Quantum Coherent Device Physics group, which focuses on connecting quantum technology with applications. He explains, “We are part of a scientific community that wants to develop the field, not simply build products.”

Staff scientist Eric Holland reviews experimental results on one of Livermore’s two quantum computing test beds. The system uses recirculating helium (hoses at top right) to cool a cryogen-free dilution refrigerator (cylindrical white tank). Two racks house electronics that control signals for quantum processing units (QPUs). (Photo by Randy Wong.)

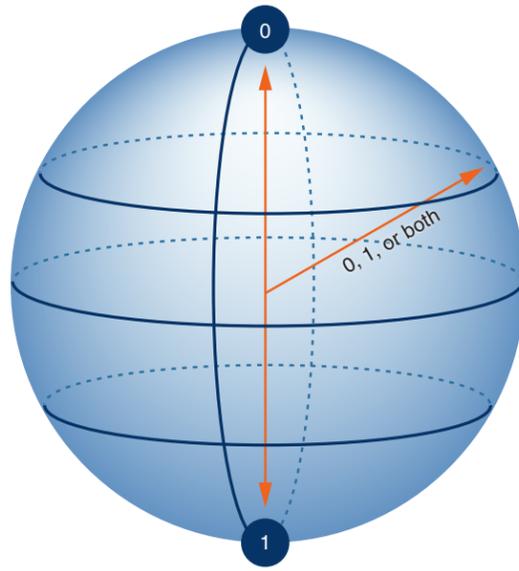
Ongoing activities include demonstrating a fully programmable quantum computing system, improving superconducting materials and devices, deploying quantum sensors, and developing quantum algorithms. Progress has been encouraging, with Livermore recently deploying two functional quantum computing test beds.

The Quantum Lexicon

At first glance, parallel computing systems such as Livermore's existing supercomputers may seem equivalent to quantum computers in that all perform multiple operations simultaneously. However, the key difference is in how the two fundamentally tackle computing problems. A classical computer uses on/off transistors to store and process information, encoding data in binary digits, or bits, in one of two states—0 or 1. In contrast, a quantum computer operates on the principles of quantum physics, storing data in quantum bits, or qubits (pronounced “cue-bits”).

Livermore's qubits are superconducting electrical circuits that can exist in multiple simultaneous states—0, 1, or both. This principle of superposition is analogous to mathematically representing the state of a heads-or-tails coin flip whose outcome is still literally up in the air. The concept was first illustrated by Erwin Schrödinger's famous 1935 thought experiment wherein a hypothetical unobserved cat is both alive and dead—but found to be one or the other when observed.

Using qubits for computation increases processing power exponentially. Two qubits can store data in four states concurrently—00, 01, 10, and 11. A 64-qubit quantum processing unit (QPU) is equivalent to 2^{64} bits—16 exabits—in a classical computer. For any number (n) of qubits, a quantum computer could perform 2^n operations at the same time. A classical computer would take far longer to do so—in some cases, years compared to seconds. This promising leap in



Superposition is a major principle in quantum physics, occurring when particles exist in multiple states. This phenomenon allows a single quantum bit, or qubit, to represent 0, 1, or both. In contrast, a bit in classical computing can only represent 0 or 1.

computing power is possible only if the superposition state can be precisely controlled to remain coherent. Otherwise, the qubit system can generate errors as it processes information simultaneously. Coherence requires preservation of the relationship between different quantum states so that superposition results, which in turn requires that changes to qubits can be reversed.

Prolonging coherence is the key to sustaining quantum calculations. The smallest changes in the environment surrounding a qubit can cause a loss of coherence, also called decoherence, so scientists are keen to reduce interference from electromagnetic waves, temperature variations, and other variables in and around quantum hardware. Quantum computing—and quantum-coherent devices in general—therefore requires both using precisely controlled low-energy pulses to sustain superposition states and preventing other energy sources

from disturbing those states. “We are working at the opposite end of the energy spectrum from explosives or galactic events,” explains Laboratory physicist Yaniv Rosen. “We are studying energies 100 million billion times fainter than the energy expended in a mosquito's flight, down to 20 microelectronvolts.”

Decoherence and other system noise can be sources of error in quantum computing. In classical computing, error correction helps make systems fault-tolerant by ensuring reliable data delivery and reconstruction, and the viability of quantum computing also depends on achieving such goals. DuBois points out, “No one experimenting in this field has yet demonstrated successful error correction, which is analogous to break-even in nuclear fusion.”

A Supercool Facility

A quantum computer does not look like a classical computer. Its refrigerator does not resemble a typical refrigeration unit, for instance. At Livermore, a quantum processor relies on superconductivity to reduce electrical resistance and interaction with the environment. The superconductive processor, consisting of particles in quantum circuits, is operated at extremely cold temperatures so that scientists can control the circuits' quantum states. This approach may offer the best chance of achieving coherence goals. The sophisticated cooling infrastructure recirculates helium-3 and -4 isotopes through layers of increasing coldness, reducing the interior temperature to -273.1°C (0.007 kelvin). The dilution refrigerator operates under vacuum and is electrically shielded to minimize heat leaks and environmental noise.

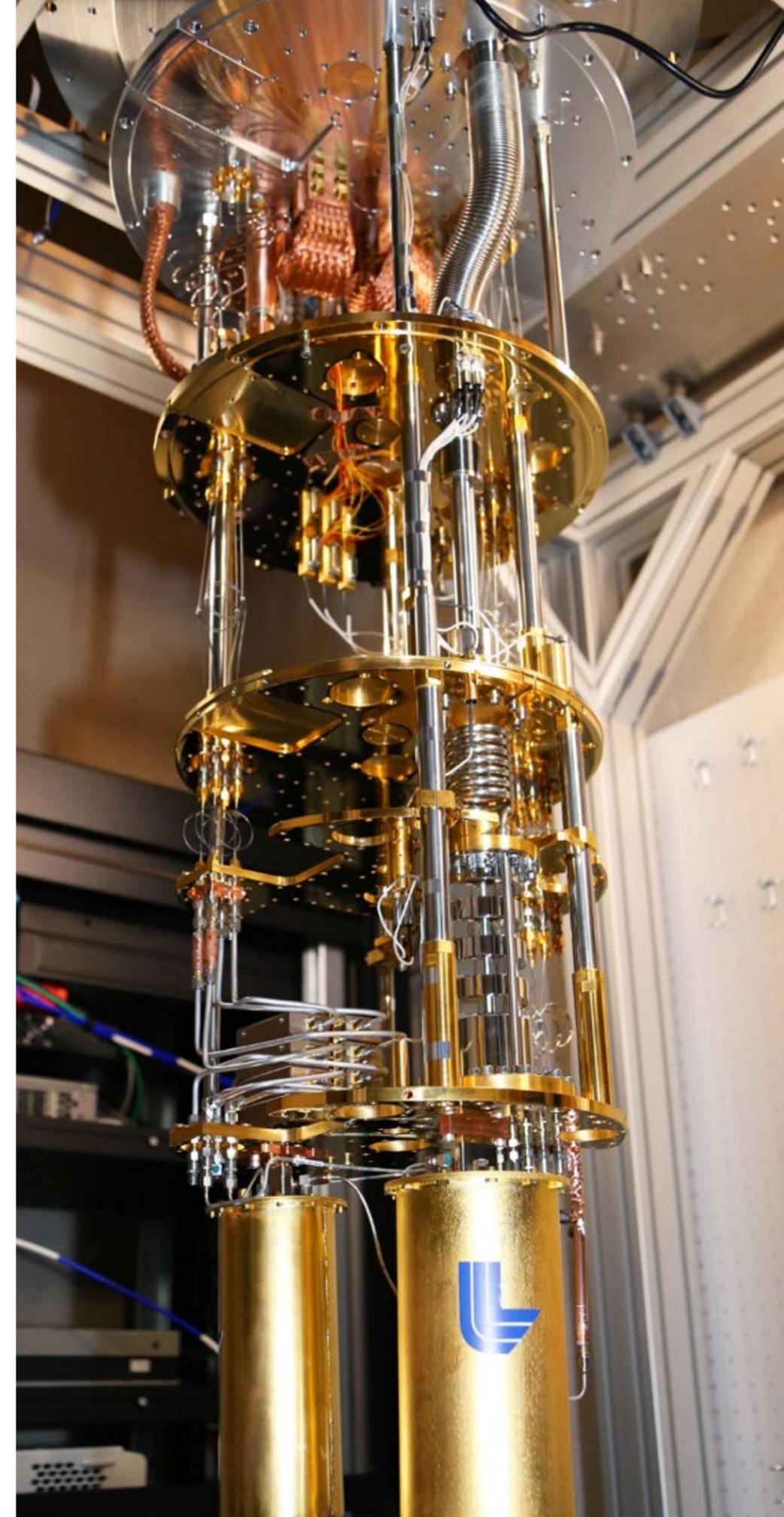
Qubits are seated inside the refrigerator and connected to a suite of electronics that control superposition with microwave pulses. An arbitrary waveform generator provides gigahertz frequencies and amplitudes to interact with the qubit, and an oscilloscope monitors the input signals.

The results of these manipulations are sent to an analog-to-digital converter to verify signal fidelity, and the calculation results are read on a standard computer. Indeed, classical computing plays an important role in calibrating, running, and maintaining the Laboratory's quantum computing test beds. The Livermore team codes instructions for pulse shape and frequency in the Python programming language and uses HPC software to adjust designs for pulse control and other variables.

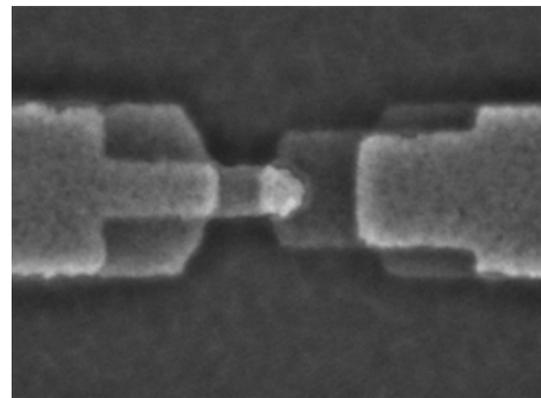
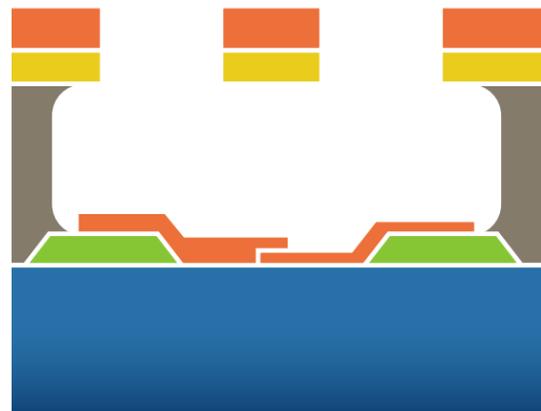
Although many of these components are available commercially, no instruction manual exists for a fully integrated quantum system. The team's hands-on experience and troubleshooting skills grow daily as they supply their own technical support. Eric Holland, Livermore's chief quantum systems architect, explains, “We are assembling quantum computing components in ways others have not. Livermore is blazing a trail.” For example, the Laboratory's qubits are housed inside canisters attached to the bottom of the refrigerator. Made of gold-plated copper to prevent oxidation and maximize thermal contact in a vacuum, the cans are designed, built, and coated at the Laboratory before being sent offsite for annealing. Special shielding protects the qubits from stray magnetic fields and prevents light leaks. Each test bed holds four cans, allowing multiple experiments to run simultaneously.

This machinery is inherently fragile. Rosen says, “On paper, a quantum system design can seem perfect, but the environment really comes into play when implementing the design.” However, DuBois cites the Laboratory's expertise in HPC, engineering, materials science, cryogenic physics, and quantum physics as

Inside a test bed's dilution refrigerator, gold-plated cans contain qubits, which are connected by wires to the rest of the assembly. Recirculating helium progressively cools the structure from top to bottom, with each circular plate introducing a colder phase. (Photo by Carrie Martin.)



a potentially game-changing combination in solving the quantum computing puzzle. “Livermore’s people have a well-defined vision of how to advance this field,” he says. The Laboratory’s two test beds are similarly assembled but serve different purposes—one for quick tests and prototyping and the other for mature experiments. The former was installed in late 2017, while the latter came online in early 2018 to support the ASCR Quantum-Enabled Simulation (AQuES) Testbed Pathfinder Program, which brings



A Josephson junction is the key component of superconducting qubit circuitry. (top) The Laboratory’s fabrication process, shown in side view, includes precisely controlled deposition of layered materials (green, orange, yellow) on a substrate (blue). (bottom) Scanning electron microscopy shows a top view of a complete Josephson junction after deposition.

Lawrence Livermore and Lawrence Berkeley national laboratories together to pursue diverse research and development in quantum computing.

Building Better Qubits

Livermore scientists are developing quantum computing components alongside a new class of superconducting materials for low-energy regimes. These efforts span qubit design, QPU configuration, quantum chip circuitry, and quantum materials science. (See *S&TR*, March 2016,

pp. 17–19.) Holland explains, “The design space is ripe for exploration. Our internal investments allow us to question others’ approaches.” Classical computing advancements typically focus on planar chip design, and industry’s prevailing quantum chip architecture is a two-dimensional (2D) lattice of qubits, each controlled by a separate oscillating signal input. However, both 2D and three-dimensional (3D) designs are being pursued at the Laboratory. DuBois states, “For better efficiency, we are trying to achieve the same computational power with one input port per system, not per qubit—a completely different paradigm for controlling the basic unit of a scalable quantum computer.”

Furthermore, industry typically offers nearest-neighbor connections between qubits, which means lattice arrays increase as more neighbors per qubit are added, making the device less efficient as it grows in size. By the end of the 5-year AQuES Testbed Pathfinder Program, the Livermore team intends to stand up a working 20-qubit QPU with all-to-all connectivity—any pair or trio of qubits, and any combination of pairs or trios, will be interconnected. “This QPU

size is the equivalent of a matrix of about a million squared, which is a good starting point for an HPC system to simulate,” says Holland.

The team is experimenting with several designs for manufacturing and positioning qubits, all aimed at minimizing energy loss and error rates while maximizing performance. The Laboratory’s qubits are based on Josephson junctions, in which two superconducting materials are connected by an insulating link. In an environment cooled nearly to absolute zero, this design allows current to flow between the superconductors with very little voltage applied. “Josephson junctions are the essential ingredient in superconducting QPUs,” says Holland. Using electron-beam lithography and evaporation, Josephson junctions are created with overlapping layers of aluminum and oxidation coatings deposited onto a substrate.

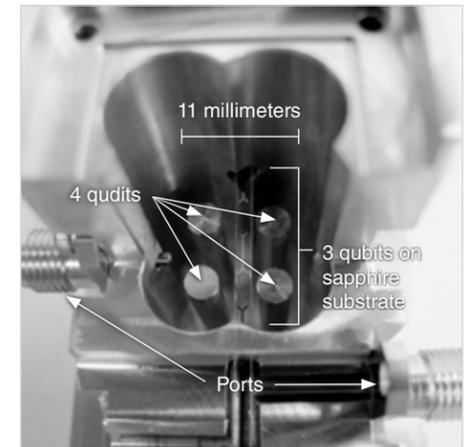
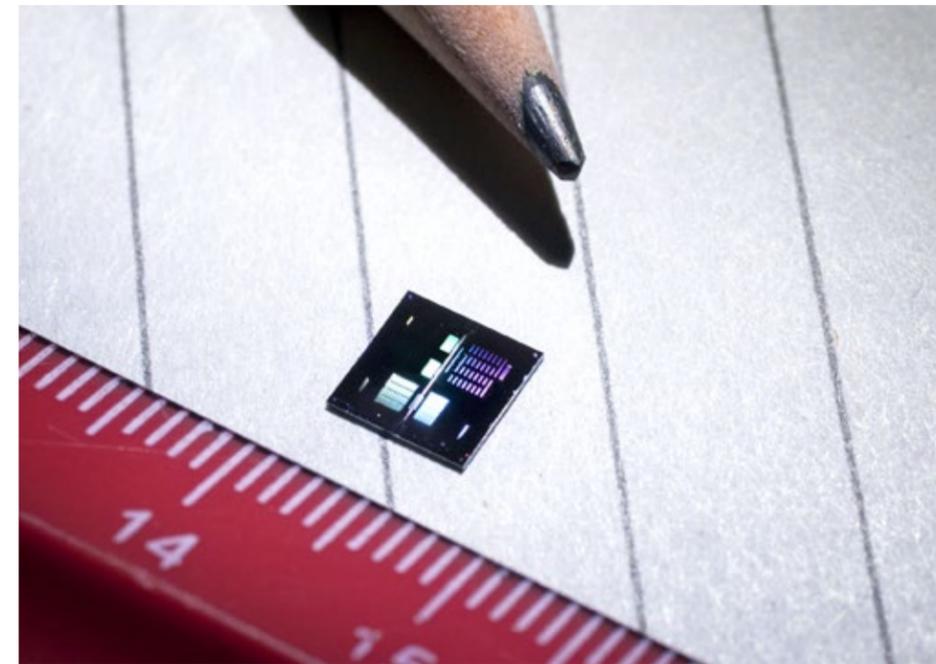
An effort at design improvement combines qubits in a new configuration known as a “qudit.” This highly efficient, multidimensional arrangement of qubits stores data in more than two states and with lower error rates. The larger the qudit, the more qubits it represents and the faster its calculation potential. A new, homegrown QPU design, nicknamed the quad core, begins with qubits fabricated on sapphire wafers, which are then cut into strips. Inside the high-purity aluminum core, a three-qubit strip is flanked by four qudits. This layout results in all-to-all connectivity.

Do-It-Yourself Materials

Beyond serving as the building blocks of quantum computing, qubits also help Livermore researchers probe low-energy and -temperature systems in general, which in turn helps the team build better qubits. Rosen explains, “Not many institutions are investigating materials development for quantum systems. While others try to improve construction, we also strive to understand the root of the problem, such as which material properties are affected by

miniscule energy changes.” For instance, Rosen studies surface defects, which behave completely differently from bulk defects. Disruption in surface-level energy is a potential source of decoherence in quantum circuits and qubits.

Livermore researchers are developing 2D quantum chips containing unique resonator geometries. A 2D resonator is a pattern of conductive material used to optimize oscillation signals, visually resembling a television antenna flattened onto a plane inside a microchip. The widths of each tine and the spaces between them affect electrical flow through the resonator. In recent experiments, Rosen used the Laboratory’s quantum computing test beds to measure surface defects in superconducting aluminum resonators. The test bed’s ultracold environment reduces electronic interference so that the team can track a single photon’s passage through a resonator pattern. The longer the photon stays inside the resonator before “ringing down,” the longer the coherence time. Rosen summarizes, “If we can store a photon indefinitely by controlling or



Livermore’s innovative “quad core” QPU provides all-to-all connectivity among three qubits and four qudits. The design also improves resource efficiency with multipurpose ports that can be used for inputs or outputs.

mitigating surface defects, we can extend the quantum computing time limit.”

Another project uses Livermore’s additive manufacturing capabilities to create a 3D resonator whose conical cavity may prolong quantum states. “Sources of energy loss in 3D resonators are different than in 2D resonators,” explains Rosen. The team seeks to understand energy loss in resonator cavity areas of high current and high electric field. They are also investigating materials with high kinetic inductance, a property describing the energy stored in a superconductor’s bound electrons. Experiments run on Livermore’s test beds characterize electrical resistance along the cavity’s surface.

The superconducting 3D resonator is made of a common alloy of titanium,

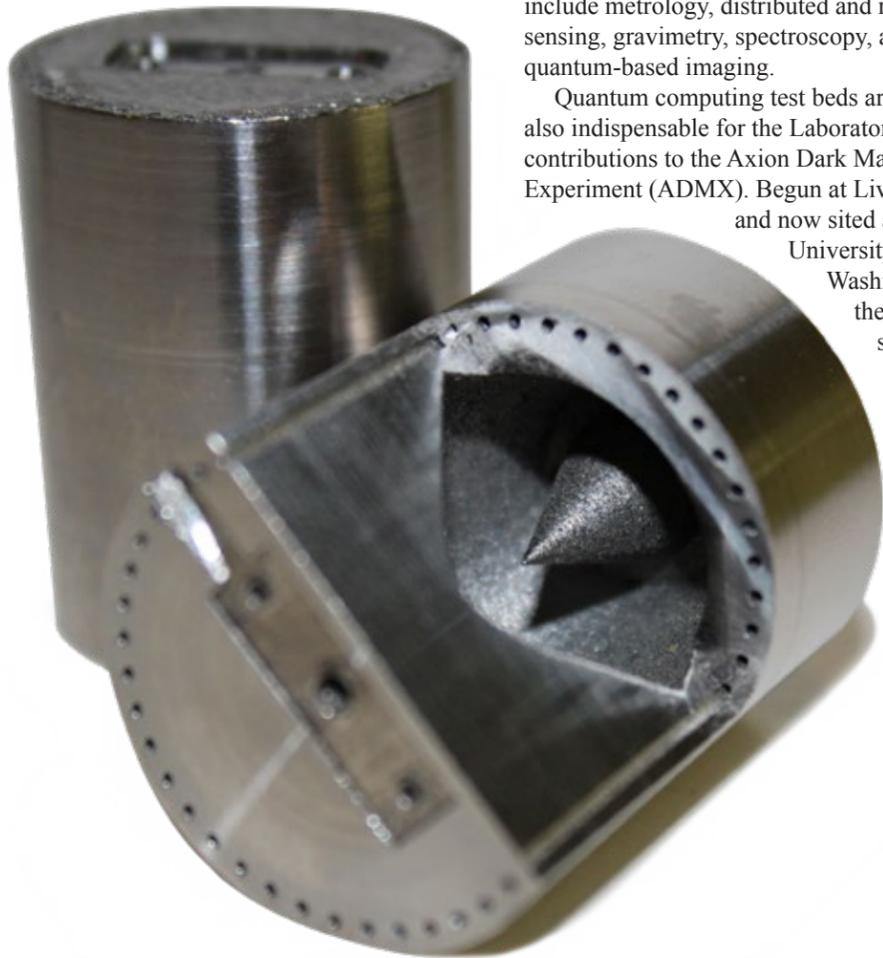
aluminum, and vanadium known as Ti64, often used in additive manufacturing at Livermore. The cylindrical device measures 25 millimeters in diameter and is fabricated with selective laser melting because conventional machining cannot create the special cavity shape. Investigating and testing the Ti64 and other cavity systems augment Livermore’s approach to quantum technologies. In 2018, physicist Gianpaolo Carosi led a workshop at the Laboratory’s Livermore Valley Open Campus to review the latest in cavity research. Attendees hailed from other national laboratories, international organizations, and academic institutions. He says, “Better cavities mean better qubit control. We see much synergy in developing these systems for superconducting qubits and accelerator experiments.”

In addition, Laboratory researchers are collaborating with the University of California at Berkeley to explore other types of resonator materials, such as amorphous silicon. Rosen says, “Growing crystalline materials for 2D resonators is very difficult, so we are considering different

Fabricated with the Laboratory’s photolithography equipment, an aluminum quantum chip is ready for testing. This chip contains 5 resonator layouts, each up to 1 millimeter wide. (Photo by Randy Wong.)

configurations of atoms in amorphous structures.” While Berkeley scientists measure defects that interact with energy vibrations, Livermore measures defects affected by electric fields. The two teams are comparing their results to learn how defects behave in amorphous materials. “This is the first attempt at correlating electrical and vibrational defects to find their origin,” states Rosen. The Laboratory’s additive manufacturing capabilities again play a role, as the two institutions contribute different fabrication methods

The cavity of Livermore’s superconducting three-dimensional resonator was fabricated with selective laser melting from a titanium–aluminum–vanadium alloy known as Ti64. This type of resonator is used to study energy loss in superconducting materials.



to the project. Livermore’s multipronged efforts to solve the coherence problem are bearing fruit for several applications, such as laser amplifiers, single-photon and low-temperature microwave detectors, high-precision quantum sensors, and more compact quantum-coherent devices. The work also advances the overall state of the art in additive manufacturing.

Ultrasensitive Detection

Another important research thrust at the Laboratory is quantum sensing, which exploits quantum superposition, entanglement, and squeezing to achieve ultrahigh resolution. (Entanglement and squeezing involve multiphoton quantum states that are dependent on or correlate to each other.) Carosi notes, “We search for changes that standard detection systems cannot find, such as a tiny frequency shift amid background noise.” Applications include metrology, distributed and remote sensing, gravimetry, spectroscopy, and quantum-based imaging.

Quantum computing test beds are also indispensable for the Laboratory’s contributions to the Axion Dark Matter Experiment (ADMX). Begun at Livermore and now sited at the University of Washington, the work searches for the dark

matter thought to comprise nearly one-fourth of the universe’s energy density. (See *S&TR*, January/February 2015, pp. 23–26.) As the project’s spokesperson, Carosi leads a team supporting the search for theorized particles called axions. Carosi explains, “The axion is one of the most likely dark matter candidates. The ADMX system is designed to detect axions by their coupling to photons, when they convert to microwaves in the presence of a strong magnetic field.” The primary background signals come from photons produced by thermal noise, and the exceptional sensitivity of quantum-coherent devices helps find the proverbial needle in the haystack. Similar to a quantum computer, the ADMX system contains a superconducting dilution refrigerator to reduce thermal background noise, along with a large-bore magnet and a resonant cavity to boost the axion-to-photon conversion signal.

The Livermore team is testing two types of devices for the ADMX project—microwave cavity systems and amplifiers based on superconducting quantum interference devices (SQUIDs). These cavity systems—which at 1 meter long are much bigger than the Ti64 cavity—are built at the Laboratory and tested for resonance quality at different frequencies. SQUID-based amplifiers decrease background noise inside the cavity, thereby clarifying potential axion signals. The team has also combined multiple SQUID amplifiers into a “SQUIDADEL” to search multiple frequencies simultaneously. In fact, Livermore is the only facility with the equipment to test the full SQUIDADEL system. Carosi states, “The more precisely we can measure, the better chance we have to solve the universe’s mysteries.”

New Programming Paradigm

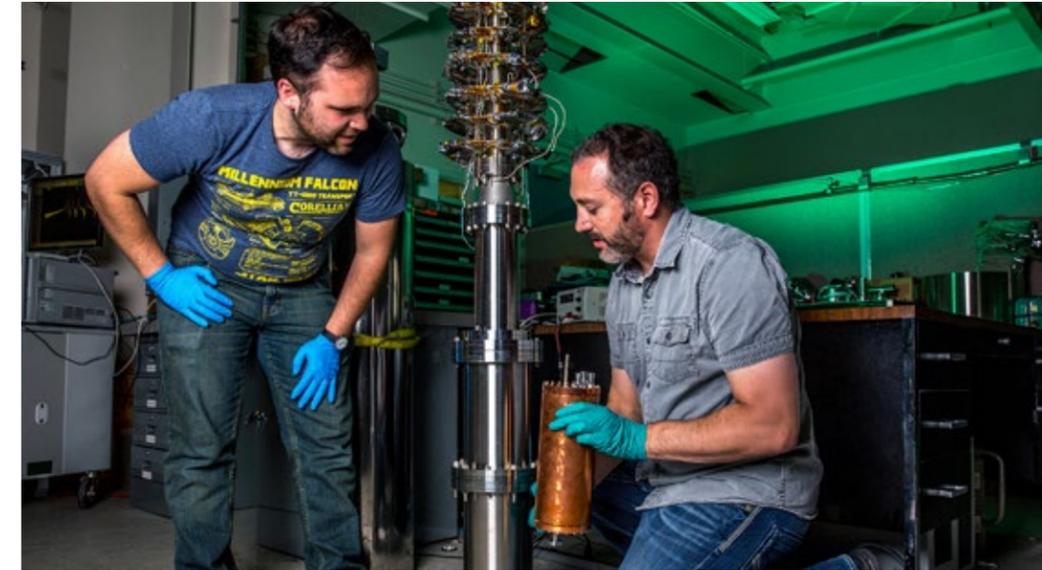
Classical computers may help run quantum computers, but classical programming is insufficient for quantum calculations. DuBois explains, “Quantum

computers need a different kind of programming, which includes intimately understanding the physics of the system to be simulated and the system running the simulation.” As part of ASC’s Beyond Moore’s Law Project, Livermore scientists are developing new algorithms to run on the quantum test beds. The project’s twin goals are improvements in basic science and scientific computing. DuBois notes, “We have the potential to achieve huge increases in scientific computing speed with this technology.”

For the basic science goal, the team strives to efficiently simulate quantum dynamics in physical systems such as chemical reactions or atomic-level material behavior. With classical computing, simulations become more computationally expensive at smaller temporal and spatial scales, and quantum phenomena cannot be simulated directly or effectively. At best, solving quantum equations on a classical computer results in approximations, but more accurate simulations on a quantum computer could feed into larger models, improving simulation quality. Key to the scientific computing goal are new algorithms to solve applied problems—such as linear equations—and optimized functions to enable large-scale multiphysics simulations. The team is therefore focusing on mapping these algorithms to the quantum hardware and demonstrating their efficacy.

Exponential Potential

Even with an already sizeable portfolio of ongoing projects, scientists are eager to evolve the Laboratory’s quantum ecosystem even further and expand collaborations with HPC experts. For instance, DuBois’s team plans to deploy a larger, more versatile test bed. Another effort may involve distributed quantum computing, integrating the test beds with the Laboratory’s HPC systems. Other plans target the user experience, revealing the inner workings of a quantum computer



so users can see how their experiments are being run. Holland adds, “If researchers want to access the system remotely, from their own office, for instance, we could enable this first at Livermore and then expand to other national laboratories and external collaborators.”

Meanwhile, work continues amid another unique challenge—finding and nurturing specialists in quantum computing. “The field requires multidisciplinary expertise and a diverse skill set,” states Holland. Few graduate programs train students to contribute to quantum computing, and mid-career staff may not consider changing paths. However, DuBois’s own career is an example of the Laboratory’s professional development opportunities in emerging science and technology in general. He points out, “I don’t know of any other institution where a theoretical computational physicist can transition to experimental quantum physics.”

Livermore embraces its pioneering role in a field Carosi calls “the Wild West.” Holland emphasizes, “Quantum computing is not a fantasy—it’s already happening. Investments are crucial for making further progress and delivering

Livermore researchers Nathan Woollett (left) and Gianpaolo Carosi inspect the cryostat used for testing prototype microwave cavity systems for the Axion Dark Matter Experiment. The exceptional sensitivity of quantum-coherent devices can help find the axion, considered one of the most likely dark matter candidates. (Photo by George Kitrinis.)

on our missions. A broad, coordinated effort is required, and Livermore is a great hub for synthesizing resources to meet this lofty but important goal.”
—Holly Auten

Key Words: additive manufacturing, algorithm, ASCR Quantum-Enabled Simulation (AQuES) Testbed Pathfinder Program, Axion Dark Matter Experiment (ADMX), coherence, high-performance computing (HPC), Josephson junction, quantum-coherent device, quantum computing, quantum processing unit (QPU), quantum sensing, qubit, qudit, superconducting quantum interference device (SQUID), superconductivity, superposition.

For further information contact Jonathan DuBois (925) 422-1406 (dubois9@llnl.gov).

Newly Created Water Phase Helps Solve Planetary Mystery



NASA's Voyager 2 spacecraft—launched in 1977 and still in operation—is one of the agency's two farthest-reaching and longest-running missions, the other being Voyager 1. The journey by Voyager 2 to the outer solar system and beyond has been marked by many scientific firsts, including the first and only study of the ice giants Neptune and Uranus by a space probe. Perhaps the most intriguing of Voyager 2's findings about these

two distant bodies is their tilted magnetic fields. Unlike Jupiter, Saturn, and the terrestrial planets, the magnetic axes of the seventh and eighth planets are offset from the axes around which they rotate—by roughly a third of Uranus's radius and even more for Neptune. In addition, the fields themselves are asymmetrical.

The magnetic fields of most planets are generated through large-scale motion of electrically conductive fluids. On Earth,

this dynamo effect occurs in the liquid iron outer core. Researchers have been split on the composition of the solar system's two most distant planets—and thus the origin of their tilted and lopsided magnetic fields. Many scientists envision these planets with fully fluid-convecting interiors, while others have proposed a more complex structure, consisting of a thin, electrically conductive liquid shell surrounding a thicker mantle of ice. If, as the latter theory suggests, the fields originate not deep within the planets but in the liquid just beneath their gassy envelopes, this unusual arrangement could explain the planets' strange magnetic nature.

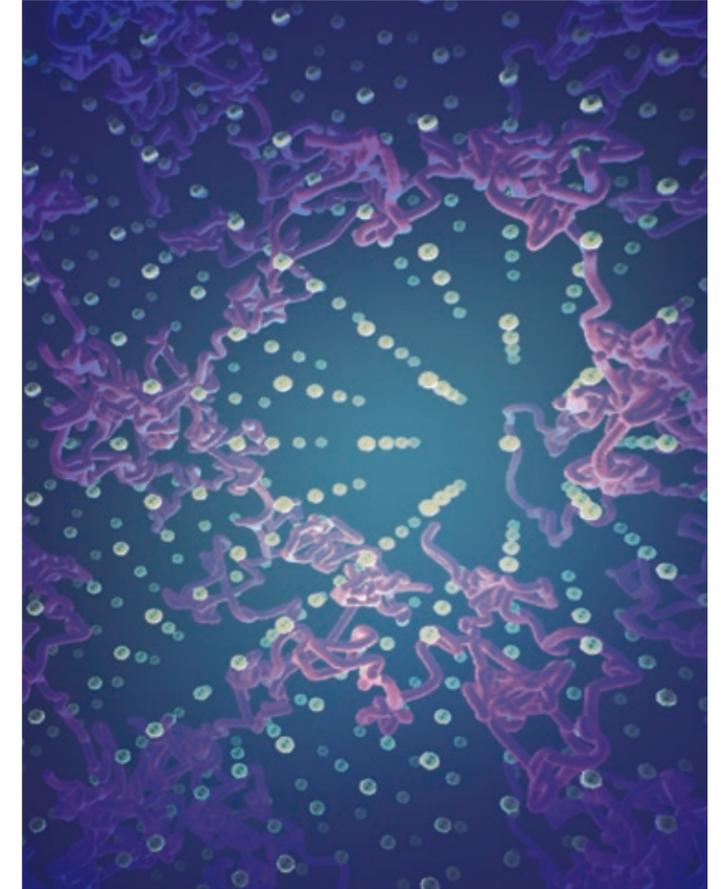
The primary ingredient in the proposed fluid and solid layers may be water, thought to make up more than 60 percent of Uranus's and Neptune's masses. Subjected to intense pressure, the ice in these planets' mantles would bear little resemblance to ice on Earth, appearing black rather than transparent and remaining solid even at temperatures approaching those of the Sun's surface. This exotic phase of water has been dubbed superionic ice. The role of superionic ice in the formation of the ice giants' odd magnetic fields was first posited nearly two decades ago and has been supported by a series of increasingly complex molecular dynamics simulations.

However, creating and characterizing superionic ice in a laboratory setting—an essential step towards validating the simulations—has until recently proven a virtually insurmountable hurdle. Now, through a novel combination of experimental techniques, a team of researchers from Lawrence Livermore, the University of California at Berkeley, and the University of Rochester have successfully produced superionic ice in the laboratory for a vanishingly brief moment. (Work at Livermore was supported by the Laboratory Directed Research and Development Program.) The properties of ice created in the laboratory agree well with simulations, lending credence to the superionic ice mantle theory.

It's Just a Phase

Water can exist in three phases—solid (ice), liquid (water), or gas (steam). On Earth, the one oxygen and two hydrogen atoms of a liquid water molecule form a loose V shape. As ice, the atoms rearrange and combine with other water molecules to form a more widely spaced hexagonal crystal structure, as seen in snowflakes—which is why water expands as it changes from liquid to solid, the opposite of most substances. This familiar form of ice is the only solid phase of water found naturally on Earth's surface but is just one of 18 known crystalline ice phases. The other phases, distinguished by their arrangements of hydrogen and oxygen atoms, form under different pressure and temperature conditions, some of which are difficult to replicate in a laboratory setting.

Once its structure has been thoroughly characterized, superionic ice may become the newest recognized ice phase,



This visualization of molecular dynamics simulations shows the fast diffusion of hydrogen ions (pink trajectories) within the solid lattice of oxygen (yellow) in superionic ice. (Image by Sebastien Hamel, Marius Millot, and James Wickboldt.)

and perhaps one of its strangest. Superionic ice forms in conditions exceeding approximately 70 gigapascals—or 700,000 times Earth's surface pressure—and 2,000 kelvins, which is approximately iron's melting temperature at ambient pressure. Above these lower boundary conditions, the hydrogen nuclei (or ions) begin to jump rapidly from one ice crystal to the next with a motion resembling that of a fluid, despite the ice being considered a solid phase of water. (Meanwhile, the larger and heavier oxygen atoms stay fixed, vibrating near their equilibrium crystal position.) Because the hydrogen ions carry a positive charge, their fluidlike diffusing motion enables a type of conductivity known as superionic conductivity. In contrast, the more familiar electrical conductivity most commonly exhibited by metals involves the flow of negatively charged electrons.

Best of Both Worlds

From molecular dynamics simulations, scientists knew the temperature and pressure conditions most likely to produce superionic ice, but the path to reach those conditions was less obvious, in part because working with water can be surprisingly difficult. Livermore physicist Marius Millot, the project's principal investigator, says, "We can normally conduct these sorts of experiments in a diamond anvil cell, a static compression platform that gradually squeezes a sample between two pieces of diamond. However, water is hard to study this way because it reacts with everything at high pressures. Diagnosing the sample's properties therefore becomes quite challenging." Computational chemist Sebastien Hamel adds, "Water becomes a 'super acid' that eats up whatever contains it. This property has ruined many past experiments."

Another possible approach is dynamic compression, which typically uses lasers or gas guns to generate shock waves that raise temperature, pressure, and density rapidly enough to bypass the acidity problem—the experiment is over before the water can react with its surroundings. However, dynamic compression can heat a water sample too much, inadvertently yielding another phase of water. (See *S&TR*, December 2015,

pp. 4–12.) Millot therefore decided instead to combine static and dynamic compression techniques in a single experiment. Hamel provided high-resolution simulations to help Millot design the experiments. "Because we precompress the water, less shock-heating occurs than when shock-compressing ambient liquid water, allowing us to access much colder states at high pressure than in previous shock-compression studies," explains Millot.

The superionic ice experiments took place in two parts, separated by over 4,800 kilometers. At Lawrence Livermore, Millot and his collaborators loaded a single microgram of water into a 5-centimeter-diameter diamond anvil cell (DAC) assembly containing tiny quartz plates, tailored antireflection and polymer coatings, and ruby microspheres. These cells were compressed at room temperature to 2.5 gigapascals, squeezing the water into an ice phase 60 percent denser than normal water. The Livermore team then transported the whole assembly from California to the University of Rochester's Omega Laser Facility in New York. There, Millot worked with the Omega operations crew to position the DAC in the laser's target chamber, where it was simultaneously bombarded with six nanosecond-long pulses of ultraviolet light. The beams sent shock waves through the sample, heating and further squeezing it. The laser-driven compression was so violent that the diamonds were vaporized by the end of each experiment.

Taking the Experiment's Pulse

During the brief, 20-nanosecond duration of the experiment, the team collected time-resolved optical pyrometry and laser velocimetry measurements to monitor the shock waves and document how the ice changed. "In our experiments, we look at the interface between shock-compressed and unshocked material. Think of it like a snow plow advancing through the ice," says Hamel. The speed of the shock wave, for instance, can be used to determine the pressure produced by the wave. The temperature of the shocked sample can be inferred by measuring the heat radiated from the object in the form of visible light. In a series of experiments, these and other measurements enabled the team to "see" the formation of superionic ice and its transition to a liquid phase at approximately 190 gigapascals and 5,000 kelvins. The melting of the superionic ice was signaled by a discontinuity in the increase of the shock temperature and density in the sample in response to increasing shock pressure.

These upper boundary conditions matched predictions and supported the magnetic field generation theory—5,000 kelvins is hotter than the probable temperature deep inside Neptune and

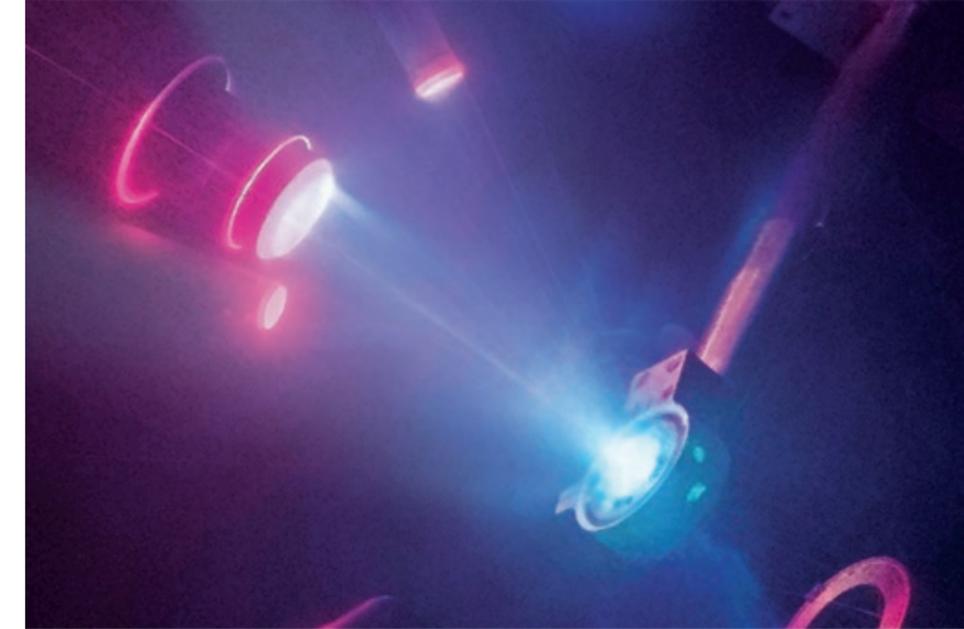
Uranus, indicating superionic ice could indeed exist in those planets. In fact, all the properties measured in the experiments were in good agreement with theoretical predictions and computer simulations. "Our experiment also showed 100 times higher ionic conductivity than other superionic solids, which was exactly what theory predicted," says Millot.

Although the experiments were successful and produced findings supportive of previous research, the journey from experiment to publication was neither easy nor quick. In all, the team painstakingly assembled and fielded more than 30 targets over the course of two years to gather data across a wide range of temperatures and pressures. They then spent two more years analyzing the data and confirming that their findings agreed with decades-old predictions. However, when the drafted journal paper was rejected for publication, the team was forced to reexamine its results. Fortunately, Millot's analysis of related metallic hydrogen experiments he had conducted at the National Ignition Facility (NIF) produced new insights. "I saw a signal in our NIF experiment similar to something seen in our superionic ice data and realized that some data we had thought was spurious was instead important," he explains. "We therefore reanalyzed our approach and conducted a few more experiments, greatly improving the whole narrative." The revised article was accepted for publication.

A Cool New Method

The experimental results not only confirmed the existence of superionic ice and lent credence to a theory for Uranus's and Neptune's odd magnetic fields. The findings also demonstrated the efficacy of a Livermore-developed experimental methodology—applicable to other laboratory astrophysics experiments—for compressing solids to high pressures and temperatures that are relatively cool by astrophysical standards. The work has also had other unexpected benefits. Millot now uses the new approach to analyze critical shock timing experiments for inertial confinement fusion research.

Furthermore, Hamel says that the experiments provide crucial validation data for his simulations. "Our molecular dynamics simulations rely on density functional theory. This theory has been validated and used repeatedly under ambient conditions but rarely verified at high pressures and temperatures because of the difficulty of conducting experiments in those regimes. Millot's experiments are some of the first to validate the theory under those extreme conditions," he notes.



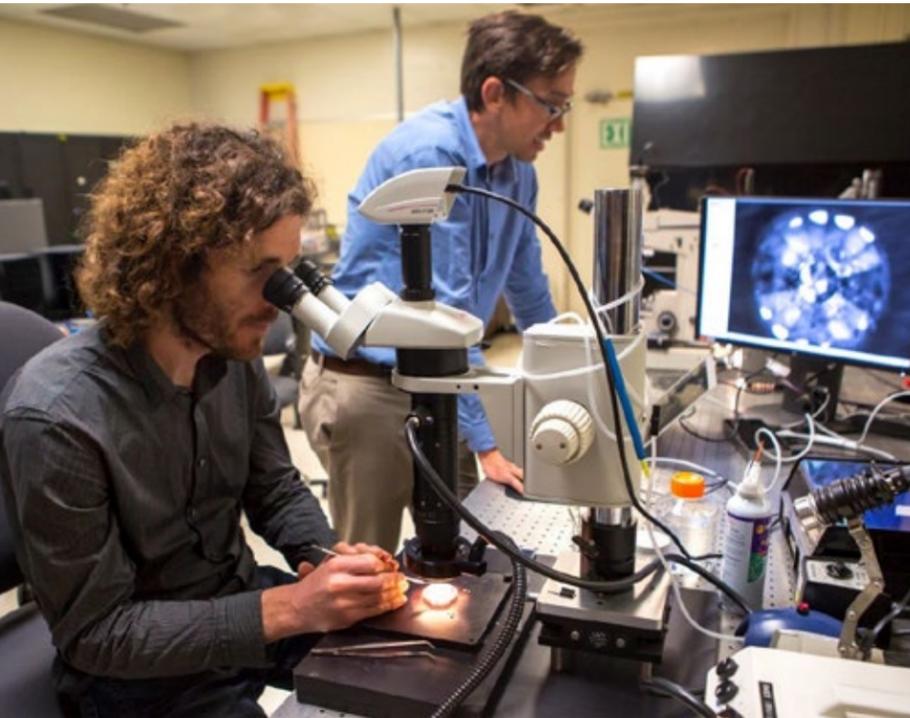
A time-integrated image depicts a laser-driven shock-compression experiment at the Omega Laser Facility. The experiment aimed to re-create planetary interior conditions and study the properties of superionic water. (Image by Marius Millot, James Wickboldt, and Eugene Kowaluk.)

These experiments are only the tip of the iceberg. After finishing their study of the crystal structure of superionic ice, the team intends to explore the properties of superionic ice combined with other elements, such as nitrogen and carbon. Such mixtures would more closely replicate the environment on Neptune, Uranus, and many water-rich exoplanets. Millot and his team relish the intellectual challenges that such experiments afford. "We can take advantage of NIF's and Omega's flexible laser systems and Livermore's great ingenuity in target design," he says. "The challenge is determining how to use these resources most effectively and design the best possible experiments. Experimental success or failure is determined long before we conduct the laser shot."

—Rose Hansen

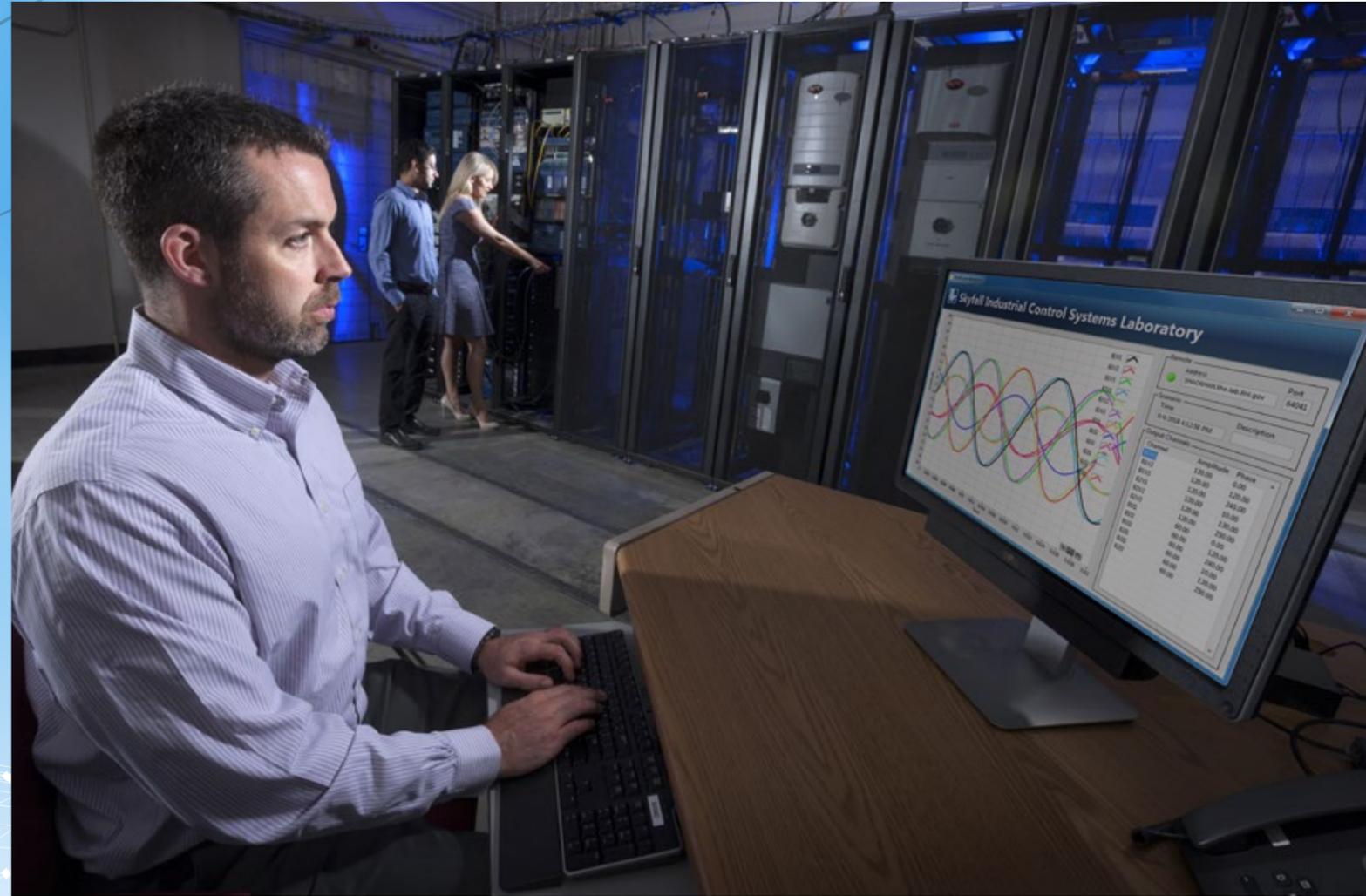
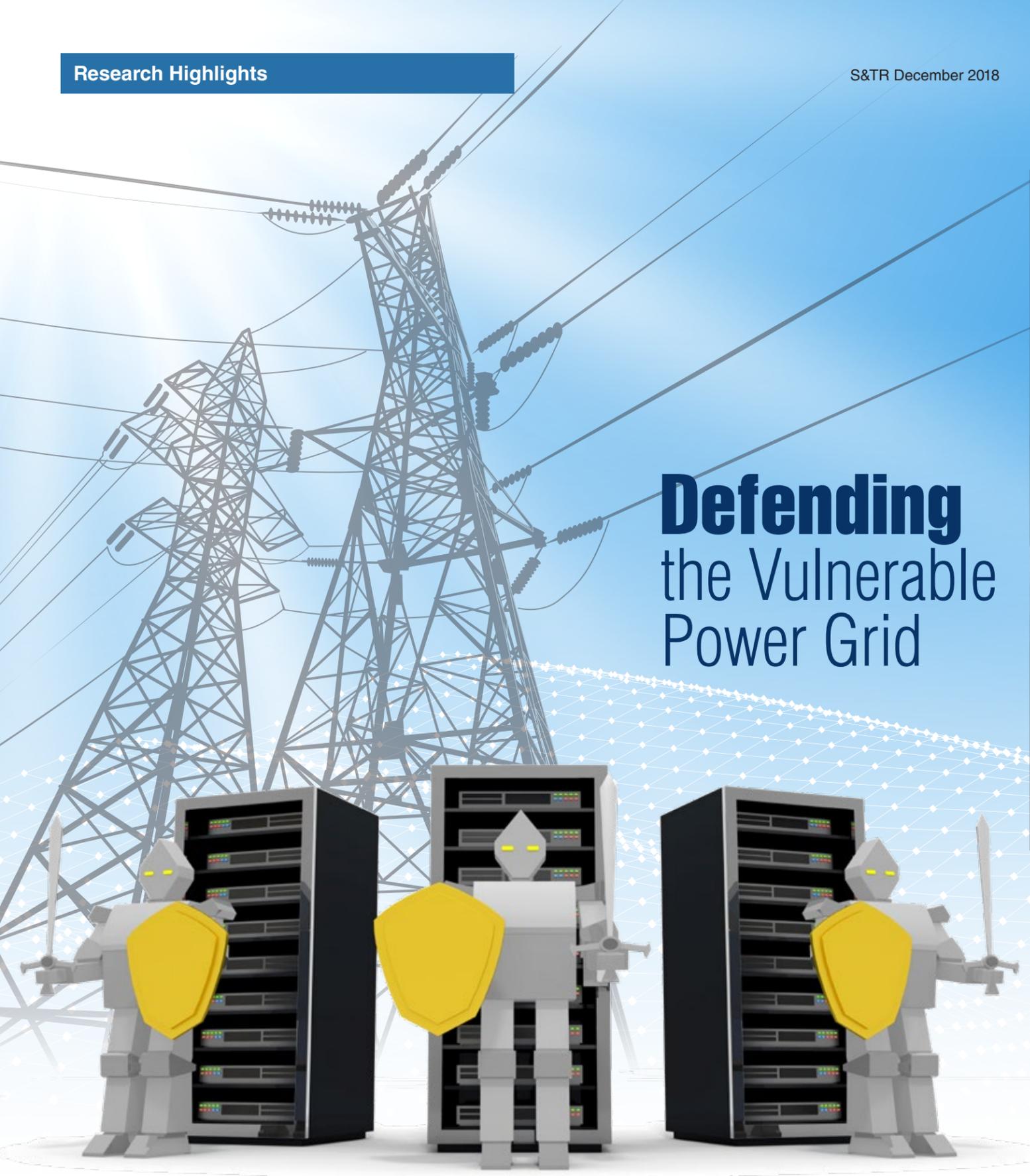
Key Words: diamond anvil cell (DAC), dynamic compression, magnetic field, National Ignition Facility (NIF), Neptune, Omega Laser Facility, pyrometry, shock compression, static compression, superionic ice, Uranus, velocimetry, water.

For further information contact Marius Millot (925) 422-6359 (millot1@llnl.gov).



At Lawrence Livermore, physicists Marius Millot (left) and Dayne Fratanduono prepare targets for shock-compression experiments. (Photo by Jason Laurea.)

Defending the Vulnerable Power Grid



IN 2015, just before the holidays, hackers shut down electricity for more than 230,000 people in and around Kyiv, the Ukrainian capital. The event is understood to be the first successful cyberattack on a power grid, but infrastructure vulnerability is everywhere. The next attack could be just over the horizon, and Lawrence Livermore’s Skyfall laboratory is working hard to blunt its force.

Skyfall is a combined cyber-physical hardware-in-the-loop test bed that connects real-world equipment with high-performance computers, strengthening the fidelity of simulations that help the United States prepare for disaster. The name “Skyfall” comes from the James Bond movie of the same name, in which villain Raoul Silva uses a cyberattack to destroy a gas pipeline in London.

Nate Gleason (seated) studies electrical sine waves on a monitor at Livermore’s Skyfall test bed facility. Behind him, Vaibhav Donde (left) and Jovana Helms examine the interior of Skyfall’s in-house relay substation. (Photo by Randy Wong.)

Although the film is fictional, the threat of cyberterrorism to many infrastructure networks is very real.

“If security is not part of the inherent design, the system will be vulnerable,” says Jovana Helms, an associate program leader in Livermore’s Global Security principal associate directorate. “One thing we hope to use Skyfall to do is understand how we can make security part of the design, rather than an afterthought. Our motto is ‘security built-in, not bolted-on.’”

Simulating a Hodgepodge

Power grids are immensely complex, interconnected systems. In Ukraine, the attack involved exploiting human weaknesses—phishing passwords from system administrators. Thankfully, the attack’s effects were kept relatively limited by reverting to manual control. In the United States, phishing is a vulnerability,

but more aspects of the grid are controlled by automated systems, broadening the risk. “The power grid is a very old system,” says Vaibhav Donde, Skyfall’s principal investigator. “With a mix of legacy and new equipment, the system always has issues and challenges on how to make everything work together, and fitting on top of all that is a cyber system.”

Past accidents can be instructive. In August 2003, a software bug led to a series of procedural mistakes that failed to correct for a simple voltage fluctuation in rural Ohio. A few hours later, an estimated 55 million people on the East Coast and in Canada were plunged into darkness. This event illustrates how small problems can rapidly cascade into a massive outage. Although the 2003 event was caused by a software error, a similar event could also be triggered by a deliberate cyberattack. The system only needs to “think” it is malfunctioning for such problems to arise.

Hardware in the Loop

Sophisticated simulations, such as those run on Lawrence Livermore’s high-performance computers, can help power providers plan for cyber-physical incidents on the grid, including accidents and attacks. However, an important difference exists between a purely software-based simulation model and a hardware-in-the-loop model. Helms explains, “Some customers may say, ‘That’s just a model, and there’s no perfect model,’ but with hardware in the-loop, we are adding a whole new level of realism and fidelity to our simulations. We can incorporate an actual device in the laboratory and mimic that behavior across a grid.”

At Skyfall’s center is a full-fledged power substation that behaves as if connected to an actual power system. A computer feeds the substation a set of conditions—such as voltages and currents—just like the signals that would be received in the real world. The researchers can then see how the Skyfall substation responds to an unexpected power surge, for example, and then extrapolate the results across the wider network. “Let’s say you have a simulation with 5,000 relays, two of which are physically represented in the laboratory,” says Helms. “Instead of talking to a modeled relay in a computer, our simulation actually talks to the physical relays.” In some ways, the difference is the same as that between trying to understand a forest with a computer and understanding a forest by growing a real tree. The resulting high-fidelity simulations are detailed, realistic models of cyber-physical systems at scale.

What sets Skyfall apart from other hardware-in-the-loop facilities is its ability to simulate a cyberattack from beginning to end, providing a realistic view of system behavior during an attack. Skyfall can cosimulate power flow and communication across the grid. Donde says, “Today, all these systems—distribution, transmission, and communications—are so tightly

coupled that one cannot simulate any single system correctly without considering its connections to the other layers.” Because of this interconnectedness, the Department of Energy has made cosimulation a priority. Future evolution of the Skyfall platform will include equipment used in the other layers, including solar panels and electric car chargers.

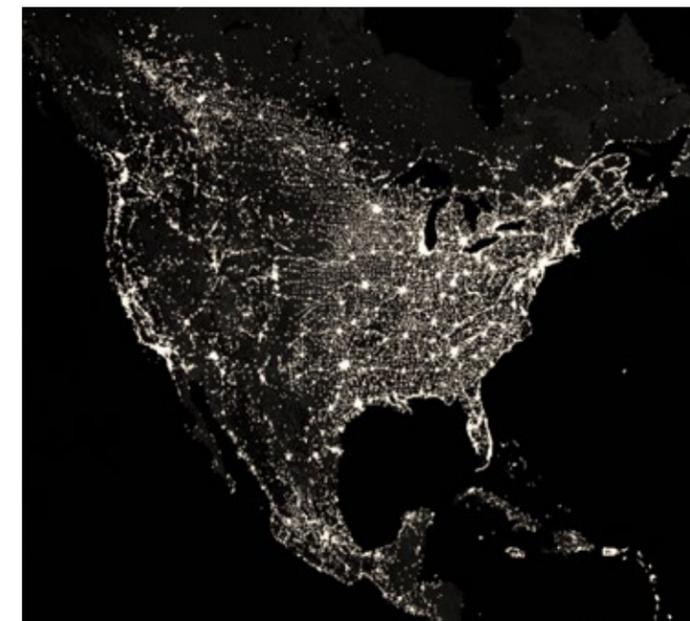
Protecting Infrastructure

One of the newest monitoring devices being incorporated into power grids are phasor measurement units (PMUs), which track power flow between locations by measuring electrical sine waves. Each PMU is calibrated to look for a shift in the wave—a change in waveform phase—to determine how differently the grid is loaded at the PMU’s specific location relative to others. A PMU in Livermore will measure Livermore’s phase, but the same PMU model in Chicago or Virginia Beach will measure a different phase there. All such PMUs will collectively use this information to accurately calculate the power that people are using at that instance of time across the grid and estimate the chances of an overload or power surge.

To determine the correct phase for its location, each PMU is synchronized to a GPS satellite clock. However, if the PMU gets an incorrect GPS signal, every resulting calculation will be wrong, creating unforetold problems. A recent outage in the Pacific Northwest was traced to such an incorrect signal, which had been supplied accidentally by the wrong satellite. Led by Helms, Skyfall was used to prove that such a “spoofed” signal could be reproduced relatively easily by malicious agents. This finding, bolstered by the improved accuracy of the hardware-in-the-loop simulation, has helped the Department of Homeland Security work with vendors to guard PMU hardware and software against future accidents and attacks.

Another component of Skyfall is the Malicious Code Analysis Center (MCAC), which focuses on understanding the vulnerabilities in firmware and software for cyber-physical systems. MCAC is a library of malicious code and analysis tools, kept totally isolated from other networks, that could someday be used against cyber-physical systems. When used against Skyfall, researchers can safely gain critical insight into the worst-case scenarios for the nation’s infrastructure. Donde explains that power relays such as the one connected to Skyfall have computer chips that run code. He says, “If someone hacks in and changes the logic of how the relay should operate, essentially the user would not know until the code were executed and something bad happened on the grid.” With MCAC, researchers can see how bad software can affect power delivery and potentially damage the integrity of grid systems. “MCAC is like a sandbox where you can play and understand how code changes would work out on the actual grid,” says Helms. “It’s a realistic but safe environment.”

The nation’s power grid is integrated coast to coast by modern devices connected to an aging infrastructure. An accident or attack on one component could create cascading problems for huge segments of the grid. Skyfall is designed to model the network’s behavior in such cases.



The Sky Isn’t Falling

Cyberattacks will target the nation’s infrastructure and accidents will happen, but Livermore’s Skyfall test bed is constantly adding capability to strengthen its predictive powers and connect more closely with the Laboratory’s missions and core competencies. In the future, Helms and Donde agree, Skyfall will further capitalize on the speed and efficiency afforded by Livermore’s high-performance computing resources and continue expanding its hardware-in-the-loop approach to more types of critical systems. With the rise of automated vehicles, telecommunications, and renewable sources of power, the need is increasing for sophisticated, realistic simulation capabilities to help protect the complex infrastructure upon which the nation depends.

—Ben Kennedy

Key Words: cosimulation, energy, cyberattack, cyberterrorism, high-performance computing, electric grid, hardware-in-the-loop simulation, malware, Malicious Code Analysis Center (MCAC), phasor measurement unit (PMU).

For further information, contact Jovana Helms at (925) 423-3877 (helms7@llnl.gov).



Skyfall’s power substation is the same as one that would be found on a real-world power grid. By using such hardware alongside sophisticated computer simulations, Skyfall can analyze a cyberattack from beginning to end.



Virtual and Augmented Reality Yield New Insights

Using virtual reality (VR), National Ignition Facility (NIF) technician Robin Issavi trains to install modified panels (blue) inside the NIF target chamber. (Image by Jason Laurea and Paul Bloom.)

THE 192 laser beams of the massive National Ignition Facility (NIF) converge at the center of its giant, spherical target chamber through 48 symmetrically distributed portholes. Interspersed among these portholes is an array of other ports used for equipment with functions ranging from holding and positioning fusion targets to detecting what happens after the targets are hit by the laser beams. Although the target chamber is 10 meters in diameter—the size of a small hot air balloon—gaining access to its outer wall proves challenging because of ever-increasing congestion. A majority of the nearly 200 ports are already in use, leaving only a small fraction unclaimed and unobstructed. As the variety of experiments running on NIF increases, so does the demand placed on this limited and valuable real estate.

Now, leading-edge simulation technologies are helping researchers go beyond reality to help answer the question of exactly what is possible at NIF. Considering the facility's enormous complexity and demanding requirements—as well as the power and energy involved with experiments and the potential hazards that must be safely contained—methods that more effectively answer this question also help NIF achieve its myriad operational goals.

Bruno Van Wonterghem, NIF's operations manager, must ensure the facility is up and running around the clock for

current users and is well prepared for future experiments and improvements. He explains, "As we fill up seemingly every cubic centimeter of space around the target chamber, it gets harder and harder to determine exactly where new equipment will go and how we will operate and maintain it all. Turning to virtual and augmented reality to evaluate scenarios ahead of time gives us insight that we never had before." These two approaches differ in that virtual reality (VR) is a completely immersive experience in which everything the user sees is simulated, similar to playing a videogame. In contrast, augmented reality (AR) superimposes computerized images over the user's real-life field of view. Besides using VR and AR for practical engineering and mechanical applications to maintain and expand operations, NIF also uses these computerized visualization tools to give hands-on, realistic experiences that connect people to a realm that is ordinarily out of reach.

Training Goes Virtual

In a building separate from the NIF facility, a technician stands alone in a room tethered to a wire dangling from the ceiling. A virtual representation of a 14-kilogram, louvred panel drifts in front of him. Wearing VR goggles and clutching handheld controllers, he explores part of one of the largest and most complex virtual environments in the world. The panel represents

part of the segmented stainless-steel wall that lines the inside of the NIF target chamber, providing a protective barrier against the shrapnel and debris generated when NIF's laser beams blow apart experimental targets. The panel also absorbs stray laser light, preventing reflections from entering the beamlines and damaging components.

To accommodate new equipment for additional experiments, panels that completely cover inactive ports are being replaced with those containing cutouts to allow access into the target chamber. These covered ports were once considered excess inventory but are now a valuable commodity. In his VR world, the technician grabs and repositions the new panel to fit it into the wall similar to a giant jigsaw puzzle piece. VR training allows him to practice this challenging replacement procedure without having to wear the usual two layers of protective hazmat suits, fully enclosed helmet, and respirator. Normally, the work requires him to spend many hours at a time suspended high above the target chamber floor, in close confinement in a hazardous environment, and tasked with potentially risky mechanical activities. Virtual training reduces risks.

Before entering the hazardous environment inside the target chamber to replace panels, technicians have already trained with VR to familiarize themselves with the replacement procedure. (Photo by Dan Linehan.)



Typically, a user inside NIF's VR world can freely move around side-to-side and up-and-down inside and outside of the target chamber as if the laws of gravity did not exist. For this particular training exercise, mechanical designer Paul Bloom, who maintains the NIF VR model for the Virtual Immersion Engineering (VIE) group, programmed a simulation to closely match the actual sequence of replacement. "The user can look in all directions while the simulation is running and also pause the sequence to manipulate parts as if they were actually being handled," says Bloom. "However, for this application, the user is anchored in space and cannot freely walk around." This limitation is in place because movement is similarly restricted in the real world. Two technicians performing actual panel replacements will work side-by-side inside a small safety cage attached to a lift that elevates them more than 12 meters above the target chamber's basement floor. Using VR training gives the technicians a feel for being inside the target chamber by providing realistic familiarization and a sense of situational awareness that translates directly to the real world.

Augmented and Virtual Outreach

NIF technicians are not the only ones gaining valuable understanding by using VR to experience the inside of the

target chamber. The technology also benefits the wide range of visitors who flock to NIF each year for one of hundreds of hour-long tours. These visits expose thousands of people to NIF's NASA-like mission control room, the master oscillator room—the source of laser light—and one of the two gigantic laser bays, where the laser light is split into 192 beams and magnified in energy by a factor of 4 quadrillion. Having doubled for the starship *Enterprise's* warp core in the movie *Star Trek Into Darkness*, the target chamber steals the show, but for tour participants it can still be as elusive as a cloaked Klingon vessel. NIF is a working research facility, where experiments take precedent over visitors. Consequently, over half of all NIF tours are prevented from seeing the target chamber while it is sealed off during operation.

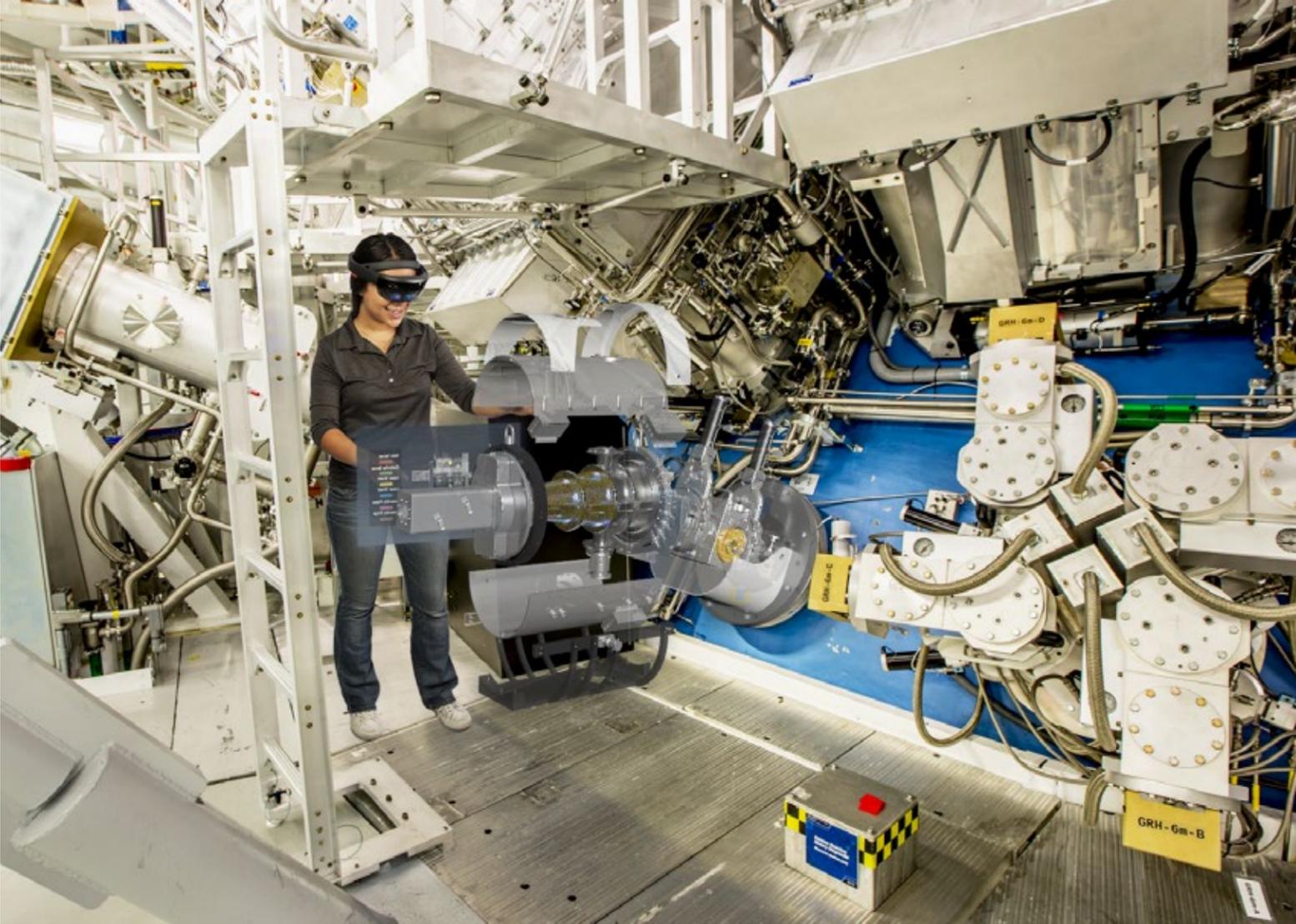
In 2015, Pam Spears, supervisor in the Technical Information Department (TID), and her team were first exposed to the VR possibilities of Bloom's decade-long three-dimensional (3D) visualization work. Just prior to this, the team had also attended an AR demonstration by 3D animators in TID's Visualization group during a student outreach event. These two meetings inspired Spears's team to develop an AR-VR tool for NIF tours with the help of the TID Visualization and NIF VIE groups.

"If you cannot see the target chamber for yourself during a tour, then AR and VR offer the next best thing. In some cases, it's even better," states Spears. "The tool allows people to quickly understand the excitement, science, tiny details, and sheer magnitude of what's happening at NIF."

On a pedestal in front of a video wall, a large model of the target chamber forms the centerpiece of the NIF facility's lobby. Around the model's equator is a series of high-contrast images that a computer tablet's camera recognizes as 3D positioning targets, which allow a high-resolution representation of the target chamber to be mapped in place of the actual model and shown on the tablet's screen and the video wall. NIF graphic designer John Jett, who managed the tool project, says, "Visitors can move all around the model, but the AR stays locked in place. The target chamber wall, the beamlines, diagnostics attached to the target chamber, and the target itself can be turned on and off. The most popular feature allows visitors to fire all the laser beams." Switching to VR mode then gives tour participants an inside view of the target chamber from the same perspective as a NIF technician.

Engineering with Augmented Reality

Inspired by TID's AR-VR tool, Bloom saw how AR could help find ports for new equipment



by looking at the problem in reverse. He realized that with an understanding of actual space constraints around available ports, equipment designs could be tested on the target chamber before any physical pieces were assembled. This goal was achieved this year with AR converted from computer-assisted design (CAD) drawings. Describing the challenges of conversion, TID 3D animator Adam Connell says, "We're interested in the outer surfaces because the objects are large, complex, and must be viewable from a distance. For instance, with the AR-VR tool in NIF's lobby, CAD drawings give us the shape and scale but also much more detail than we need. For the images to appear realistic without looking jittery, we have to remove all excess geometry and then run smoothing algorithms."

After such initial simplifications, yielding believable AR then requires adding detail. Jake Long, a TID 3D animator who provided the finishing touches, says, "We want to match the actual properties of the object to make it look photo realistic, including textures and lighting. The more such detail we add, the more the objects look as if they are really there."

With AR goggles containing a computer and multiple cameras, an engineer can walk around inspecting equipment clearances from

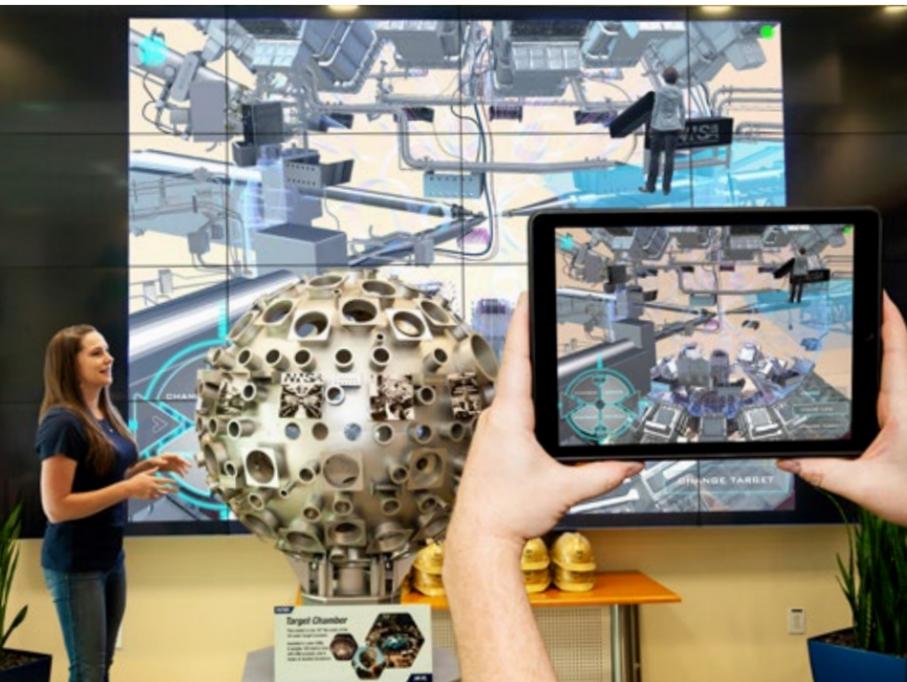
A composite image shows the exploded view that mechanical engineer Samantha Clements sees of a diagnostic (gray) that, in photo-realistic AR, is attached to an unclaimed port on NIF's target chamber wall. (Image by Jason Laurea and Brian Chavez.)

every angle. The equipment is visualized by AR and attached to a port with the help of technicians using VR. Similarly, NIF visitors can use both AR and VR to gain a better understanding of how the pieces all fit together. As additional needs and applications arise, the mixture of AR and VR will continue inspiring advancements and yielding new insights.

—Dan Linehan

Key Words: augmented reality (AR), computer-assisted design (CAD), laser, National Ignition Facility (NIF), outreach, simulation, target chamber, Technical Information Department (TID), training, virtual reality (VR), Virtual Immersion Engineering (VIE) group, Visualization group.

For further information contact Pam Spears (925) 423-8272 (spears10@llnl.gov).



A computer tablet transforms a scale model of NIF's target chamber into augmented reality (AR) and VR views, which are also displayed on a giant video wall inside NIF's lobby. (Image by Mark Meamber.)

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- or eight-digit number in the search box at the U.S. Patent and Trademark Office's website (<http://www.uspto.gov>).

Patents

Portable Medical Diagnosis Instrument

Tore Straume, David J. Loftus, Jing Li, Cristina E. Davis, Anup K. Singh, Matthew A. Coleman
U.S. Patent 9,824,870 B2
November 21, 2017

Method for Efficient, Narrow-Bandwidth, Laser Compton X-ray and Gamma-Ray Sources

Christopher P. J. Barty
U.S. Patent 9,986,627 B2
May 29, 2018

Ion Conductive Inks and Solutions for Additive Manufacturing of Lithium Microbatteries

Eric B. Duoss, Patrick G. Campbell, William C. Floyd, III, Julie A. Jackson, Matthew Merrill, Conner T. Sharpe, Christopher M. Spadaccini, Michael Stadermann, Cheng Zhu
U.S. Patent 10,003,059 B2
June 19, 2018

Awards

The **National Nuclear Security Administration's** (NNSA's) Office of Safety, Infrastructure, and Operations (NA-50) awarded three Laboratory teams with **NA-50 Excellence Awards**. 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 **Applied Materials and Engineering Area Plan** team was recognized for outstanding teamwork in developing an infrastructure area plan through innovative application of real property asset management principles. The team's efforts resulted in a multiyear, synchronized, multi-investor plan to repurpose, consolidate, build and dispose of equipment and facilities to achieve productivity more quickly than alternative approaches can. The award's recipients are held up as an example for other NNSA sites.

The **Creation of the Cooling and Heating Asset Management Program** team received the award for extraordinary efforts in developing an innovative contract instrument that allows, for the first time, rapid evaluation, design, and construction delivery of heating and air-conditioning (HVAC) systems to all eight NNSA sites. In less than two years, the recipients established a comprehensive master task agreement and process for the program. Their efforts greatly reduced mission risks, costs, and schedule in addressing HVAC issues NNSA-wide.

High-Density Carbon Nanotube-Based Monolith and Related Materials, Methods, and Devices

Marcus A. Worsley, Theodore F. Baumann, Juergen Biener, Supakit Charnvanichborikarn, Sergei Kucheyev, Elizabeth Montalvo, Swanee Shin, Elijah Tylski
U.S. Patent 10,014,090 B2
July 3, 2018

Expandable Implant and Implant System

Thomas S. Wilson, Ward Small, IV, William J. Benett, Jason M. Ortega, Duncan J. Maitland, Jonathan Hartman
U.S. Patent 10,010,327 B2
July 3, 2018

Chemical, Biological, and Radioactive Contamination Remediation with Lasers

Joseph C. Farmer, Alexander M. Rubenchik
U.S. Patent 10,016,844 B2
July 10, 2018

The **Injury-Free Construction Delivery** team was recognized for outstanding teamwork and dedication in safely executing \$60 million of construction projects at Livermore in FY 2017 without a single worker injury. This track record was achieved while scaling up construction work from only \$10 million in FY 2013.

Fady Najjar, a design physicist at Lawrence Livermore, has been elected a **fellow** of the **American Society of Mechanical Engineers** (ASME). Najjar was recognized for "significant contributions and innovations in computational techniques for fluid flows, for advances in understanding of high-speed gas particle flows including shock physics, and for advances in simulations of flow fields in solid rocket motors and high-speed reacting flows."

Najjar has a Ph.D. in mechanical engineering from the University of Illinois and has applied his skill simulating ejecta and fluid dynamics of energetic materials as a design physicist in Livermore's Weapons and Complex Integration Principal Directorate. During the 22 years Najjar has been an ASME member, he has co-authored more than 40 refereed publications and 30 technical reports and delivered more than 60 presentations at international conferences and technical meetings.

Less than 4 percent of ASME's 91,078 members are fellows. Najjar's nomination was sponsored by his former Ph.D. adviser from the University of Illinois, Surya Vanka, who also is an ASME fellow, and was supported by three nomination letters.

Abstract

Livermore Leaps into Quantum Computing

With the potential to exponentially transform processing speed, quantum computing has emerged as the next frontier of high-performance computing. Unlike classical computing, this technology exploits principles of quantum physics and requires new paradigms in how scientists approach computer hardware and programming. Accordingly, many opportunities exist for Lawrence Livermore to advance the state of the art in quantum computing architectures and related technologies. Activities in the Laboratory's diverse research portfolio include demonstrating a fully programmable quantum computing system, improving superconducting materials and devices, deploying quantum sensors, and developing quantum algorithms. Experiments are designed to minimize energy loss and error rates while reducing interference and maximizing performance. Livermore's two quantum computing test beds are cooled near absolute zero and precisely tuned to control the quantum properties of superconducting circuits. The future of this relatively young field depends on strategic investments in innovative scientific endeavors and multidisciplinary staff.

Contact: Jonathan DuBois (925) 422-1406 (dubois9@llnl.gov).

Small Satellites Bolster a Space Program



The Laboratory's work developing small, modular cube satellites is enabling other "out-of-this-world" technologies.

Also in January/February

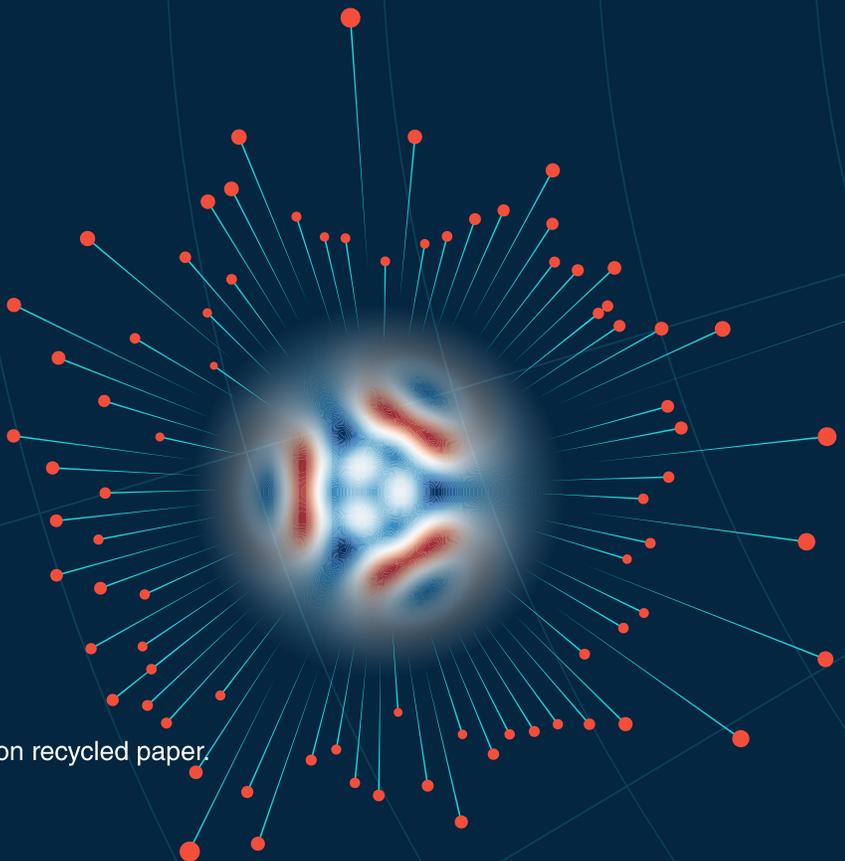
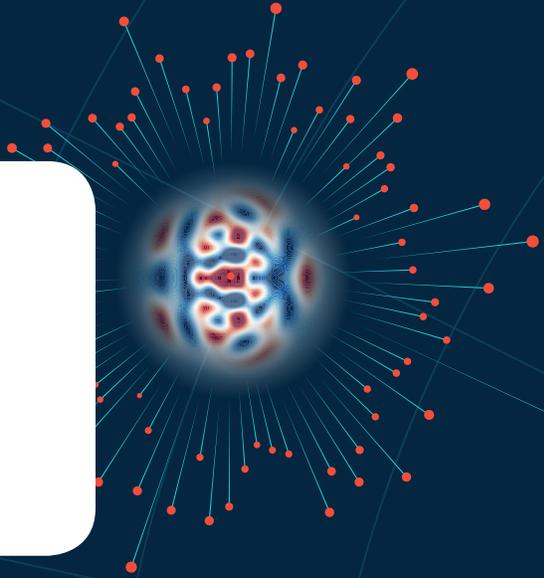
• *On the road to fusion ignition, researchers at the National Ignition Facility are nearing a critical milestone called burning plasma.*

• *An innovative Wolter optic for pulsed-power x-ray diagnostics creates sharper images, potentially opening new doors for fusion research.*

• *The Laboratory's engagement with the military includes a variety of onsite education opportunities, such as the Air Force Fellows program.*

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