Lawrence Livermore National Laboratory

Science & Technology Review

September 2016

INNOVATIONS FOR EXTREME-SCALE COMPUTING

Also in this issue:

Modernizing the Format for Nuclear Data

An Enterprise Model of Lick Observatory

Improved Hydrogen Storage and Delivery

About the Cover

High-performance computing is used to tackle many outstanding scientific and engineering challenges pertaining to climate, energy, biosecurity, and stockpile stewardship. Users continue to need faster, massively parallel computer systems that can perform billions or trillions of calculations concurrently, access and process vast amounts of data efficiently, and run ensembles of simulations. Through funding avenues such as the Laboratory Directed Research and Development (LDRD) Program, Livermore computer scientists are contributing to the progress of extreme-scale (exascale or greater) computing, in which machines perform 10^{18} or more floating-point operations per second. LDRD-funded projects aim to establish methods for efficiently using machines with increasingly complex computer architectures.

Cover design: Alexandria Holmberg and Max Rodriguez.

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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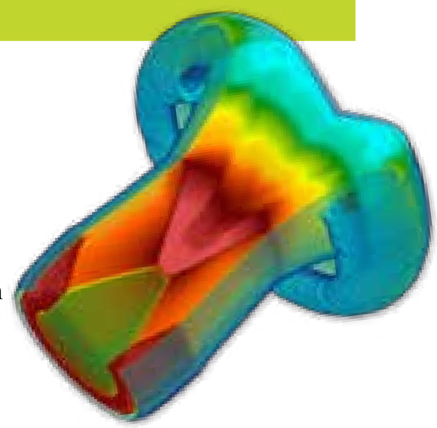
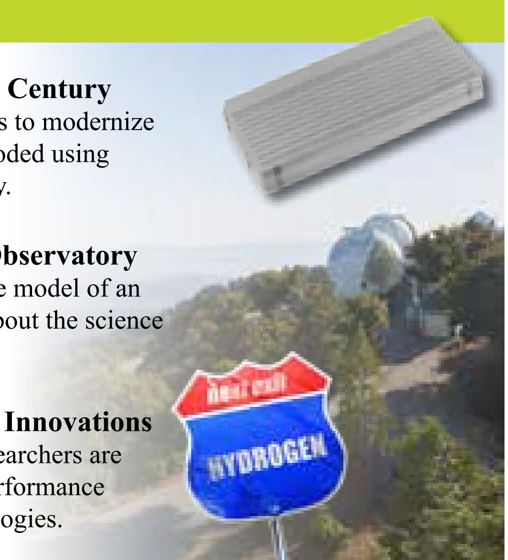


Research Highlights



Departments

Carbon Allotrope Could Mark Meteor Impacts

Scientists speculate that lonsdaleite, a hexagonal form of diamond found in meteorite fragments around the world, is created when graphite-bearing meteors strike Earth. The violent impact generates incredible heat and pressure, transforming the graphite into diamond while retaining the graphite's original hexagonal structure. Recent Livermore dynamic high-pressure experiments, which mimic meteor-impact conditions, created a lonsdaleite structure for the first time in a laboratory. The research appears in the March 14, 2016, edition of *Nature Communications*.

The research team, which includes scientists from Livermore, the University of California (UC) at Berkeley, SLAC National Accelerator Laboratory, and international institutions, conducted the experiments at SLAC's Linac Coherent Light Source. Graphite samples were shock-compressed to pressures of up to nearly 203 gigapascals (2 million atmospheres) to trigger the structural transitions from graphite to diamond and lonsdaleite. The results indicate that the lonsdaleite found in nature could serve as evidence of violent meteor impacts.

"Our experiments show that above the pressure range studied in our experiments, the lonsdaleite structure can be generated in a very pure form. Since pure lonsdaleite is supposedly even harder than diamond, our results already have important industry applications," says Dominik Kraus, who conducted this research while working as a postdoc within Livermore's National Ignition Facility and Photon Science Principal Directorate. Kraus now serves as the Helmholtz Young Investigator group leader at Helmholtz-Zentrum Dresden-Rossendorf in Germany.

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Scientists Pump Up Batteries with Metal Oxides

Graphene metal oxide (GMO) nanocomposites are renowned for their potential energy storage and conversion applications. For lithium-ion batteries, nanosize metal oxide particles and highly conductive graphene are considered beneficial for shortening lithium diffusion pathways and reducing polarization in the electrode, leading to enhanced performance. In research featured on the cover of the March 21, 2016, edition of the *Journal of Materials Chemistry A*, Livermore materials scientists synthesized and compared the electrochemical performance of three GMO nanocomposite structures and found that two of them greatly improved reversible lithium storage capacity.

As part of the experiments, the team dipped prefabricated graphene aerogel electrodes in solutions of metal oxide nanoparticles, which became anchored on the surface of the graphene pores (shown in image below), making them fully accessible to the electrolyte. The method can deposit most types of metal oxides onto the same prefabricated three-dimensional graphene structure, allowing for direct comparison of electrochemical performance of a wide range of GMOs.

"Surprisingly, we saw that the graphene's capacity is mainly determined by active materials and the type of metal oxide bound onto the graphene surface," says Morris Wang, a Livermore materials scientist and author of the paper. The work was funded through Livermore's Laboratory Directed Research and Development Program.

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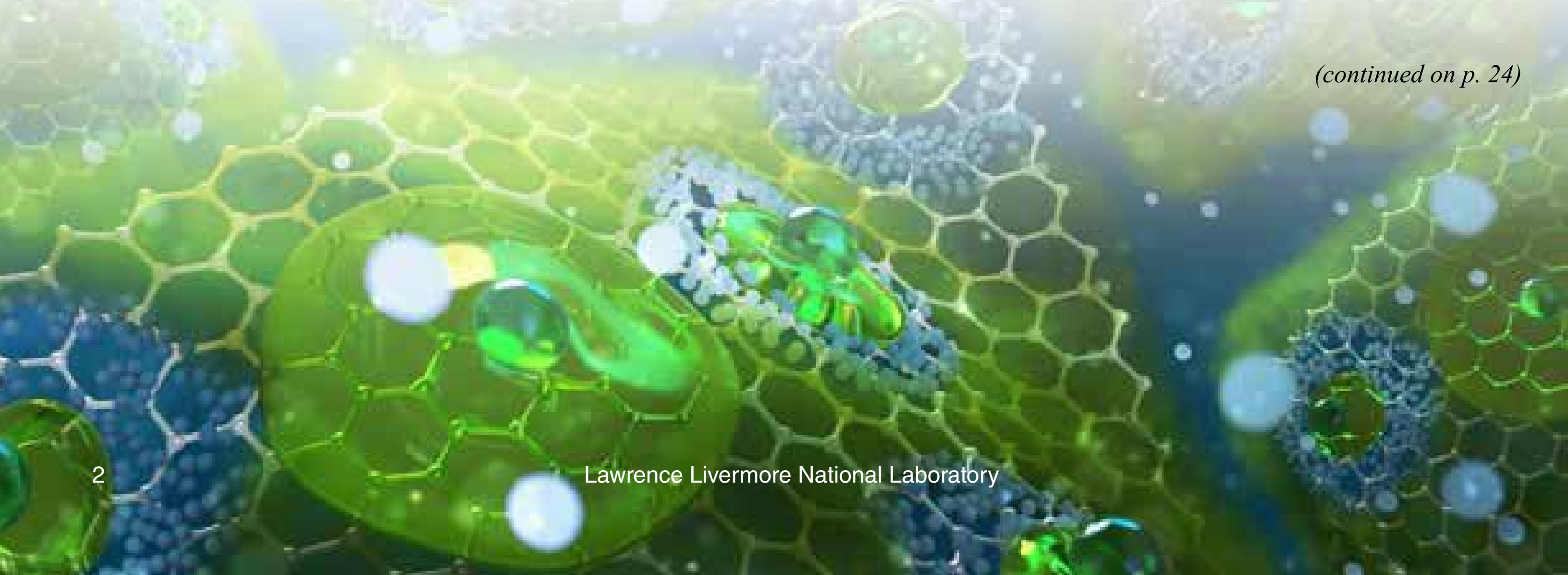
Building a New Brain-Inspired Supercomputer

In March 2016, Lawrence Livermore received a first-of-its-kind, brain-inspired supercomputing platform for deep learning developed by IBM Research. Based on a breakthrough neurosynaptic computer chip called IBM TrueNorth, the scalable platform processes the equivalent of 16 million neurons and 4 billion synapses yet consumes the energy equivalent of a hearing-aid battery—a mere 2.5 watts.

The brain-like, neural network design of the IBM Neuromorphic System can infer complex cognitive tasks such as pattern recognition and integrated sensory processing far more efficiently than conventional chips. The system will be used to explore new computing capabilities important to the National Nuclear Security Administration's (NNSA's) missions in cybersecurity, stockpile stewardship, and nonproliferation. NNSA's Advanced Simulation and Computing (ASC) Program will evaluate machine-learning applications as well as deep-learning algorithms and architectures and conduct general computing feasibility studies.

The Laboratory also acquired an end-to-end ecosystem to create and program energy-efficient machines that mimic the brain's

(continued on p. 24)



Commentary by Rokaya Al-Ayat

Laboratory Investments Drive Computational Advances

HIGH-PERFORMANCE computing (HPC) has been a defining strength of Lawrence Livermore since its founding. Indeed, Livermore scientists have designed and used some of the world's most powerful computers to drive breakthroughs in nearly every mission area. Today, the Laboratory is recognized as a world leader in the application of HPC to complex science, technology, and engineering challenges. Most importantly, HPC has been integral to the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program—designed to ensure the safety, security, and reliability of our nuclear deterrent without nuclear testing. The program celebrated its 20th anniversary in 2015, and much of the credit for its overwhelming success belongs to HPC capabilities and the expertise of scientists at NNSA's national security laboratories.

A critical factor behind Lawrence Livermore's preeminence in HPC is the ongoing investments made by the Laboratory Directed Research and Development (LDRD) Program in cutting-edge concepts to enable efficient utilization of these powerful machines. Congress established the LDRD Program in 1991 to maintain the technical vitality of the Department of Energy (DOE) national laboratories. LDRD has been, and continues to be, an essential tool for exploring anticipated needs that lie beyond the planning horizon of our programs and for attracting the next generation of talented visionaries. Through LDRD, Livermore researchers can examine future challenges, propose and explore innovative solutions, and deliver creative approaches to support our missions. Examples of LDRD successes are numerous and encompass all Laboratory mission areas. For HPC, we developed scalable algorithms in areas including adaptive mesh refinement and algebraic multigrid solvers, created a new paradigm in statistical debugging techniques, and produced methodologies that have resulted in the largest discrete event simulations ever performed. The present scientific and technical strengths of the Laboratory are, in large part, a product of past LDRD investments.

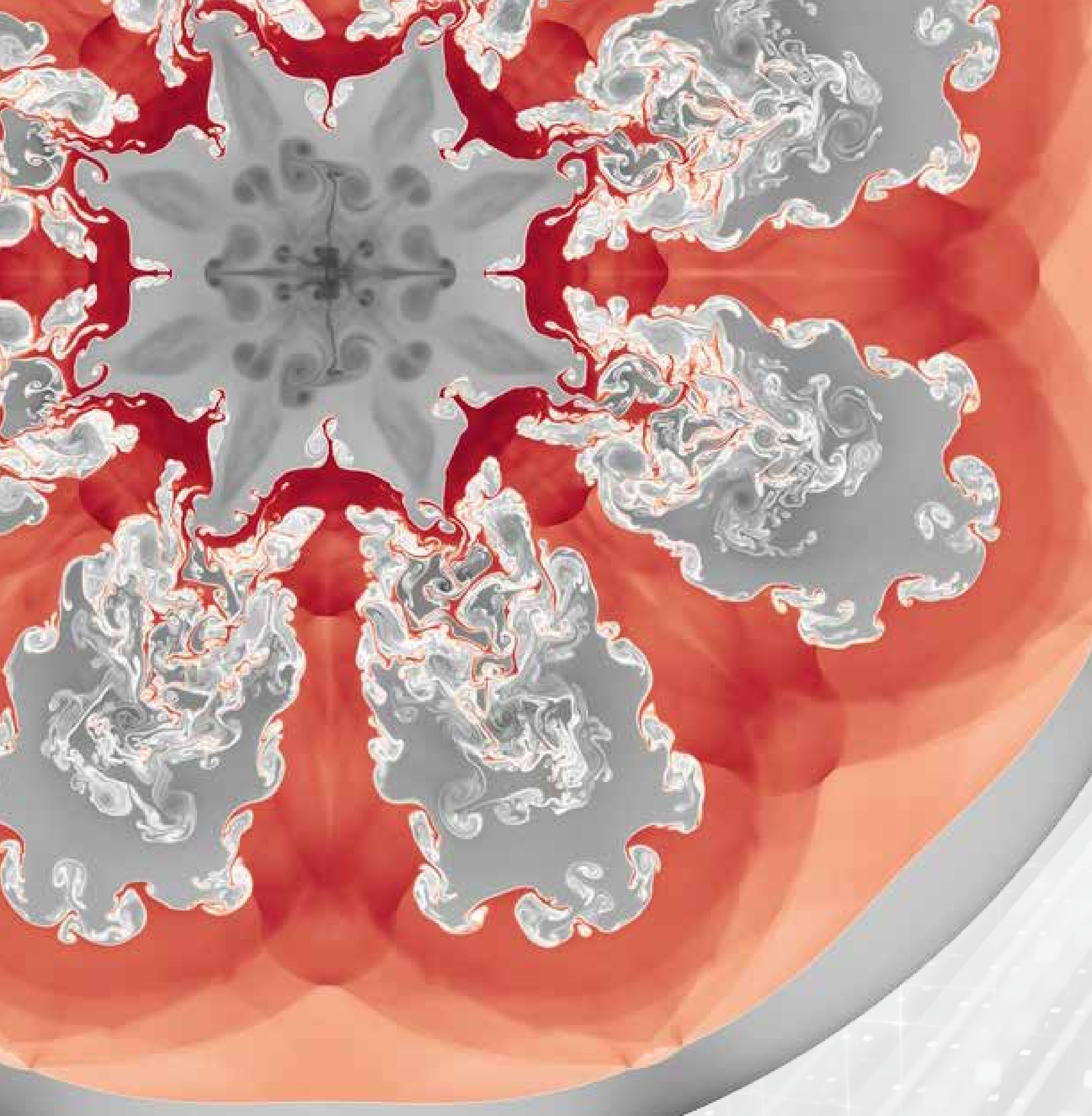
Despite the enormous power of today's supercomputers, we continue to demand even more capable machines to predict, with the requisite confidence, the behavior of complex physical systems. LDRD researchers are looking ahead to when the first exascale supercomputer arrives at Livermore. Exascale machines are expected to contain an estimated one billion processing elements (compared to today's several million), making them capable of performing a quintillion (10^{18}) floating-point operations per second.

Extreme-scale (exascale and higher) systems architecture will entail a significant departure from present-day hardware, and the methods and tools we use will have to change dramatically to exploit these systems' capabilities. In many ways, extreme-scale computing requires that we rethink our current algorithms, simulation codes, and many other aspects of supercomputing. To the extent possible, advanced computer architectures must be co-designed with software experts. Lawrence Livermore is one of only a handful of institutions worldwide with expertise in vertical integration that enables this co-design process—from understanding and developing leading-edge hardware to implementing multiphysics applications and data-science analytics.

The article begining on p. 4 describes how we are focusing some of our LDRD investments on addressing longer term research and development for extreme-scale computing. Six current LDRD-funded research projects are described. These projects involve ways to reduce, monitor, and manage power consumption; make systems more resilient to hardware and software faults and failures; lessen the required communication between hardware components; and create advanced algorithms that solve computing steps in parallel rather than in sequence for faster results. In addition, new algorithms are being developed for producing better quality simulations of shock hydrodynamics and first-principles molecular dynamics simulations that encompass far more atoms. Together, these efforts help Livermore simulation codes to efficiently utilize exascale and potentially other extreme-scale computers.

World-class HPC attracts new talent to Livermore and is a foundation upon which we continue to build new programs to meet national security challenges. When the Laboratory receives its first exascale machine, we are confident that our early LDRD investments in extreme-scale computing will have helped develop the requisite computational tools to ensure these machines meet their enormous potential for advancing national security and keeping Livermore at the forefront of HPC.

■ Rokaya Al-Ayat manages the Laboratory Directed Research and Development Program.



The BLAST code accurately simulates the interactions between multiple materials in a high-order Arbitrary Lagrangian–Eulerian (ALE) hydrodynamics calculation. Shown here is the image of this simulation, which was recently featured as part of an "Art of Science" exhibit at the City of Livermore's public library.

Laying the Groundwork for EXTREME-SCALE COMPUTING

Hardware, software, and code innovations are helping overcome the power and reliability challenges of next-generation supercomputers.

To tackle many outstanding scientific and engineering challenges such as climate, energy, biosecurity, and stockpile stewardship, users need faster, massively parallel computer systems that can perform billions or trillions of calculations concurrently, access and process vast amounts of data efficiently, and run ensembles of simulations for assessing uncertainties in results. Making the transition from today's petaflop (10^{15} floating-point operations per second) systems to future exaflop (10^{18} floating-point operations per second) systems will require new computer hardware, software, and scientific codes. (See *S&TR*, March 2015, pp. 11–15.) These changes are needed to efficiently use machines with increasingly complex computer architectures, minimize power consumption, and ensure reliability.

As machines become larger and more elaborate, the need for power also grows. "We could build an exascale machine now, but it would take 100 megawatts to run it," notes Lori Diachin, manager of the Computation Directorate's project portfolio that is funded by the Laboratory Directed Research and Development (LDRD) Program. An extreme-scale—exascale or greater—system will likely contain far more processing elements than the largest present-day machines—an estimated 70–100 million cores. These elements will operate at fairly low speeds, which saves energy but increases the likelihood of performance issues, such as those related to hardware failures. (Essentially, more components increase the odds that a component will fail.) In addition, programmers seeking speed boosts must redesign their codes and algorithms to complete more tasks in parallel, maintain accuracy, and accommodate the growing number of processing elements.

The Department of Energy (DOE) has launched an ambitious effort to prepare for U.S. exascale computing within the next decade by helping to solve these complex and interrelated hardware and software challenges. As a DOE laboratory that is home to an esteemed high-performance computing (HPC) program, Lawrence Livermore is contributing to many areas of exascale research through its Advanced Simulation and Computing (ASC) Program, the DOE Office of Science's HPC programs and initiatives, as well as various LDRD-funded projects. Diachin observes, "HPC as a whole is facing a fundamental architectural shift, and these changes create a lot of uncertainty. We are using LDRD investments to explore options, develop solutions, and in some instances direct the future of computing." This article highlights six LDRD-funded research projects designed to lay groundwork for exascale computing and potential subsequent scientific breakthroughs.

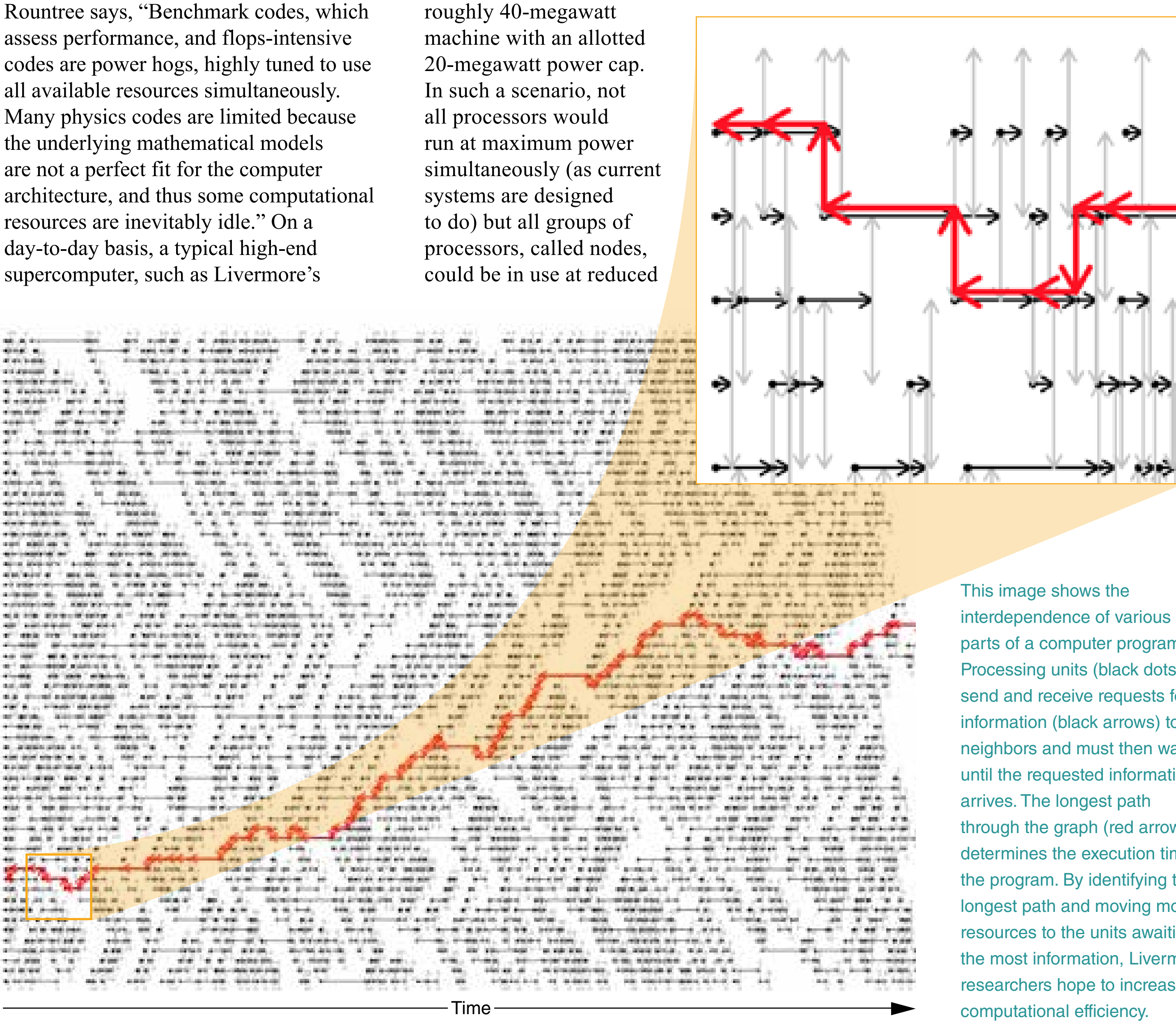
A Supercomputing Power Boost

DOE's target for exascale machine power is 20 megawatts or less—a number aimed at balancing operating costs with computing performance gains. To help achieve this goal, application developers and hardware experts are exploring ways to reduce data movement, a process that is projected to dominate the power demands of future systems. In addition, software developers are looking at new methods for monitoring and managing power.

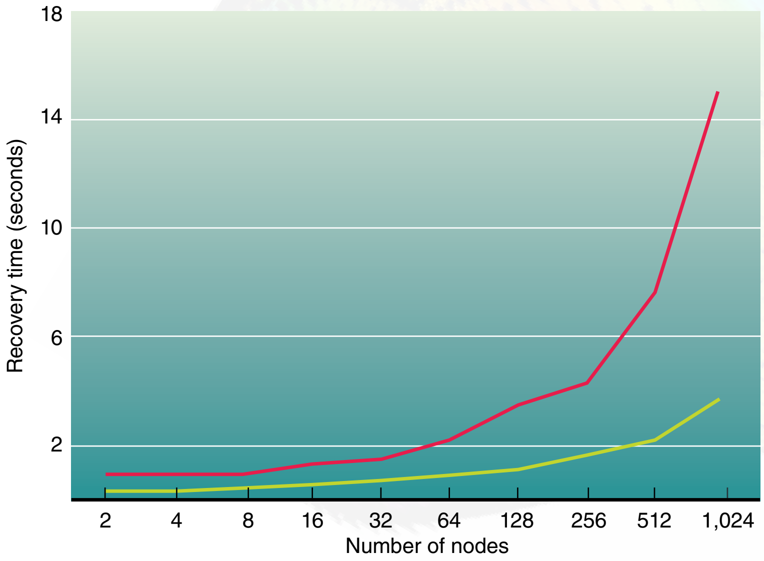
A supercomputer's flops rating represents a calculation speed (and level of capability) that the system only rarely achieves. Computer scientist Barry Rountree says, "Benchmark codes, which assess performance, and flops-intensive codes are power hogs, highly tuned to use all available resources simultaneously. Many physics codes are limited because the underlying mathematical models are not a perfect fit for the computer architecture, and thus some computational resources are inevitably idle." On a day-to-day basis, a typical high-end supercomputer, such as Livermore's Vulcan machine, uses 60 percent of its peak power.

Entirely rewriting all of Livermore's large and complex scientific codes to run more like flops-intensive ones, which complete calculations faster, is unfeasible or even impossible, according to Rountree. He and his team instead propose designing an exascale supercomputer that uses the maximum power allotment for any code it is running by overprovisioning the hardware—for example, by building a roughly 40-megawatt machine with an allotted 20-megawatt power cap. In such a scenario, not all processors would run at maximum power simultaneously (as current systems are designed to do) but all groups of processors, called nodes, could be in use at reduced power levels. Initial modeling and tests have indicated that overprovisioning can improve—even double—application performance.

Rountree's LDRD is focused on fundamental research for developing the system software to make overprovisioning practical. "The goal is not to save power—it's to use all the available power all the time," he explains. "We're looking at power as a schedulable resource. We would like to control power usage between nodes,



This image shows the interdependence of various parts of a computer program. Processing units (black dots) send and receive requests for information (black arrows) to their neighbors and must then wait idle until the requested information arrives. The longest path through the graph (red arrows) determines the execution time of the program. By identifying the longest path and moving more resources to the units awaiting the most information, Livermore researchers hope to increase computational efficiency.



Livermore computer scientists have designed and implemented Reinit, a novel backward recovery approach, to handle certain hardware failures. As indicated by recovery time measurements for failures in Livermore's Sierra machine, Reinit (green line) allows high-performance computing applications to recover up to four times faster than with traditional job restarts (red line).

within nodes, within the whole machine, and between jobs."

The team has developed and validated a model that predicts application-execution time for a given hardware configuration, accounting for factors such as the number of processors and nodes running, how tasks are divided up and completed within the processors, and how power is distributed to processors and memory. Livermore is considering this model for future one-of-a-kind, leading-edge systems.

Based on their findings thus far, the team has created two systems software tools for helping users set processor power caps and measure and monitor various power and performance indicators. These tools have been incorporated into cluster software at all three of the National Nuclear Security Administration's (NNSA's) laboratories. Next, Rountree's team will focus on how to dynamically identify and redistribute power to the slowest pieces of a calculation, which will further enhance performance.

Faster Failure Recovery

Hardware problems—referred to as faults and failures—are expected to occur more frequently in exascale systems than in petascale machines, primarily because of the new systems' greater number of processors and larger amounts of memory. (See *S&TR*, June 2012, pp. 13–15.) "Right now, our systems experience failures about once every two days. With exascale systems, failures could be as frequent as once every few hours," says computer scientist Ignacio Laguna. Ensuring that exascale systems are resilient—that hardware, software, and codes continue to function as they should despite frequent interruptions—will require a combination of hardware improvements and changes to how applications address errors and failures.

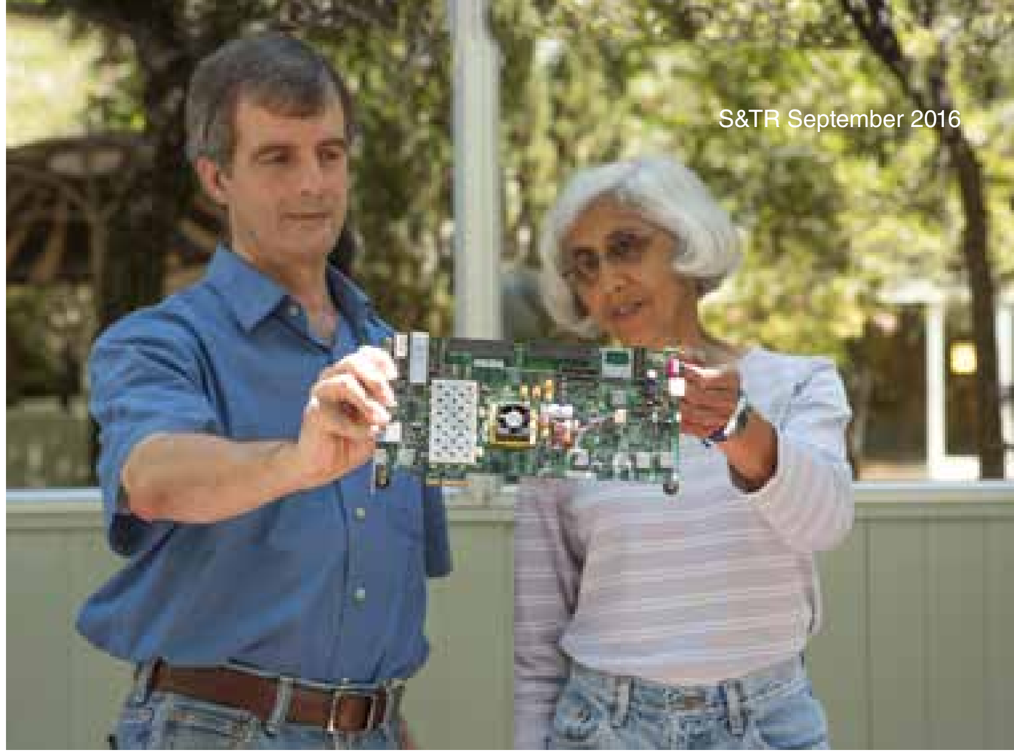
Failures are typically resolved through "backward" recovery approaches. Using this technique, a system is returned to the last checkpoint at which the data were saved and restarted from there, a process that wastes time and resources. "We want to recover from failures faster and to do so with fewer changes to the code," explains Laguna. He is leading an LDRD project to create simplified models, called programming abstractions, which allow developers to evaluate the complexity, performance, reliability, and applicability of various failure-recovery methods. The goal is to aid developers in identifying the best programming methods for meeting their recovery and performance goals.

Laguna and his team have used the Livermore-developed domain decomposition molecular dynamics code (ddcMD) to explore two types of abstractions—a backward recovery approach and a forward technique that allows the system to move ahead with a calculation using healthy, unaffected nodes. Forward recovery eliminates the need for a restart but results in a small piece of the calculation being lost, affecting accuracy. Reinit, the Livermore team's new backward approach, is an improvement when compared to existing recovery schemes. Reinit was more effective than forward recovery methods because of its easy implementation, efficiency, and broad applicability.

Laguna observes, "With HPC, speed is the measure people talk about, but productivity also matters. The time it takes to write a program is just as important as the time it takes to run it." His team will continue to explore various recovery programming models, not just forward and backward approaches. In time, they aspire to have their approaches recognized and adopted within the developer community for the message-passing interface (MPI). Used by academia, government, and industry alike, MPI is the most popular programming model for large-scale HPC.

Memory Reduces Data

Component costs and power constraints are driving a trend toward chips with more processors and correspondingly less on-chip, cache memory. Reduced local memory requires operations to fetch data from other locations to complete their calculations. The result is longer data-access times and increased stress on memory bandwidth, both of which affect code performance. Computer scientist Scott Lloyd notes, "Many



Computer scientists (from left) Scott Lloyd and Maya Gokhale inspect a memory unit emulator on a circuit board. (Photo by Lanie L. Rivera.)

newer applications have unstructured and irregular data-access patterns or other complex memory demands. These programs are much more sensitive to data-access time.” Given the far greater number of processors expected in exascale systems, without technology innovations, this memory dilemma could become a memory nightmare.

Lloyd and colleague Maya Gokhale have been exploring opportunities for reducing data movement using relatively new three-dimensional (3D) memory packaging technology, such as the Hybrid Memory Cube. These 3D units, which comprise a stack of memory layers and a basic logic layer, offer orders-of-magnitude greater bandwidth and shorter access times than is available off-chip. Additional computing functionality can be introduced on the logic layer to process data within the memory package. Gokhale and Lloyd have developed a novel method to dynamically order data to suit a code’s needs using a data rearrangement engine (DRE) in the logic layer. DRE reorganizes and filters data into local scratchpad memory—a temporary, high-speed internal memory—for use by the code. Gokhale explains, “Often, the computer fetches a whole column or row of data from memory when only part of it is needed. With a scratchpad, we can dynamically change how the data are presented for the processor.” After substantial DRE tuning and testing, the researchers demonstrated bandwidth savings, energy reductions, and up to four times faster performance, with the best performance occurring in applications featuring irregular memory-access patterns.

In-memory computing and 3D memory units are of growing interest to the HPC community. For instance, through DOE’s FastForward-2 Program, an initiative designed to accelerate the development of technologies critical to extreme-scale computing, the Livermore researchers have partnered with several vendors to explore DRE applications.

Multiple Timelines, Faster Solutions

Even though the exact architecture for exascale computers is not yet known, Livermore computational experts are preparing scientific applications, and the algorithms anchoring these codes, to run on prospective machines. As part of this effort, they are developing algorithms that account for known architectural trends such as reducing data movement and allowing for many more actions to happen in parallel, or simultaneously. The latter is particularly critical because future speedups for applications will likely happen only through greater parallelism.

Computer simulations often rely on solving time-dependent problems, such as the evolution of a supernova, the propagation of seismic waves, or the metabolism of pharmaceuticals in the human body. Until now, most solutions to these problems have addressed time steps sequentially, but this traditional time-stepping process scales up poorly on very large machines. Computational mathematicians Rob Falgout, Jacob Schroder, and their colleagues have developed a method for solving all of the time steps simultaneously with the help of a new code called XBraid—an approach that has dramatically decreased solution time for various simulations by as much as 49 times. XBraid eliminates the need for a complete code rewrite, which could be an enormous time investment. Schroder observes, “Unlike other parallel-in-time approaches, XBraid is largely nonintrusive and has a conceptually simple interface.”

The parallel-in-time approach offers a fundamentally new way to run simulations. The XBraid multigrid solver first “guesses” a solution to the problem and then uses an algorithm to generate an improved guess. This procedure repeats until the iterations converge to the final solution. The iterative process is accelerated by feeding solutions from coarser (and less computationally expensive) versions of the same problem into finer scale versions. Since the computational cost is proportional to the number of equations, a large problem can be solved in the same time as a smaller one simply by increasing the number of processors working on the calculation. Importantly, solutions from XBraid and sequential time stepping are identical, up to a user-defined tolerance.

In addition to helping researchers perform calculations more quickly, XBraid also better exploits the processing capabilities of HPC systems. "Exascale computers will be even more massively parallel than Sequoia—Livermore's 20 petaflop, 1.5-million processor flagship supercomputer," says Schroder. "We need our algorithms to make the best use of that level of parallelism."

The XBraid team is now refining and optimizing their algorithm for a range of problem types. Recent applications have included power-grid simulations and various fluid-dynamics calculations. In the future, the team will make XBraid compatible with more of the Laboratory's physics codes by exploring enhancements, such as on-the-fly refinement of spatial and temporal resolution, a significant technical challenge.

Framework Offers Greater Efficiency

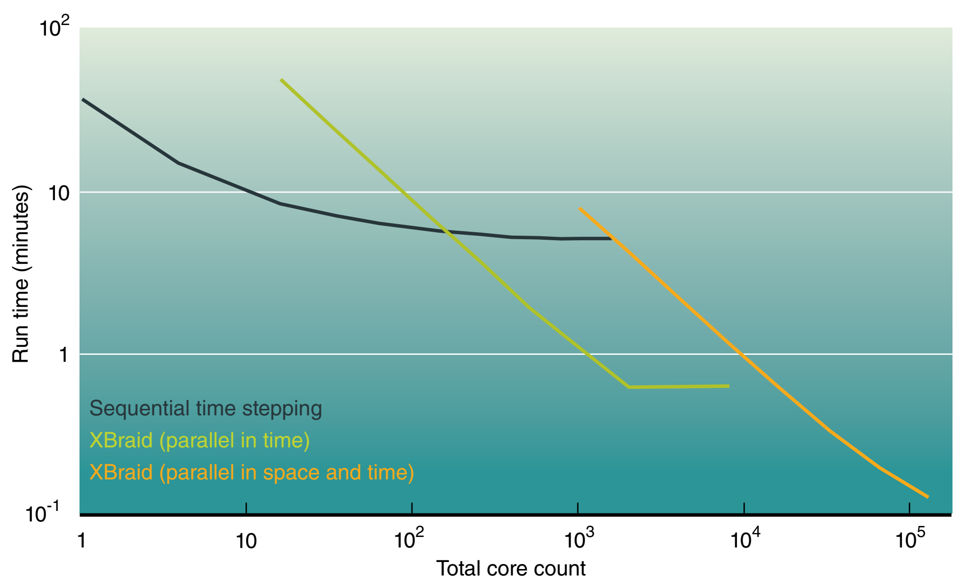
At the National Ignition Facility, researchers who study the complex shock wave interactions occurring within high-pressure experiments have found that standard low-order finite difference simulation techniques sometimes fail to satisfactorily represent material behavior under experimental conditions, particularly at material interfaces. A series of LDRD projects conducted by a team of computational mathematicians, physicists, and computer scientists led by applied mathematician Tzanio Kolev aims to remedy this issue and achieve higher fidelity simulations of shock hydrodynamics by developing more advanced numerical algorithms.

Kolev and colleagues have created a new, high-order arbitrary Lagrangian–Eulerian (ALE) framework. Standard low-order ALE methods are based on approximating the solution to a complex equation by breaking down the problem into many smaller parts (elements) along an unstructured grid, or mesh. The team's high-order ALE framework uses elements with more control points within the mesh, allowing them to curve element boundaries and the geometry inside them. "This approach helps us more accurately follow the material flow," explains Kolev. In addition, high-order methods spend less time moving data and more time crunching numbers than their lower-order counterparts, which helps offset the growing cost of data movement and enables faster calculations.

Over the past few years, the team has successfully demonstrated that the high-order ALE framework can produce accurate and robust simulations of various shock hydrodynamics problems through the method's implementation in the Livermore-developed BLAST code. The team recently incorporated a new remapping algorithm into the framework, allowing BLAST to simulate larger time steps and to more accurately model multiple materials within one element.

During a simulation, the shape of the elements in the mesh follows the movement of the simulated material, but sometimes the elements insufficiently conform to a physics field and the mesh distorts. For those portions of the calculation, the remapping algorithm "stops time" for the affected function while the mesh evolves. Once the field has been translated, along with the rest of the problem, to a more compatible mesh, the calculation continues from the point where it left off. When the mesh changes, multiple materials can be contained within the same element—a mathematically challenging situation that the BLAST team has successfully resolved, demonstrating a mix of materials can be captured at a very detailed level.

Overall, the remapping algorithm has demonstrated excellent parallel scalability, geometric flexibility, and accuracy on several model problems and single- and multiple-material ALE simulations. One of the most demanding calculations to date was a 3D BLAST simulation involving



Most solutions to time-dependent problems have addressed time steps sequentially, one at a time. The XBraid code, a parallel-in-time approach, solves all the time steps simultaneously. In this heat equation example, XBraid allows the calculation to progress up to 49 times faster.

three materials performed on 16,000 cores of Vulcan.

The team is now applying high-order solution methods to other types of physics components required for realistic multiphysics simulations, beginning with radiation diffusion. Interest in high-order methods is growing, thanks in part to the LDRD initiatives, spurring Kolev and his colleagues to propose creating a DOE high-order co-design center at Lawrence Livermore to foster greater collaboration between computer hardware, code, and algorithm developers. “To enable the high-order applications of tomorrow,” he notes, “we have to ensure that we have the hardware to make these applications run well.”

First-Principles Scaled Up

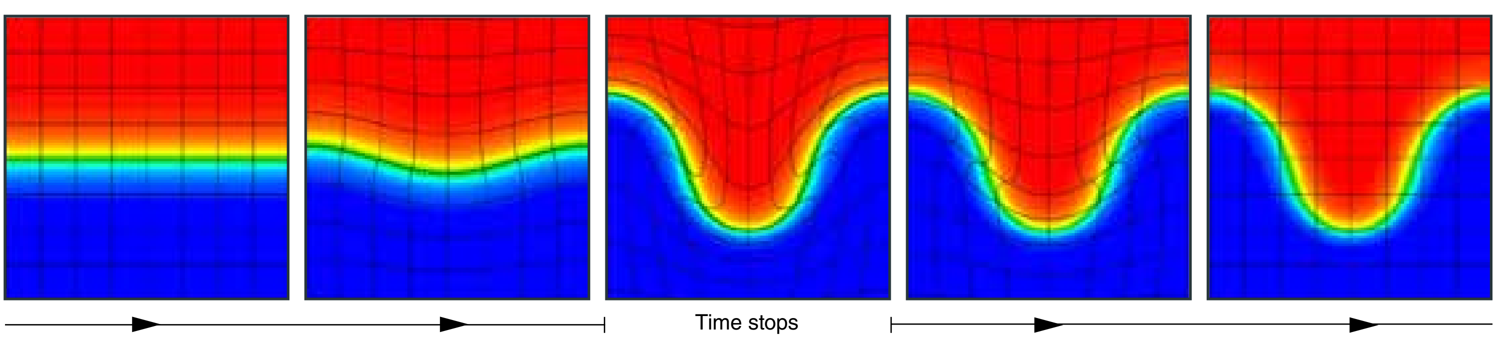
Biologists, chemists, and physicists use first-principles molecular dynamics (FPMD) codes to calculate properties of materials and molecules. These codes are based on quantum mechanics modeling, which is computationally demanding because it calculates many interactions for every atom in the problem and requires intensive communication between processors and memory. With traditional algorithms, simulation size is limited to a few hundred atoms, which is much too small for simulating complex systems or realistic materials. “The problem with FPMD methods,” explains computational mathematician Jean-Luc Fattebert, “is that the cost of computing goes up faster than the size of the physical problem. Many elements of these computations are proportional to the square or cube of the system size. Given the same run time, a ten-times bigger computer will only let us solve a problem possibly twice as big.”

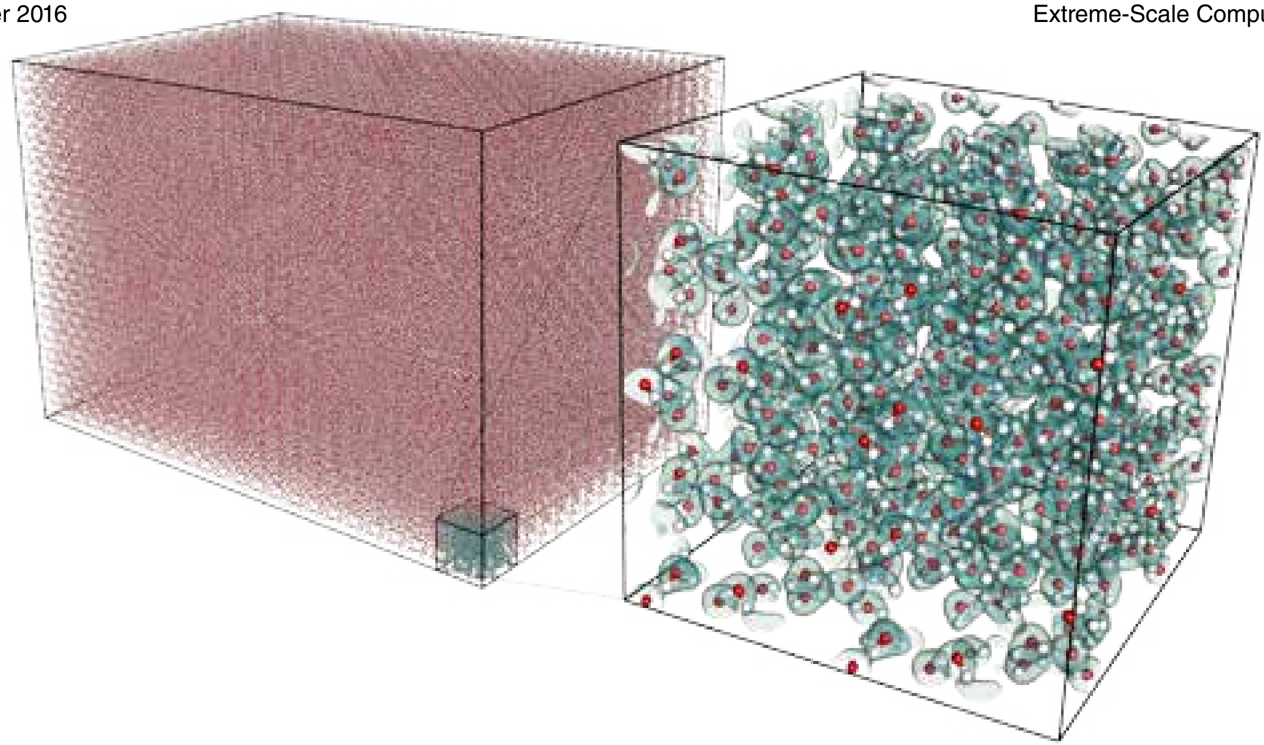
Livermore researchers, led by Fattebert, are developing new algorithms with reduced complexity and better parallel scaling to efficiently use the largest supercomputers available now and in the future to run FPMD simulations with many thousands or even millions of atoms. With these algorithms, the number of atoms that can be simulated is directly proportional to the number of processors required. The method represents only the interactions between an atom’s electrons and a certain (and adjustable) number of its neighbors. In a large system, interaction across wide distances is less significant than between nearby electrons and can be safely neglected. With this approach, the number of atoms and the complexity of the systems that can be simulated go up dramatically.

The team has demonstrated excellent scaling using the novel algorithm and an accompanying new FPMD code called MGmol. For example, simulating the motion of 1,200,000 atoms for 98 time steps on roughly 1,500,000 processors of the Sequoia machine took less than 3 hours. If the team were to solve the same problem using traditional algorithms and the same number of processors, the problem would take about two years to solve and require a computer with far more memory than any currently available. This advancement earned Fattebert and his team a 2016 Gordon Bell Prize finalist spot for outstanding achievement in high-performance computing.

However, notes Fattebert, “It is one thing to show that we scale, but we also have to show that we are not sacrificing accuracy,” as has occurred in many previous attempts to speed up FPMD calculations. Fortunately, validations of their solutions for nonmetallic systems, used for studying problems such as the dilute solutions in energy-storage devices, are progressing well. For instance, when calculating a problem involving 512 water molecules, both MGmol and Livermore FPMD code QBox, which uses more traditional algorithms, produced virtually identical results. The researchers have also recently begun developing similar methods for simulating metallic systems—a more challenging problem because fewer electron interactions can be ignored,

When the shape of grid elements in a simulation insufficiently conforms to a physics field, the BLAST remapping algorithm “stops time” (center) and institutes a remap phase, wherein the field stays the same while the mesh evolves. The field, along with the rest of the problem, is then translated to a new mesh, and the simulation is restarted from where it left off.





Livermore's MGmol code and a novel algorithm made possible a massive first-principles molecular dynamics simulation involving 1,179,648 atoms (393,216 water molecules). The simulation was performed on Livermore's Sequoia machine using 1,572,864 processors. The inset, showing a small subset of the simulation, illustrates the challenge of representing all the atoms accurately. This simulation would not be feasible using traditional algorithms. (Image courtesy of Liam Krauss.)

making computational cost reductions more difficult to achieve.

In the realm of metals, very large and accurate simulations will help researchers create better alloys. At low concentrations in particular, the percentage contribution of a given component can dramatically change an alloy's physical properties. Fattebert is also looking down the road to the next algorithmic and computational challenge: lengthening the duration of simulations to enable studies of slower processes, or a longer stretch of a specific process, thereby making FPMD a practical solution for more researchers, including biologists.

Beyond Exacale

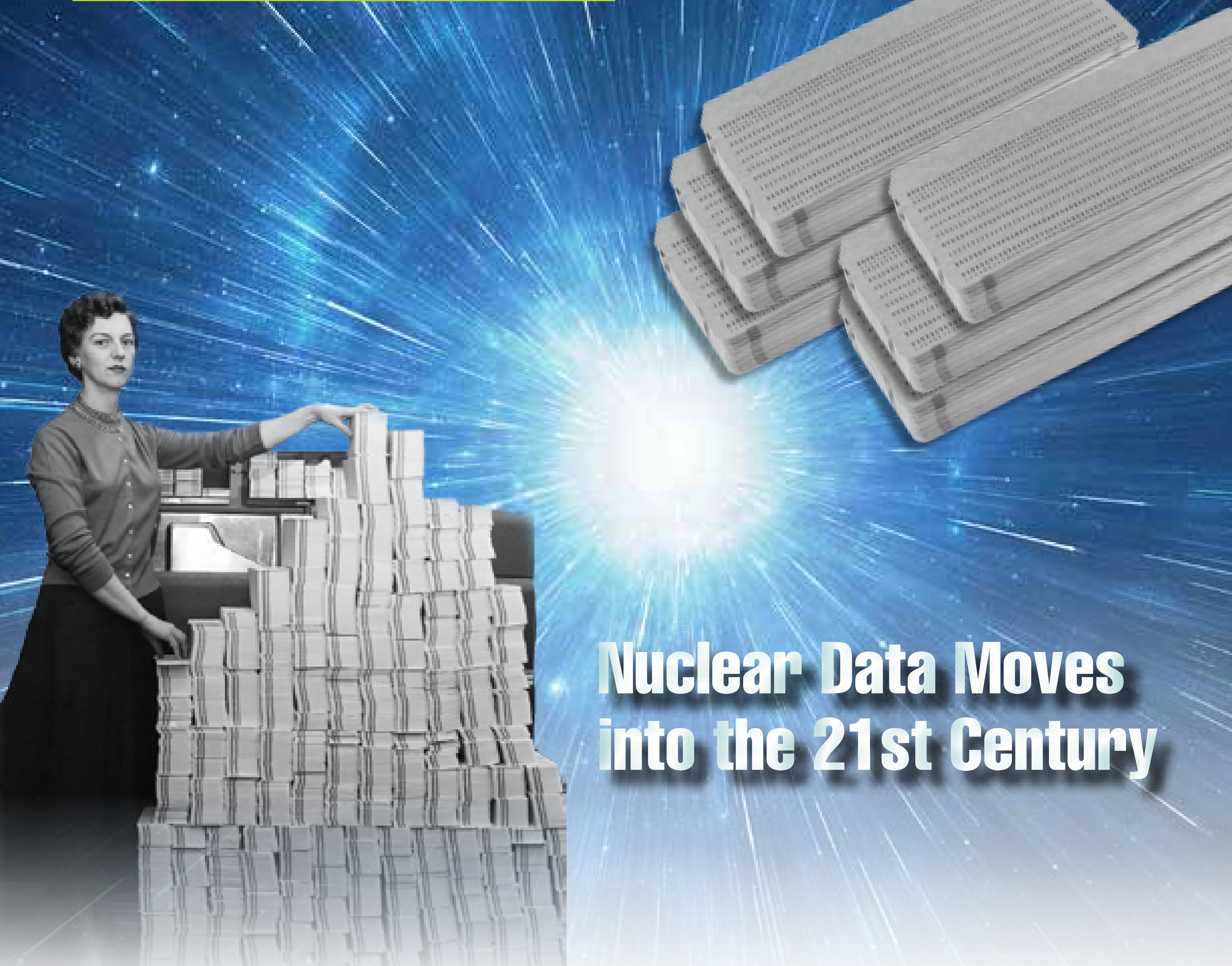
Exascale is the crucial next step in the evolution of HPC, but it is far from the final one. Livermore researchers have already begun planning for more radical shifts in computing. "The Laboratory is making 'beyond Moore's Law' investments," says Diachin. "At some point, we cannot get more speed by making transistors smaller and putting more on a chip, as there's a physical limit to the technology. The question is, what will architectures look like when these limits are reached?"

One such investment by the ASC Program supports research on neuromorphic, or brain-inspired, computing systems that can perform tasks such as pattern recognition and image processing more efficiently than standard computers. (See *S&TR*, June 2016, pp. 16–19.) The Laboratory acquired its first neuromorphic platform from IBM in March 2016. (See *S&TR,* September 2016, p. 2.) Also, several LDRD projects have been exploring how to make quantum computing practical. This type of computing exploits the laws of quantum mechanics to complete tasks, in some instances far more quickly than standard computers. Bringing these and other exotic computing concepts to fruition will take patience, creativity, collaboration, and dedication—characteristics Livermore researchers have already abundantly demonstrated in their efforts to build a foundation for exascale computing.

—Rose Hansen

Key Words: Advanced Simulation and Computing (ASC) Program, algorithm, arbitrary Lagrangian–Eulerian (ALE), BLAST code, data rearrangement engine (DRE), domain decomposition molecular dynamics (ddcMD) code, exascale, extreme-scale computing, FastForward-2 Program, first-principles molecular dynamics (FPMD), floating-point operations per second (flops), Laboratory Directed Research and Development (LDRD) Program, Message-Passing Interface (MPI), MGmol code, neuromorphic computing, programming abstraction, QBox code, quantum computing, Reinit code, Sequoia, Sierra, three-dimensional (3D) memory, Vulcan, XBraid code.

For further information contact Lori Diachin (925) 422-7130 (diachin2@llnl.gov).



Nuclear Data Moves into the 21st Century

WHEN atomic nuclei collide with other nuclei or subatomic particles, a large number of reactions can occur, resulting in many possible products. High-quality data describing these nuclear reactions are essential for many important scientific, engineering, and commercial applications. These applications include nuclear reactor design and safety, radioactive waste disposal, stockpile stewardship of nuclear weapons, medical radioisotope therapy and diagnostics, fusion energy experiments, astrophysics, nuclear forensics, and more. At Lawrence Livermore, accurate and complete nuclear data are critical for both theoretical and experimental research.

Despite the importance of nuclear data to so many fields, the format for storing, evaluating, and using these data goes back to the 1960s, when computing was based on 80-column punch cards—small, stiff sheets of paper that contain information represented by the presence or absence of holes in predefined positions. As a result, existing formats, principally Livermore's Evaluated Nuclear Data Library (ENDL) and the widely adopted Evaluated Nuclear Data Format (currently in version 6, or ENDF-6) are badly outdated. In response to the long-recognized need for modernization, the Nuclear Data and Theory group at Lawrence Livermore has developed a far more capable and flexible format called Generalized Nuclear Data (GND), which takes advantage of many recent advances in computer technology. GND is readable by both computers and humans, flexible, and extensible for supporting new types of nuclear data.

Livermore physicist Bret Beck, who leads the group responsible for the update, explains that the nuclear data tables in either the ENDL or ENDF-6 format describe the probabilities of various complex physical interactions, for example, the collision of neutrons with nuclei. Nuclear databases include physical quantities such as energy spectra, scattering cross sections, nuclear structure, nuclear decay, and angular distributions of the reaction products, together with estimates of uncertainties. ENDL alone includes all stable isotopes and many unstable isotopes for every element in the periodic table up to californium.

To be accepted into nuclear data libraries, scientists must first conduct formal evaluations of the data to ensure they are complete. Evaluations define data over a broad range of energies (usually 10^{-11} to 20 megaelectronvolts for incident neutrons), even when no measured data exist. Many nuclear decay mechanisms remain poorly understood because some of their products, namely neutrons and neutrinos, are difficult to track. Also, nuclear reactions involving short-lived nuclei are difficult to measure. Nevertheless, evaluators must do their best to combine experimental data with nuclear models to extend or interpolate the available information for incorporation into the data libraries. Without these formal evaluations, nuclear simulations and calculations would be impossible or unreliable.

Evaluation work is done under the auspices of national and international agencies, including the Cross-Section Evaluation Working Group, which controls the United States' ENDF/B data library and the ENDF-6 format. Its work is coordinated through the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory. Although the Japanese and European nuclear communities have adopted ENDF-6 for their own nuclear data libraries, each has its own organization for using nuclear data, reviewing and performing evaluations, and testing results.

Origins Date to the 1960s

Lawrence Livermore's first adopted nuclear database format, ENDL, was originally developed at the United Kingdom's Atomic Weapons Establishment in the early 1960s for storing and exchanging evaluated nuclear data. ENDF was created a few years later under the purview of a U.S. national committee that included representatives from Lawrence Livermore. "Some people wanted

The Evaluated Nuclear Data Format (ENDF) and Evaluated Nuclear Data Library (ENDL) are strongly influenced by their 1960s origins. Livermore researchers are working to modernize the way nuclear data are stored, evaluated, and used by eliminating the (left) punch-card-based format and developing one with (right) a hierarchical structure and nesting capability.

increased flexibility to store information in more complicated formats," says Livermore physicist Dennis McNabb, who has played a large role in GND's development.

In the last decade, scientists worldwide recognized that both ENDF-6 and ENDL formats had serious limitations and were showing signs of age. "The formats have been stretched way beyond their 1960s-era origins," says Livermore physicist and team member Caleb Mattoon. Both formats were designed to store data on 80-column punch cards. ENDF-6 and ENDL are designed to compactly fill the space on punch cards at the expense of human readability and, in the case of ENDF-6, numerical precision. (Fourteen characters in each line of ENDF-6 cards are reserved for identifiers to indicate the card's order.) Data are often repeated, which can lead to possible internal discrepancies. Also, neither format can accommodate all types of reactions. For example, they can store values of the energy distribution of all neutrons emitted from a reaction but cannot handle information for reactions where the neutron energy distribution depends on the number of neutrons emitted. The obfuscated formats can sometimes contain small errors that go undiscovered for decades.

"People complained for years about ENDL and ENDF, but they were heavily invested in them," says team member David Brown, who currently works at NNDC. "We went to great lengths to make square pegs fit into round holes, to make data fit the existing structure. At some point the process became unbearable, and we realized we needed a modern replacement." Furthermore, a new generation of nuclear scientists and engineers must overcome a steep learning curve on how data are stored in the legacy formats before they can use the data for experiments and simulations. Mattoon says, "Younger researchers want to adopt more modern software concepts than the 1960s-vintage formats. We don't want artificial barriers to growing the number of data evaluators."

Livermore physicists began formally developing GND in 2009 with internal funding from the Weapons and Complex Integration Principal Directorate and additional support from the American Recovery and Reinvestment Act. The developers focused on reducing data redundancies, updating the data structure hierarchy of GND to reflect current understanding of nuclear reactions and radioactive decay, and making it user friendly. For example, "GND's hierarchical structure and data nesting capability represents a significant advancement," says Beck. "It reflects how physicists think about nuclear reactions experimentally and theoretically, and also how data are used in nuclear transport codes."

Listening to the Community

Early versions of GND were presented to the national and international nuclear data communities for feedback. This effort resulted in the formation of Subgroup 38, an international collaboration led by the GND team at Livermore, to oversee development of a modern nuclear data structure that will capture the current and future needs of the nuclear data community. Brown says, "GND represents a revolution in nuclear data, but it has not been a fast process. We've been working at it for 11 years

At a Subgroup 38 meeting in Tokai, Japan in 2013, two meeting participants, (left) Bret Beck from Livermore's Generalized Nuclear Data (GND) team and Morgan White from Los Alamos National Laboratory, frequently held different opinions. During a tour of the Japan Accelerator Research Complex, the two overcame their differences and put their heads together, literally.

because we've deliberately taken a consensus-driven approach." The team expects that GND will be formally adopted as the new international standard by the end of 2017.

"We need to assure a smooth transition to GND," says Mattoon. The team recognizes that GND must fit the existing nuclear data infrastructure by supporting backwards compatibility with ENDF-6 and ENDL for as long as 10 years. This compatibility will enable benchmarking and testing data and tools using the new structures against legacy results. A potential obstacle to early and widespread adoption of GND is the large number of legacy codes that only read ENDF-6 or ENDL-formatted nuclear data. As a result, Livermore physicists have developed Fudge, a "translator" code that processes nuclear data in multiple formats. The team is optimistic that GND will prompt researchers to update legacy codes, some of which were written in the 1960s and 1970s, so that they can also handle GND.

The new GND format is designed to support not only the traditional nuclear application areas of fission reactors, nuclear waste handling, criticality safety, and defense, but also emerging areas in nonproliferation, research accelerators, and uncertainty quantification. Other applications are certain to appear, and the Livermore team is confident GND will accommodate them. Beck also anticipates that GND will attract new people to the nuclear data community who prefer working with modern computational tools. In that respect, GND should open the field of nuclear data to a broader group of developers and users.

—Arnie Heller

Key Words: Atomic Weapons Establishment, Evaluated Nuclear Data Format (ENDF), Evaluated Nuclear Data Library (ENDL), Generalized Nuclear Data (GND), National Nuclear Data Center (NNDC), neutrons, nuclear data, punch card.

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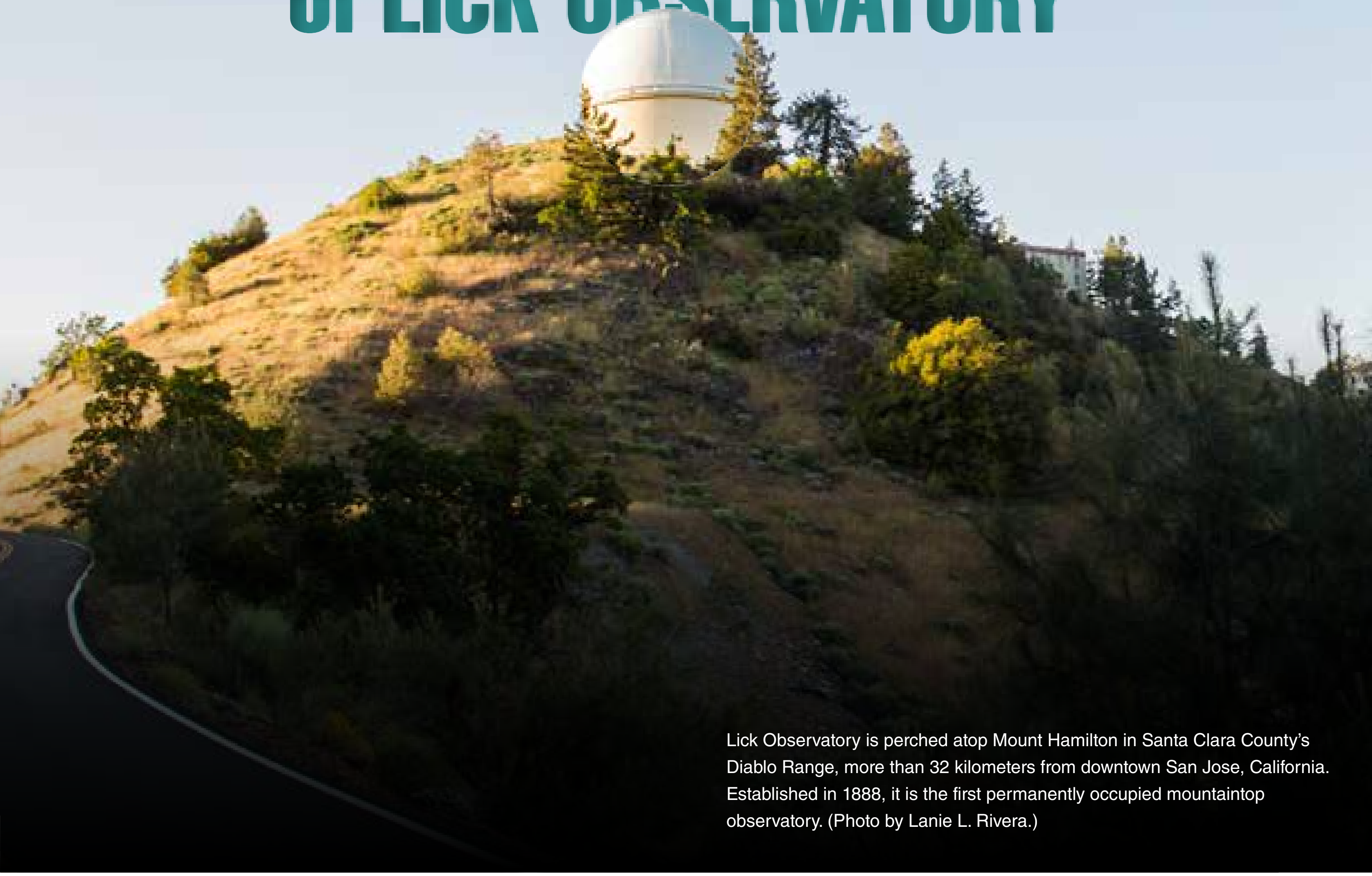
Peering into the FUTURE of LICK OBSERVATORY



Lick Observatory is perched atop Mount Hamilton in Santa Clara County's Diablo Range, more than 32 kilometers from downtown San Jose, California. Established in 1888, it is the first permanently occupied mountaintop observatory. (Photo by Lanie L. Rivera.)

SINCE 1888, the University of California's (UC's) Lick Observatory—built on the summit of Mount Hamilton near San Jose, California—has been the site of important astronomical breakthroughs. Notable contributions include the discovery of numerous extrasolar planets around other stars and measuring the redshift of distant supernovae to understand the universe's accelerating expansion. In addition to Lick's research mission, the observatory serves as a training ground for young scientists and as UC's main test bed for developing new instruments and technologies for optical astronomy—for instance, the novel adaptive-optics-based laser guide star, which was created with help from Livermore scientists. (See *S&TR*, June 2002, pp. 12–19.) Approximately 35,000 adults and children visit Mount Hamilton every year to participate in education and outreach programs.

In 2013, UC's future funding for Lick, the world's first modern mountaintop observatory, came into question. To support decision makers during that time, the UC Office of the President

(UCOP) and UC Observatories (UCO) investigated the cost of different operating options for Lick's facilities. As part of this effort, UC's provost and UC at Santa Cruz professor Sandra Faber (then the Interim Director of UCO) turned to Lawrence Livermore scientists who were experts at enterprise modeling—a tool for projecting how funding influences the future health of an organization's infrastructure, assets, and resources over time.

The Laboratory's weapons program had pioneered an enterprise modeling tool to support funding decisions for the National Nuclear Security Administration (NNSA) and Lawrence Livermore. (See *S&TR*, October/November 2013, pp. 19–22.) Armed with this tool, the Livermore–UCO team, led by Laboratory physicist Cliff Shang, created the first-ever, time-dependent lifecycle model of an observatory. The model considered the effects of different funding levels on Lick's operations given the condition of the on-site facilities and helped inform UC's decision on future funding for the observatory's services.

Every Last Detail

While considering options for Lick's future, decision makers had to comply with the terms of the original 1876 bequest from philanthropist James Lick, which stated that he would donate funds to UC for building the Lick Observatory if the facility would be used for both research and public education. Shang notes, "The bequest aligns with UC's historic mission and was at the forefront of deliberations on the observatory's future."

At the request of UCO stakeholders, Livermore's Lick enterprise model calculated three options for operating the observatory: sustaining only the assets needed for public outreach and education and keeping two, low-cost, robotic telescopes open for research to comply with Lick's bequest; sustaining only those assets needed for research; or sustaining current assets for serving both public education efforts and research.

A large and complex site, the Lick Observatory infrastructure includes nearly 15,000 square meters within 64 buildings, worth approximately $60 million, not including the scientific equipment. The Lick enterprise model incorporated facility data, such as building type, age, size, condition, utilization, value, and current operational status. The model was then calibrated to cost (labor, materials, equipment rental, and utilities) and climate considerations for the San Jose area. "This project required very detailed modeling," says Livermore computer scientist Lisa Clowdus. "We had to be sure every facet was correct, from physical building elements to weathering effects on infrastructure."

The enterprise model calculates the operations, maintenance, and repair costs at Lick Observatory. These factors can be adjusted to simulate the site's operations at different funding levels. With these results, UCOP was able to estimate infrastructure costs over time. The model's decision-analysis tools ultimately enabled decision makers to compare the cost–benefit trade-offs of various alternative approaches to managing the facility's lifecycle from acquisition to demolition.

A Unique Place

Although the Livermore team's past experience with modeling the nuclear weapons complex provided an excellent foundation for this more recent work, simulating Lick Observatory facilities

Lick Observatory's 3-meter Shane telescope has been used for testing many new instruments for astronomy research, including the novel adaptive-optics-based laser guide star—developed with help from Livermore scientists. (Photo by Lanie L. Rivera.)

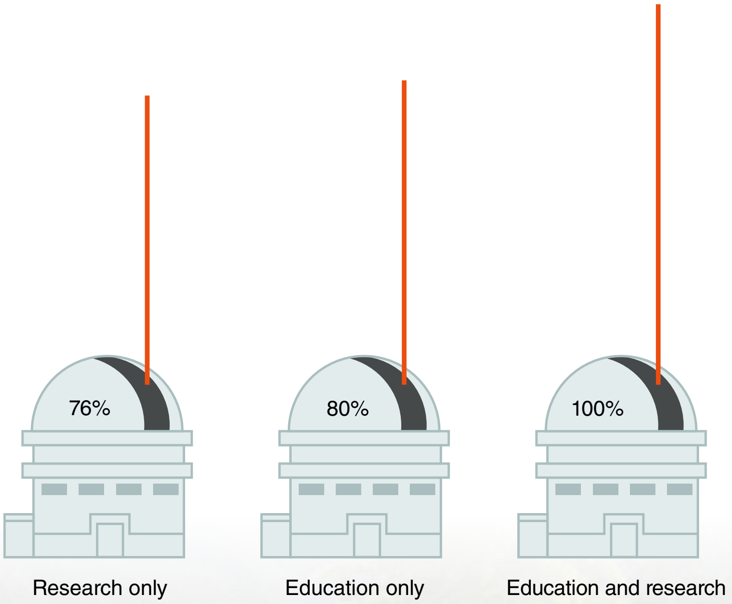
posed many unique challenges. "This new brand of modeling involves many fields of expertise, including real-property experts, modeling and simulation specialists, computer scientists, and astrophysicists," says Bernie Mattimore, Livermore's former associate director for plant engineering, who provided facilities expertise for the Lick modeling effort. The site is remote, at an elevation of nearly 1,300 meters. Its hard-to-reach location and changing weather conditions complicate maintenance operations and costs. Further, Lick's unique facilities have widely different utility needs. In contrast with its residential buildings and visitor's center, the domed-shaped research facilities—where most activity occurs at night with a small staff—do not use heat, ventilation, or air-conditioning systems.

The model indicated that Lick's funding for infrastucture, maintenance, and repair needed to double just to maintain current facility conditions. "Because of budget constraints, Lick had a 'repair it as it breaks' maintenance approach," says Clowdus. Without proper preventive and corrective maintenance, systems have a shorter service life and an increased risk of failure. The model made it clear that if operations, maintenance, and repairs remained underfunded, it would have a significant negative effect on facility and system conditions, thus increasing future operating costs.

When comparing the options of reducing Lick Observatory's scope of operations to either serving public education efforts or research, the model revealed that the cost savings of choosing one mission area over the other was marginal. Mattimore notes, "If either service were cut, great scientific and educational contributions would have been lost for little financial gain."

Contributions of Astronomical Significance

With the Livermore modeling results in hand, UCO and UC senior staff had a more quantitative understanding of Lick's maintenance needs and ultimately decided to sustain Lick at full operation with increased financial support from UCOP. In a letter to the Livermore contributors, the project's sponsors from the UC provost's office acknowledged, "Finding a team with the right expertise and knowledge of UC, who could take a fresh and rigorous look at the facilities on [Mount] Hamilton, has proven invaluable…We now have a common understanding about the



The enterprise model for Lick Observatory revealed that funding one mission area (research or education) rather than both resulted in marginal cost savings. As depicted in the graphic shown here, while sustaining both education and research was the most expensive option—requiring 100 percent of allowable funds—maintaining research or education alone would have cost only 24 or 20 percent less, respectively.

costs and ongoing challenges to operating and maintaining these facilities according to industry-based standards."

Claire Max, former Livermore astrophysicist and UCO's director since 2015, notes that this effort proved beneficial for both the site and her position at the observatory. She says, "This project was a great learning experience for me, and it continues to provide a guide for needed site maintenance and expenses." The model data also help Lick explore private or corporate financing, as potential contributors have a more concrete idea of what their donations can accomplish.

With the success of the Lick Observatory project, Livermore has begun applying enterprise modeling to new scenarios. For example, the Laboratory Strategic Infrastructure group, led by Shang, is currently collaborating with NNSA and the U.S. Army Corps of Engineers to accurately model the nuclear weapons complex. Such models are highlighting the significance of sound infrastructure for accomplishing mission objectives. At Livermore, infrastructure is the most expensive investment, followed by stockpile stewardship, safeguards and security, and science and technology. "Many people don't know how essential infrastructure is for meeting mission needs," says Clowdus. "Our models provide evidence that our success depends upon reliable facilities and infrastructure." As shown by the work with the Lick Obsevatory, the same holds true for research facilities outside the Laboratory.

—Lanie L. Rivera

The Great Lick Refractor, a type of telescope that uses a lens to form an image, is 17.3 meters long, 1.2 meters in diameter, and weighs over 12.5 tons. Among today's refracting telescopes, it is second in size only to the refractor at the University of Chicago's Yerkes Observatory in Williams Bay, Wisconsin. (Photo by Lanie L. Rivera.)

Key Words: astronomy, enterprise model, infrastructure, Lick Observatory, lifecycle, maintenance, University of California (UC), University of California Observatories (UCO), University of California Office of the President (UCOP).

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Facility Drives
Hydrogen Vehicle Innovations

As demand for limited fossil fuels grows, so does the need for viable alternatives to their use. In particular, researchers are working hard to replace these resources in transportation vehicles, which account for 70 percent of worldwide petroleum consmption. Lawrence Livermore scientists have been at the forefront of research for nearly two decades on one of the most promising long-term solutions: hydrogen.

Offering several advantages over fossil fuels, hydrogen is in limitless supply and has potential for pollution-free, high-efficiency use in fuel cells. However, the gas is difficult to store compactly, making today's hydrogen-powered vehicles costly and limited in their driving range. With funding from the Department of Energy's Fuel Cell Technologies Office, a Livermore team is using the Laboratory's new Cryogenic Hydrogen Test Facility to improve hydrogen storage and delivery. Through their efforts, the researchers aim to help make hydrogen-powered vehicles that meet customer expectations for range, cost, passenger and cargo space, and refueling time a reality.

Gas versus Liquid

Today's hydrogen-powered vehicles carry a tank of compressed-gas fuel. These vessels, made of lightweight, ultrastrong carbon fiber, store the hydrogen at ambient temperature and high pressure—about 70 megapascals (MPa). Yet hydrogen, the lightest chemical element, remains at low density even when highly pressurized. Thus, obtaining enough energy for a practical vehicle range requires large fuel tanks, which are expensive and occupy valuable vehicle space.

Hydrogen gas becomes liquid at low temperatures, around 20 kelvins. Liquid hydrogen is 60 percent denser than its compressed-gas counterpart, which could make it feasible for compact, high-energy-density storage. But liquid hydrogen is extremely volatile, rapidly vaporizing and increasing pressure because of heat transfer from the environment. Therefore, liquid-hydrogen tanks must have a safety valve to vent excess gas when it pressurizes beyond the vessel's limit. Even in well-insulated tanks, hydrogen venting is common and could fully deplete the supply.

Previous hydrogen research conducted at Livermore demonstrated that increasing liquid hydrogen's containment pressure kept fuel storage compact and eliminated venting under all but the most extreme conditions. (See *S&TR,* June 2007, pp. 11–16.) "This work was key in achieving high-density storage without fuel losses," says Salvador Aceves, the program leader for Livermore Hydrogen Technologies. However, such cryogenic liquid-hydrogen tanks are not yet commercially available.

Fueling under Pressure

While several automobile brands have compressed-gas hydrogen vehicles on the market, the technology's widespread adoption is limited by high vehicle cost and the scarcity of fueling stations. The United States has approximately 50 hydrogen fueling stations, 20 of which are located in California, and the number is anticipated to increase to 100 stations within the next few years. Many filling stations store hydrogen in its liquid form, but dispense it as a cooled, compressed gas by evaporating the liquid and pressurizing it in a series of compressors. Although inefficient and expensive, this method is necessary to facilitate hydrogen distribution and storage at the station.

At Livermore's Cyrogenic Hydrogen Test Facility, researchers are evaluating the feasibility of eliminating many of these steps by directly pressurizing liquid hydrogen in a pump. Manufactured by Munich-based Linde Corporation, the pump takes low-pressure (0.3 MPa) liquid hydrogen from an insulated vessel called a dewar and pressurizes it to the vehicle's vessel pressure (up to 87.5 MPa) before dispensing. Because pressurizing liquid is more thermodynamically efficient than pressurizing gas, the pump delivers a continuous stream of high-pressure cryogenic hydrogen while considerably reducing electricity consumption at the station. What's more, the pumping equipment occupies a smaller footprint and is easier to maintain.

The new liquid-pumping process offers two main advantages for the consumer. First, a relatively small piston pump can deliver 100 kilograms of liquid hydrogen per hour. As a result, refueling time is reduced to just five minutes per vehicle. The increase in pumping efficiency also benefits the station owner as more vehicles can be serviced in less time and the overall pump cost per vehicle is lower. The second advantage to consumers is increased vehicle range. Unlike water, which can be highly pressurized without significantly increasing its density, liquid hydrogen becomes considerably denser when pressurized. The research team, which includes Livermore engineers Guillaume Petitpas, Francisco Espinosa-Loza, and Nick Killingsworth as well as high-pressure technicians Rick Buskey and Vernon Switzer, expects to fill a high-pressure vessel to 80 grams per liter (double the density of today's compressed-gas tanks) from a 65-grams-per-liter dewar. This increase in hydrogen density offers the potential for longer vehicle driving range when compared to vehicles with conventional compressed hydrogen.

The pumping station at the Cryogenic Hydrogen Test Facility currently refuels vehicles with the highest density molecular hydrogen in the Western Hemisphere. Aceves says, "Higher

The two main components of Lawrence Livermore's Cryogenic Hydrogen Test Facility are (left) the stainless steel containment unit used to test prototype hydrogen storage vessels and (right) the liquid-hydrogen pump built by Munich-based Linde Corporation.

density hydrogen can only be found in minute amounts in physics laboratories, including in the tiny capsules of compressed hydrogen produced at Lawrence Livermore's National Ignition Facility."

Building a Better Fuel Tank

After researching several key parts of the hydrogen fueling process, the team turned its attention to improving on-board vehicular storage vessels. Livermore, in partnership with Spencer Composites and BMW, has designed and built several prototypes. To test these prototypes safely, the research team uses another critical component of the Cryogenic Hydrogen Test Facility—the remotely controlled and monitored stainless-steel containment unit. More than 3-centimeters thick and weighing almost 5 metric tons, the test vessel can contain the equivalent energy of 1.8 kilograms of TNT, making it possible to test full-scale vessels and hydrogen systems safely.

The containment unit is used to repeatedly test prototype hydrogen storage vessels with pumped cryogenic hydrogen to see how they perform. As part of these experiments, the team continuously fills and empties prototype vessels to simulate a lifetime of wear. Test results are then analyzed to assess the prototype's strengths and weaknesses.

The Future of the Hydrogen Highway

Today, car manufacturers such as Toyota, Honda, Hyundai, and Mercedes-Benz are actively commercializing vehicles powered by hydrogen fuel cells. Furthermore, several of the San Francisco Bay Area's Alameda–Contra Costa counties transit buses are hydrogen fuel-cell vehicles with a range of 355 kilometers per fill. In 2015, one of these buses achieved 20,000 hours of continuous operation, about four times longer than expected. In California, the 2016 Toyota Mirai—a hydrogen fuel-cell vehicle—sells for approximately $57,000. To make the price of hydrogen vehicles more competitive will require an increase in consumer demand, but the lack of fueling infrastructure is keeping the market small.

"The improvements we are making to the pumping process and our research into complementary storage vessels could potentially lower cost and improve performance," says Petitpas. "However, big changes are needed across many areas, and these advancements will take some time—we need more testing, more charging stations, and improvements to other capabilities…but we are getting there."

The work done by Aceves and the team directly supports an agreement from the 21st Conference of the Parties, or COP21, held in Paris. COP is the decision-making body of the United Nations Framework Convention on Climate Change. "Through our efforts, we are enabling practical, long-range hydrogen vehicles that can help reduce climate-changing carbon-dioxide emissions," says Aceves. In addition, recent progress on hydrogen technology will be highlighted at the National Hydrogen and Fuel Cell Day, celebrated annually on October 8. "This event is a great opportunity to increase awareness of current developments in the area of hydrogen technologies, including research organizations, refueling infrastructure, and commercially available vehicles."

—Maren Hunsberger

Key Words: alternative fuel, Cryogenic Hydrogen Test Facility, fossil fuel, fuel efficiency, hydrogen, hydrogen fuel cell, hydrogen-powered vehicle, liquid hydrogen.

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Livermore engineers (from left) Salvador Aceves and Guillaume Petitpas examine a liquid-hydrogen fuel tank inside the containment unit. (Photo by Julie Russell.)

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 (http://www.uspto.gov).

Patents

Apparatus for Point-of-Care Detection of Nucleic Acid in a Sample
Jane P. Bearinger, Lawrence C. Dugan
U.S. Patent 9,315,858 B2
April 19, 2016

Microfluidic Ultrasonic Particle Separators with Engineered Node Locations and Geometries
Klint A. Rose, Karl A. Fisher, Douglas A. Wajda, Raymond P. Mariella, Jr., Christopher Bailey, Dietrich Dehlinger, Maxim Shusteff, Byoungsok Jung, Kevin D. Ness
U.S. Patent 9,321,050 B2
April 26, 2016

Fluorescent Lighting with Aluminum Nitride Phosphors
Nerine J. Cherepy, Stephen A. Payne, Zachary M. Seeley, Alok M. Srivastava
U.S. Patent 9,337,010 B2
May 10, 2016

Porous Media Heat Transfer for Injection Molding
Neil Reginald Beer
U.S. Patent 9,352,502 B2
May 31, 2016

Device, Array, and Methods for Disease Detection and Analysis
Rupa S. Rao, Stephen M. Lane, Dennis L. Matthews, Matthew A. Coleman
U.S. Patent 9,366,668 B2
June 14, 2016

Diffractive Optical Elements for Transformation of Modes of Lasers
Arun K. Sridharan, Paul H. Pax, John E. Heebner, Derrek R. Drachenberg, James P. Armstrong, Jay W. Dawson
U.S. Patent 9,373,928 B2
June 21, 2016

Awards

Lawrence Livermore researchers **John Elmer**, **Holly Carlton**, and **Randy Pong**, along with Jay Vaja of the United Kingdom's Atomic Weapons Establishment, received the **American Welding Society's McKay-Helm Award** for their 2015 *Welding Journal* paper describing the effect of argon and nitrogen shielding gas on reducing, or even eliminating, porosity in laser welds in steel, stainless steel, and nickel. The findings could have implications for improving metal laser-powder-bed or wire three-dimensional printing, which often result in porous final products.

Bioinformatics scientist **Jonathan Allen** has been selected to serve on a **National Academies of Sciences Engineering and Medicine Panel** that will study the interface between microbiomes—microbial communities—and human-built environments. Allen, a researcher in Lawrence Livermore's Global Security Principal Directorate, will be part of the 15-member committee that will identify key research gaps in understanding how building infrastructure design affects human health. The panel is sponsored by the Sloan Foundation, the Environmental Protection Agency, the National Institutes of Health, and the National Aeronautics and Space Administration.

Christopher Barty, the chief technology officer for the Laboratory's National Ignition Facility and Photon Science Principal Directorate, has won the **2016 Society of Photo-optical Instrumentation Engineers** (SPIE) **Harold E. Edgerton Award** for his work on ultrafast lasers and laser-based x-ray and gamma-ray science.

The Harold E. Edgerton Award is presented annually for outstanding contributions to optical or photonic techniques in the application and understanding of high-speed physical phenomena. Edgerton (1903–1990) was an MIT professor known for his pioneering efforts to photographically capture fast physical events. In the 1950s, he produced the first photographs of the initial phases of nuclear explosions.

(*continued from p. 2*)

perception, action, and cognition abilities. Jim Brase, Livermore's leader for the Data Science Initiative, says, "Neuromorphic computing represents the potential that machine intelligence will change how we conduct science."

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Tiny Tubes Move into the Fast Lane

For the first time, Lawrence Livermore researchers have shown that carbon nanotubes as small as 0.8 nanometers in diameter are 10 times faster than bulk water at transporting protons. The transport rates in these nanotube pores, which form one-dimensional (1D) water wires, also exceed those of biological channels and human-made proton conductors, making carbon nanotubes the fastest known proton conductor. The research appears in the April 4, 2016, online edition of the journal *Nature Nanotechnology*.

The Livermore team, along with colleagues from Lawrence Berkeley National Laboratory and the University of California at Berkeley, created a simple and versatile experimental system for studying transport in ultra-narrow carbon nanotube (CNT) pores. The researchers used CNT porins, a technology developed earlier at Livermore that uses CNTs embedded in a lipid membrane to mimic biological ion-channel functionality. The team's key breakthrough was creating nanotube porins with a diameter of less than 1 nanometer, which allowed the researchers for the first time to achieve true 1D water confinement.

"Our results show that when you squeeze water into the nanotube, protons move through that water even faster than through normal water," says Aleksandr Noy, a Livermore biophysicist and a lead author of the paper. Practical applications include proton exchange membranes, proton-based signaling in biological systems, and the emerging field of proton bioelectronics, called protonics.

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Cloud "Brightening" Effects in Climate Models

Lawrence Livermore and Yale University researchers found that climate models aggressively make clouds "brighter" as the planet warms, causing the models to underestimate how much global warming will occur from increasing atmospheric carbon dioxide. The research appears in the April 8, 2016, edition of *Science*.

As the atmosphere warms, clouds become brighter as ice within them turns to liquid. This "cloud-phase feedback" acts as a brake on global warming as liquid clouds reflect more sunlight back into space than ice clouds. Clouds in most climate models contain too much ice, causing the stabilizing cloud-phase feedback to be unrealistically strong.

The researchers used a state-of-the-art climate model to modify parameters that brought relative amounts of liquid and ice in the model's clouds into agreement with those observed in nature. Correcting the bias led to a weaker cloud-phase feedback, and thus an increase in global warming.

In nature, clouds containing both ice crystals and liquid droplets are common at temperatures well below freezing. The relative amount of liquid in these "mixed-phase" clouds increases as the atmosphere warms. Lawrence Livermore coauthor Mark Zelinka says, "Most climate models are a little too eager to glaciate below freezing, so they are likely exaggerating the increase in cloud reflectivity as the atmosphere warms."

Recent studies indicate that other cloud-feedback mechanisms involving changes in cloud altitude and coverage may also exacerbate global warming. Zelinka says, "Clouds do not seem to want to do us any favors when it comes to limiting global warming."

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New Method of Measuring Crystalline Equation of State

In research appearing in the April 7, 2016, edition of *Journal of Applied Physics,* Livermore physicists describe a new experimental method to determine the equation of state (EOS) of low-symmetry anisotropic crystalline materials. A material's EOS describes how material properties such as volume and internal energy are affected by intense pressure and temperature. For most materials, a prescribed set of experiments, including high-pressure x-ray diffraction (XRD), are conducted to determine sample volume under various pressure–temperature conditions.

While experimenting with an unusual insensitive explosive compound, the research team discovered the material's complicated crystal structure limited their ability to determine its volume with high-pressure XRD. "To accurately predict performance characteristics of the material, we needed another method for determining its equation of state," says Sorin Bastea, a Livermore computational physicist and the project leader. Based on pioneering research at Cornell University demonstrating direct volume measurements with large crystals, Livermore physical chemist Joe Zaug theorized a similar method could work with smaller structures. He conducted microscopy and interferometry measurements on a 10-micrometer-size triaminotrinitrobenzene (TATB) crystal pressurized in a diamond anvil cell. The results matched remarkably well with published x-ray results and helped the team extend the pressure range of TATB's EOS.

Team member and Livermore physicist Elissaios Stavrou later applied the method to measure the EOS of a sample up to 30 gigapascals (300,000 times normal atmospheric pressure), which enabled the researchers to calculate performance characteristics for the insensitive explosive they were studying. This new experimental approach provides researchers with a simple and direct method for measuring the high-pressure EOS of complex crystalline materials.

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Abstract

Laying the Groundwork for Extreme-Scale Computing

Livermore computer scientists are contributing to the progression of extreme-scale (exascale or greater) computing through avenues such as the Laboratory Directed Research and Development (LDRD) Program. This article highlights six LDRD-funded computational research projects designed to help explore options and advance such systems. Barry Rountree is designing software to monitor and control power usage within and between jobs to make better use of a limited resource. Ignacio Laguna is exploring various approaches for helping an application efficiently recover from hardware and software failures. Scott Lloyd and Maya Gokhale have demonstrated the utility of performing some computing functions within a computer's memory, and organizing information within it to limit the amount of communication between components. Jacob Schroder and Rob Falgout have developed an algorithm that works with many applications to solve time steps in parallel rather than in sequence for faster results and better utilization of massively parallel systems. A team led by Tzanio Kolev has developed advanced algorithms that achieve higher quality simulations of shock hydrodynamics and other complex physics that are well-suited for future architectures. Finally, Jean-Luc Fattebert has designed methods for performing large-scale, first-principles molecular dynamics simulations without sacrificing accuracy.

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Coming Next Issue

Predictive Medicine Points Way to Cure

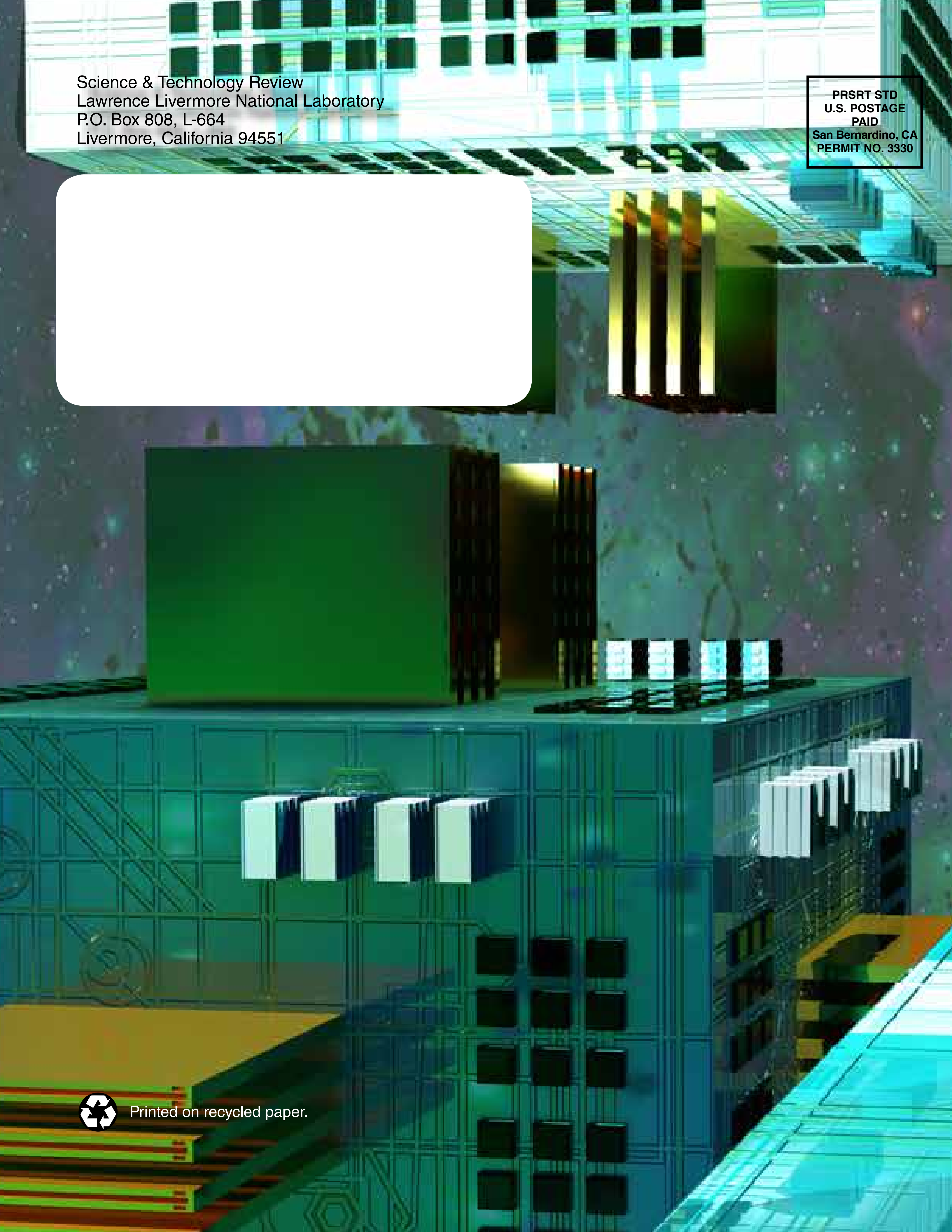
High-performance computing efforts aim to eradicate cancer and improve biological understanding, human health, and biosecurity.

Also in October/November

- *Collaborative studies help identify necessary steps for quick restoration of an underground transportation system following a biological attack.*

- *Livermore scientists answer long-standing questions about lithium hydride's equation of state.*

- *Implantable brain sensors may help in developing better treatments for Parkinson's disease, chronic depression, and post-traumatic stress disorder.*



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