THE MIGHTY
SEQUOIA

Also in this issue:
Celebrating Johnny Foster at 90
Diamond under Pressure
Z-Pinch Ups the Voltage
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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About the Cover

Sequoia (shown on the cover) is Lawrence Livermore’s newest and largest supercomputer. Developed in collaboration with IBM and Argonne National Laboratory, Sequoia once again demonstrates the Laboratory’s leadership and expertise in the design, commissioning, and application of high-performance computing systems. As the article on p. 4 describes, Sequoia will execute highly complex physics simulations for the National Nuclear Security Administration’s stockpile stewardship mission as well as help the Laboratory explore and prepare for exascale, the next great milestone in computing.

About S&TR

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Water Signature Revealed in Extrasolar Planet

Laboratory astrophysicist Bruce Macintosh, along with a team of international scientists, has made the most detailed examination yet of a Jupiter-size planet’s atmosphere beyond our solar system. Using the OSIRIS instrument on the Keck II telescope in Hawaii, the team has uncovered the chemical fingerprints of specific molecules, revealing a cloudy atmosphere containing water vapor and carbon monoxide. “With this level of detail,” says Travis Barman, an astronomer at Lowell Observatory in Arizona, “we can compare the amount of carbon to the amount of oxygen present in the atmosphere, and this chemical mix provides clues as to how the planetary system formed.”

The planet is one of four gas giants known to orbit a star called HR 8799, 130 light-years from Earth. (See artist’s rendering; courtesy of Dunlap Institute for Astronomy and Astrophysics and Media Farm.) Although the planet’s atmosphere shows clear evidence of water vapor, that signature is weaker than would be expected if the planet shared the composition of its parent star. Instead, the planet has a high ratio of carbon to oxygen—a fingerprint of its formation in a gaseous disk tens of millions of years ago.

As the gas cooled with time, grains of water ice formed, depleting the remaining gas of oxygen. Planetary formation began when ice and solids collected into planetary cores—similar to how our solar system formed. “This spectrum is the sharpest ever obtained of an extrasolar planet,” says Macintosh. “The exquisite resolution afforded by these new observations has allowed us to begin to probe the planet’s formation.” The team’s findings appeared in the March 22, 2013, edition of Science.

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Scientists Find New Materials to Capture Methane

Scientists at Lawrence Livermore and the University of California at Berkeley have discovered new materials to capture methane, the second highest concentration greenhouse gas in our atmosphere. Methane is a substantial driver of global climate change, contributing 30 percent of today’s net warming. Concern of methane is mounting because of leaks associated with rapidly expanding unconventional oil and gas extraction. In addition, as Arctic ice cover continues to melt, the potential exists for large-scale release of methane from decayed material. At the same time, methane is a growing source of energy.

The research team, which includes Livermore’s Amitesh Maiti, Roger Aines, and Josh Stolaroff, performed computer simulation studies on the effectiveness of methane capture using two different materials—liquid solvents and nanoporous zeolites. Zeolites are unique structures that can be adapted for many types of gas separation and storage applications because of their diverse topology. The porous materials are commonly used as commercial adsorbents.

While the liquid solvents were not effective for methane capture, a systematic screening of about 100,000 zeolite structures uncovered a few nanoporous candidates that appear technologically promising. In the team’s simulations, one specific zeolite, dubbed SBN, captured enough medium-source methane to convert it to high-purity methane, which in turn could be used to generate efficient electricity. The team’s research was reported in the April 16, 2013, edition of Nature Communications.

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Moon’s Core Active Later Than Thought

New evidence from ancient lunar rocks suggests that the Moon’s long-lived dynamo—a molten, convecting core of liquid metal that generated a strong magnetic field—lasted 160 million years longer than originally estimated. Lawrence Livermore scientist William Cassata and a group of international collaborators analyzed two rocks gathered during the Apollo 11 mission and found that the samples were magnetized in a stable and surprisingly intense magnetic field. The study of these slowly cooled, unshocked rocks demonstrates that the Moon had a core dynamo as late as 3.55 billion years ago.

“The Moon possessed a magnetic field much later than would be expected for a body of its size,” says Cassata. The study shows that the Moon likely possessed a long-lived core dynamo, much like the one that currently exists on Earth, but generated by a different mechanism. Earth’s core dynamo is generated by thermally driven convective motions in the liquid outer core. However, because of its size, the Moon was too cool to sustain core convection as late as 3.55 billion years ago.

In the past, however, when the Moon was closer to Earth, its greater angle of precession would allow for mechanical stirring of the liquid metal core by the overlying rocky mantle. These motions can induce a global magnetic field. A gradual decrease in the Moon’s precession angle as it moved further away from Earth and an increase in its core viscosity as it cooled may have caused the dynamo to decline between 1.8 and 2.7 billion years ago. According to Cassata, “The lifetime of the ancient lunar core dynamo has implications for mechanisms of field generation on other planetary bodies.” The research appeared in the May 6, 2013, edition of Proceedings of the National Academy of Sciences.

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Mighty Challenges Call for Computing on a Grand Scale

Commentary by Bruce T. Goodwin

Given the sheer scale of modern supercomputers, it is tempting to assume that they are powerful enough to solve almost any problem imaginable. However, some of the computing challenges Laboratory researchers face are so complex that they compel us to persistently push computing’s boundaries. One of these challenges is maintaining a safe, secure, and effective nuclear stockpile in the absence of testing—an effort that relies in large part on supercomputers and the skilled computer scientists needed to perform sophisticated computer simulations.

As discussed in the article beginning on p. 4, Sequoia, the first IBM BlueGene/Q machine and one of the world’s fastest computers, was installed at Lawrence Livermore in 2012. With Sequoia, the Laboratory has demonstrated once again its leadership and expertise in designing, commissioning, and using high-performance computing (HPC) systems. BlueGene/Q was developed by IBM and Lawrence Livermore and Argonne national laboratories through an iterative and equitable design process. This process ensured that all three partners were involved in the decision making and that the resulting system could support both laboratories’ mission needs.

Since the start of the Accelerated Strategic Computing Initiative (ASCI)/Advanced Simulation and Computing (ASC) era, we have worked closely with IBM researchers for the delivery of five generations of Livermore supercomputers—ASCI Blue, ASCI White, ASC Purple, BlueGene/L, and now Sequoia. These projects have demonstrated that complex and ambitious computing technology development efforts are best accomplished through collaborations between government and industry. By sharing risk and expertise, we can achieve astonishing outcomes.

Now that Sequoia has been commissioned, tested, and tuned, we are eager to put it to work, executing sophisticated physics simulations and calculations for the National Nuclear Security Administration’s stockpile stewardship mission. With Sequoia, we will produce higher fidelity simulations with more accurate physics that will help us improve our existing models and codes. The machine will also allow us to routinely perform large sets of uncertainty quantification (UQ) calculations to better understand and reduce sources of uncertainty in our weapons codes. Working through the 100 to 200 potential failure modes in a nuclear weapon system, determining the margins of uncertainty for each, and then integrating and balancing these uncertainties across the system requires tens of thousands of simulations.

UQ can be challenging and computationally intensive, but in time, it could become an essential element of the design process for many large engineered objects, especially those that cannot easily be physically tested before use. For instance, UQ techniques were used during the development of BLU-129/B, a low-collateral-damage conventional munition co-developed by Livermore for the U.S. Air Force. BLU-129/B also serves as a great example of how robust simulations can shorten design and development time. With supercomputing support, we moved from concept to field deployment in 18 months. Even accelerated Department of Defense design cycles typically take 4 to 6 years.

Supercomputing reduces the investment in time and testing needed to bring a product to market—not just for defense equipment but a full spectrum of high-quality goods. The industrial facet of computing matters because computational excellence is both a national and economic security issue, and countries such as China are offering intense competition on both fronts. Investing in computing and encouraging wider adoption of HPC simulation in product development is essential if our nation wishes to prevail in this competition.

For our part, we continue to support both national security and competitiveness through our computing. We routinely partner with companies and other laboratories to develop new software and systems that further our mission-centered science and engineering work and the field of computing itself. Vulcan, a smaller BlueGene/Q machine procured along with Sequoia, will be used to power industrial research through Livermore’s HPC Innovation Center. The Laboratory may hold an unmatched record of achievement in supercomputing, but we are not resting on our laurels.

Bruce T. Goodwin is associate director at large for National Security Policy and Research.
REACHING FOR NEW COMPUTATIONAL HEIGHTS

After demonstrating stellar performance in early science runs, Livermore’s newest and largest supercomputer has assumed dual roles as a platform for stockpile stewardship research and exascale computing preparation.
At Lawrence Livermore and across the National Nuclear Security Administration’s (NNSA’s) complex, leadership in supercomputing is not only a core competency but also essential to the national security mission. Demands on computer systems used for weapons assessments and certification continue to grow as the nuclear stockpile moves further from the test base against which simulations are calibrated. Simulation capabilities are also strained because weapons behavior spans such a range of timescales, from detonation, which happens on the micro- to millisecond scale, to nuclear fusion, which lasts mere femtoseconds.

The perpetual push for higher resolution computer simulations and faster number crunching is motivated by a desire to verify, with high confidence and without resorting to nuclear testing, that a critical national resource remains secure and functional. Says Fred Streitz, director of Livermore’s High Performance Computing Innovation Center, “Every time we jump to a new generation of supercomputers, we open another window through which we can look to discover new science, and that helps in our quest to understand materials and phenomena with a high degree of accuracy.”

In 2006, the 100-teraflop (trillion floating-point operations) Advanced Simulation and Computing (ASC) Purple supercomputer delivered the first-ever three-dimensional, full-physics nuclear weapons simulation, and the 360-teraflop BlueGene/L was in the midst of its three-year reign as the world’s fastest computer. While these two Livermore systems were still setting records, leaders in NNSA’s ASC Program—the organization that integrates work by researchers at Los Alamos, Lawrence Livermore, and Sandia national laboratories to develop nuclear weapons simulation tools—were planning for a new computing system that would be delivered in 2012. Supplying the next level of performance necessary for supporting stockpile stewardship work, they soon realized, would require the most ambitious leap in computing ever attempted. They needed a machine that could deliver 12 to 24 Purple-class weapons calculations simultaneously to credibly evaluate the uncertainties in weapons physics. The machine also needed to have 20 to 50 times the capability of BlueGene/L for running materials science codes.

These performance milestones formed the design basis for Sequoia, the “serial number one” IBM BlueGene/Q machine. The newest and largest member of
Livermore’s supercomputing arsenal, Sequoia has a peak performance speed of 20 petaflops (quadrillion floating-point operations per second). IBM designed BlueGene/Q in partnership with Lawrence Livermore and Argonne national laboratories, with national laboratory researchers providing user input at every stage of development. Livermore experts worked to create a machine that could be programmed with relative ease, while helping to explore and prepare for future computer architectures. Most critically, the machine would provide an effective platform for the existing trove of weapons codes, in which NNSA has invested several billion dollars and more than 15 years of effort.

**Energy Drives Hardware Decisions**

A breakthrough system with over 1.5 million processor units, or cores, and 1.6 petabytes of memory, Sequoia serves as a bridge, design-wise, between supercomputers of the past 15 years and exascale machines some 100 times faster than today’s top performer (an exaflop machine would perform at least 1 quintillion floating-point operations per second). While BlueGene/Q is still grounded in today’s computer architecture, it introduces hardware features and supports programming models likely to carry over to and potentially proliferate in tomorrow’s systems.

According to Michel McCoy, ASC program director at Livermore, computer architecture is undergoing its toughest transition in the past 70 years. The last truly revolutionary design shift came in the mid-1990s, when groups of interconnected cache-based microprocessors became standard in computers of every scale. Succeeding generations of these microprocessors have grown faster by boosting the speed and shrinking the size of transistors, effectively packing more calculations into every unit of time and space occupied by the computer. But now transistors are approaching a lower limit in size and an upper limit in speed. Although individual transistors could be pushed to run yet faster, further speeding up the millions of transistors on a typical microprocessor would drive energy demands and operational costs for large-scale computing to unsustainable levels.

Researchers are therefore seeking new ways of designing processors to increase their performance, while reducing energy consumption enough to make the units affordable to operate. One promising approach, exemplified by IBM’s BlueGene series, is using large numbers of relatively low-frequency, simple processing units to achieve high cumulative performance with moderate energy usage. With a peak power requirement of less than 10 megawatts and the capability to perform 2.1 billion floating-point operations per second per watt, BlueGene/Q is among the world’s most energy-efficient supercomputers.

BlueGene/Q’s ingenious hardware design begins with the chip. Processors, memory, and networking logic are all

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This chart shows the evolution of Lawrence Livermore supercomputers throughout the Laboratory’s history. Performance advances in early systems came through increases in the number of vacuum tubes and other components. In the late 1970s, hardware companies started building machines that used vector processing to manipulate data and speed up computing. Beginning in the mid-1990s, cache-based microprocessors were tied together through a message-passing interface; subsequent increases in speed resulted from processor technology improvements. Sequoia stands on the threshold of yet another era, which could be dominated by energy-efficient, multicore systems.
integrated into an exceptionally energy-efficient single chip that operates at both lower voltage and lower frequency than many of the chips found in leading supercomputers of the past decade. Each BlueGene/Q compute chip contains 18 cores—more than four times the core density of its recent predecessor, the BlueGene/P chip. Sixteen cores are used for computation, while one runs the operating system and another serves as a backup to increase the yield of usable chips. Each core has a relatively small amount of nearby memory for fast data access, called a Level 1 cache, and all the cores on the chip share a larger Level 2 cache. Each compute chip is packaged with memory chips and water-cooling components into a compute card, and compute cards are organized in sets of 32 (called a node card). Thirty-two node cards comprise a rack, and Sequoia has 96 of these racks, for a total of just fewer than 100,000 16-core processors.

**Bandwidth as Performance Inhibitor**

Modern supercomputers, including BlueGene/Q, have several types of on-chip memory storage. “However, real problems don’t fit in the cache,” says Bronis de Supinski, Livermore Computing’s chief technology officer. Most operations cannot simply access data from a nearby memory cache but instead must fetch data on a separate memory chip or another module. As the volume of cores and tasks has grown, the rate at which the system can retrieve data for the processor in order to complete calculations (known as bandwidth) has gradually become the limiting factor in computer performance, more so than how fast the processor can theoretically perform calculations.

The 20-petaflop (quadrillion floating-point operations) Sequoia supercomputer boasts more than 1.5 million processing units, or cores, arranged in a compact, water-cooled, energy-efficient system. Its processing power is compressed into 96 racks, each the size of a large refrigerator, arrayed across just 3,400 square feet of floor space. Hardware features of the BlueGene/Q compute chip are highlighted in the dye photograph at far left, where L1, L2 = Level 1, 2.
Hardware designers have implemented various methods to ameliorate delay and improve performance. BlueGene/Q uses hardware threading, an energy- and space-efficient alternative. Each processor supports four execution threads that share resources. The situation is analogous to four workers who must share a single tool. While one worker (thread) is waiting for data retrieval, it can lend the tool to another worker so that the core’s resources are always being used.

Keeping otherwise idle threads or cores occupied was a goal for the BlueGene/Q hardware designers. Many parallel programs contain shared data and portions of code that must be executed by a single process or thread at a time to ensure accurate results. Threads attempting to update or access the same data must take turns, through locks or other mechanisms, which can cause a queue to form. As the number of access attempts increases, program performance deteriorates. BlueGene/Q’s multiversioning Level 2 cache supports two new alternatives to locks: speculative execution and transactional memory. Together, they may improve application performance and ease the programmer’s task compared with traditional locking methods.

Using either memory feature requires that a programmer designate regions in the code as speculative. Instead of waiting for up-to-date versions of all the data it needs, which might depend on another core finishing a computation, a thread is allowed to begin speculatively performing work with the available data. The cache then checks the work. If the data are fresh, the work will be saved, and the system will gain a performance bonus because the labor was completed before the relevant value was changed by another thread. If the data are stale, the speculative work is discarded, and the operation is reexecuted with the correct value.

Another innovative memory element is BlueGene/Q’s intelligent Level 1 cache list prefetcher. This cache can learn complex memory access patterns and retrieve frequently visited data sets from the more distant memory devices, making them available in the cache when needed.

Improving computational performance and bandwidth through threading and special memory functions would largely be for naught without a high-speed method for moving the data between nodes. Most supercomputers use commodity interconnects or Infiniband for their primary connections. BlueGene/Q has a novel switching infrastructure that takes advantage of advanced fiber optics at every communication level. With the latest generation of BlueGene, IBM has also upgraded the toroidal connection between node cards from three to five dimensions for more robust interconnection and to halve the maximum latency. In this configuration, each node is connected to 10 others (instead of 6), thereby reducing the maximum distance between nodes from 72 hops to 31.

Accompanying Sequoia and connected via high-speed parallelized interconnect is one of the world’s largest file storage systems. The 55-petabyte Grove is designed to manage and store the immense amounts of data needed for Sequoia’s research functions.

Greater Parallelism in Codes

Knowing that supercomputer hardware and software must function as a team, Livermore experts have worked to ensure not only that Sequoia’s hardware will be compatible with ASC codes, but also that these codes are tuned to run on Sequoia. Because one goal is to improve the codes’ predictive capability, code preparation has required new physics models, new mathematical representations for the models, and algorithms for solving these representations at a new scale. In addition, researchers have begun analyzing threading techniques and other hardware features to determine how and where to incorporate these innovations into the codes. The undertaking began in 2009, a full three years before Sequoia arrived. Dawn, a 500-teraflop BlueGene/P machine, served as the primary platform for code preparation and scaling. Additional support was provided by BlueGene/Q simulators, other Livermore high-performance computing (HPC) systems, and starting in 2011, some small-scale BlueGene/Q prototypes.

Physicist David Richards observes, “With parallel computers, many people mistakenly think that using a million processors will automatically make a program run a million times faster than with a single processor, but that is not necessarily so. The work must be divided into pieces that can be performed independently, and how well this can be done depends on the problem.” For instance, Richards has found that running a 27 million particle molecular-dynamics simulation on 2,000 nodes of Sequoia is barely faster than doing so on 1,000 nodes. Determining the optimal level of task division for the given problem is essential.

Computational physicist Bert Still divides the code readiness work into two distinct components—scaling out and scaling in. Scaling out is modifying the code to perform effectively across a greater number of nodes by breaking a problem or calculation into smaller but still functional chunks. Using more nodes allows researchers to save on calculation time, increase the problem size or resolution, or both.

Essentially, the scaling-in task entails streamlining operations within each node. In the past, programmers focused on parallelism exclusively at the node level. Sequoia offers parallelism opportunities at lower levels within the node as well. Sequoia’s individual cores are comparatively slow and equipped with rather simple logic for deciding which tasks to run next. The programmer is largely responsible for efficiently organizing and apportioning work, while...
programming that combines MPI with hardware-threading methods.

Several projects were launched to assist Livermore computer scientists with applying these hybrid methods and implementing new programming styles. One such project investigated accomplishing larger tasks using a group of threads. Strategically deciding when, where, and how much threading to add to the code is crucial. Shifting to a more thread-focused scheme allows code writers to worry less about communication and more about coordinating thread activity through a strategic combination of locks, speculative execution, and transactional memory. The latter two features have just begun to be explored, but Livermore programmers suspect that the new memory features could boost performance in code sections not already optimized for threading and locks.

Code preparation, enhancement, and testing have been challenging, surprising, and even gratifying. Livermore researchers have found that MPI programming functions better than anticipated on Sequoia. In addition, says Still, “While we knew that Sequoia would be a good HPC throughput engine, we were surprised how good it was as a data analytic machine. Graph analytics is representative of a large class of data science and is relevant to mission work at the Laboratory.” Sequoia maintains the highest ranking on the Graph 500 list, which measures the ability of supercomputers to solve big data problems. (See S&TR, January/February 2013, pp. 4–11.)

Sequoia has also presented new scaling complications. While preparing the laser–plasma code pf3D for a simulation requiring 1 trillion zones and 300 terabytes of memory, Langer realized that scaling up the code for Sequoia would require him to parallelize every aspect of the effort, including preparatory calculations and post-simulation data analysis. Tasks
previously considered relatively trivial or not particularly data intensive were now too large for a typical workstation to handle. Langer notes, “Sequoia is so big, it challenges our assumptions. We keep bumping against the sheer size of the machine.”

**Integrating Sequoia into the Family**

While software experts were beginning code optimization and development work for Sequoia, engineering and facilities teams were preparing to install the new system in the two-level space previously occupied by ASC Purple at Livermore’s Terascale Simulation Facility. (See *S&TR*, January/February 2005, pp. 22–24.) The teams first created a three-dimensional model of the computer room to determine how to best use the available space, with consideration for sustainability and energy efficiency. They then made changes to the facility on a coordinated schedule to avoid interrupting existing operations. Changes included gradually increasing the air and chilled-water temperatures to meet Sequoia’s requirements and to save energy.

Sequoia is equipped with energy-efficient features such as a novel 480-volt electrical distribution system for reducing energy losses and a water-cooling system that is more than twice as energy efficient as standard air cooling. Incorporating such systems into the space necessitated two significant modifications to IBM’s facility specifications. First, the facilities team designed innovative in-floor power distribution units to minimize congestion and reduce, by a factor of four, the conduit distribution equipment bridging the utilities and rack levels. Second, although IBM specified stainless-steel pipe for the cooling infrastructure, the team selected more economical polypropylene piping that met durability requirements and relaxed water-treatment demands. The polypropylene piping also contributed to the building’s already impressive “green” credentials as a Leadership in Energy and Environmental Design gold-rated facility. Facilities manager Anna Maria Bailey notes, “Sequoia’s electrical, mechanical, and structural requirements are demanding. Preparing for Sequoia really pushed us to think creatively to make things work.”

Integrating any first-of-its-kind computer system is challenging, but Sequoia was Livermore’s most grueling in recent history because of the machine’s size and complexity. System testing and stabilization spanned a full 14 months, but the integration schedule itself was unusually tight, leaving a mere 5 weeks between delivery of the last racks and the deadline for completing Linpack testing—a performance benchmark used to rank the world’s fastest computers.

Issues ranged from straightforward inconveniences, such as paint chips in the water system during pump commissioning and faulty adhesives on a bulk power module gasket, to more puzzling errors, such as intermittent electrical problems caused by connections bent during rack installation. Sequoia’s cooling infrastructure also presented some initial operational challenges, including uneven node-card cooling and false tripping of a leak-detection monitor.

A more serious manufacturing defect was encountered during the final integration phase. During intentionally aggressive thermal cycling as part of the Linpack testing, the team experienced a high volume of uncorrectable and seemingly random memory errors. In effect, compute cards were failing at alarming rates. The integration team began removing cards while IBM performed random dye-injection leak tests. The tests revealed that the solder attaching chips to their compute cards was, in some instances, exhibiting microscopic cracks. Investigation revealed that unevenly applied force during manufacturing tests had damaged the solder on a portion of Sequoia’s cards. These cracks had widened during thermal cycling, overheating the memory controllers beneath.

The Livermore team overcame this and other integration hurdles with assistance from IBM computer scientists and
BlueGene/Q’s unusually sophisticated error-detection control system software. Within 40 days of detecting the memory errors, IBM and Livermore troubleshooters had pinpointed the cause and replaced all 25,000 faulty cards. Although the system was accepted in December 2012, IBM continued to work with Livermore to fine-tune Sequoia hardware and software until the machine converted to classified operations in April 2013, demonstrating a notable level of dedication and partnership in machine deployment.

Performance on a Grand Scale

None of the integration challenges prevented Sequoia from completing, with only hours to spare, a 23-hour Linpack benchmark run at 16.324 petaflops and assuming the lead position on the Top500 Supercomputer Sites list for a 6-month period in 2012. Kim Cupps, a division leader in Livermore Computing, observes, “We’re proud that Sequoia was named the world’s fastest computer, but really, what’s important about the machine is what we can do with it. When we hear people talk about the work they’re doing on the machine and what they’ve accomplished, that’s what makes all the work worthwhile.”

The speed, scaling, and versatility that Sequoia has demonstrated to date is impressive indeed. For a few months prior to the transition to classified work and the access limitation that entails, university and national laboratory researchers conducted unclassified basic-science research on Sequoia. These science code and multiphysics simulation runs helped unearth a number of previously undetected hardware and software bugs and provided scientists with a preview of Sequoia’s capabilities, while accomplishing compelling research.

Over the course of the science runs, Sequoia repeatedly set new world records for core usage and speed.

The Livermore–IBM-developed Cardioid code, which rapidly models the electrophysiology of a beating human heart at near-cellular resolution, was the first to use more than a million cores and the first to achieve more than 10 petaflops in sustained performance. Cardioid clocked in at nearly 12 petaflops while scaling with better than 90-percent parallel efficiency across all 1,572,864 cores on Sequoia. Scientists hope to use Cardioid to model various heart conditions and explore how the heart responds to certain medications. (See S&TR, September 2012, pp. 22–25.) In another study, HACC, a highly scalable cosmology simulation created
by Argonne National Laboratory, achieved 14 petaflops on Sequoia (or 70 percent of peak) in a 3.6 trillion particle benchmark run. Argonne’s code is designed to help scientists understand the nature of dark matter and dark energy. The HACC and Cardioid projects were 2012 finalists in the prestigious Gordon Bell competition for achievement in HPC.

Using a sophisticated fluid-dynamics code called CharLES, researchers at Stanford University’s Center for Turbulence Research modeled noise generation for several supersonic jet-engine designs to investigate which design results in a quieter engine. A calculation that had taken 100 hours to run on Dawn took just 12 hours on Sequoia. In one of the final science runs, a plasma physics simulation performed by Livermore scientists using the OSIRIS code also displayed magnificent scaling across the entire machine. This run demonstrated that, with a petascale computer, researchers can realistically model laser–plasma interactions at the necessary scale and speed for optimizing experimental designs used in a fusion approach called fast ignition.

In July, following a period for classified code development, science runs, and system optimization, Sequoia will become the first advanced architecture system to shoulder ASC production environment simulations for Livermore, Los Alamos, and Sandia national laboratories. Before now, stockpile stewardship and programmatic milestones were met using commercial-grade capability systems. Sequoia will serve primarily as a tool for building better weapons science models and quantifying error in weapons simulation studies. By supporting computationally demanding, high-resolution, three-dimensional physics simulations, Sequoia will allow researchers to gain a more complete understanding of the physical processes underlying past nuclear test results and the data gathered in nonnuclear tests. Weapons science results such as these may be used to improve integrated design calculations, which are suites of design packages that simulate the safety and reliability of a nuclear device.

Integrated design calculations are the target for Sequoia’s uncertainty quantification (UQ) efforts. Researchers have endeavored to incorporate UQ into their annual weapons assessments to better

Uncertainty quantification (UQ) uses statistical methods to determine likely effects of minor differences in input parameters. This chart displays the primary roles of key past, present, and future National Nuclear Security Administration resources responsible for performing UQ calculations of weapons codes. Trinity and Cielo are located at Los Alamos National Laboratory, while Purple, Sequoia, and Sierra are Livermore supercomputers. (D = dimensional.)
understand and reduce sources of error in these studies. Until now, they lacked the computing resources to perform UQ at the desired scale and level of mathematical rigor. Scientists conducting UQ analyses will run many integrated design calculations simultaneously on Sequoia and examine how the outcomes are affected by slight variations in the input parameters. A complete study could involve hundreds or thousands of runs. Sequoia will be the first system to allow for the routine use of twodimensional UQ studies at high resolution; it will also be capable of entry-level three-dimensional UQ studies. Routine, highly resolved, three-dimensional UQ must await more powerful platforms, such as the Livermore Sierra system slated to go into production in 2018.

As a platform for both UQ and weapons science research, Sequoia is a powerful resource that will improve the predictive capability of the ASC Program. These capabilities have broader national security applications as well, according to computational physicist Chris Clouse. “It’s not just about predicting an aging stockpile,” says Clouse. “We also need powerful computers and UQ to understand the weapons design of proliferant nation states or organizations, for instance, where we don’t have a large test base for calibration.”

Experts Prepare for the Unknown

Sequoia serves a vital function beyond weapons research. Still remarks, “Sequoia is both a production platform for UQ and weapons research and an exploration platform for future architectures. It really serves an amazing role as a prototype for advanced technology and as a way to develop a system strategy that will propel us forward.” Finding the ideal recipe for an exascale computer that balances power-consumption limits, memory and communications requirements, programmability, space limits, and many other factors may take some years. However, using Sequoia, Livermore programmers can explore how best to exploit both new and potentially enduring architectural elements, such as shared memory, vast quantities of cores, and hardware threading. Whatever the future of computing might bring, ASC codes need to be compatible. To that end, Still is leading a Laboratory Directed Research and Development project, using Sequoia, to make codes more architecturally neutral.

Livermore computational experts aim to do far more than simply react to computer architecture trends, though. Even during Sequoia’s integration, Laboratory researchers were developing a research portfolio to propel innovation and prepare for exascale computing. Through efforts such as NNSA’s Fast Forward Program and in partnership with HPC companies, they have begun exploring potential computer technologies and testing prototype hardware in Livermore environments and with Livermore simulations. Given NNSA laboratories’ expertise in leading-edge HPC and their history of successful code development with hardware companies, a collaboration between laboratory and industry experts has an excellent chance of addressing the obstacles on the path to exascale supercomputing, while ensuring that next-generation computer designs continue to meet ASC Program and other mission-driven needs.

Says McCoy, “Our Laboratory’s intellectual vitality depends on our staying in a leadership position in computing, from the perspective not only of the weapons program but also of every scientific endeavor at Livermore that depends on vital and world-class computing. The 21st-century economy will depend on using HPC better than our competitors and adversaries.” The knowledge and vision that have helped make Sequoia a success have also positioned Lawrence Livermore to help forge a path to a new era of computing.

—Rose Hansen

Key Words: Advanced Simulation and Computing (ASC); BlueGene; Cardioid; exascale; hardware threading; high-performance computing (HPC); Leadership in Energy and Environmental Design; Linpack; message-passing interface (MPI); parallel computing; single-instruction, multiple-data (SIMD) unit; stockpile verification; uncertainty quantification (UQ).

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EMPLOYEES, retirees, and friends of Lawrence Livermore gathered earlier this year to celebrate the achievements of one of the Laboratory’s pioneering scientists and greatest leaders. Recognized for six decades by presidents from Dwight D. Eisenhower to George W. Bush, Johnny Stuart Foster, Jr., was honored during a celebration on January 24 marking his 90th birthday, which occurred four months earlier on September 18, 2012.

In hosting the daylong celebration, Director Parney Albright called the Laboratory’s fourth director “one of the truly great leaders of our nation” and “one of the founding and continuously guiding fathers” of Lawrence Livermore. Albright thanked him for a lifetime of contributions to the Laboratory, including counseling every succeeding Livermore director. In recognition of Foster’s 70 years of service to the nation that established an unparalleled level of technical credibility, Director Albright announced the establishment of the Johnny Foster Medal for outstanding contributions to national security.

Ernest O. Lawrence Protégé

A protégé of Livermore cofounder Ernest O. Lawrence, Foster is widely respected for his frank, impartial, and perceptive advice to national leaders covering a broad range of defense issues. One of the earliest physicists to arrive at the Laboratory from the University of California (UC) Radiation Laboratory in Berkeley, California, Foster was the first leader of Livermore’s B Division (the group that focuses on the nuclear weapon’s “primary” or so-called nuclear trigger). He later became director of the Laboratory in 1961. Foster wrote several classified technical papers during his Livermore career that remain the foundation of the entire U.S. nuclear deterrent. The September 1962 issue of LIFE magazine named him one of the 100 most important young men and women in the nation. In 1965, Foster was named director of Defense Research and Engineering for the Department of Defense, serving for eight years under former presidents Lyndon B. Johnson and Richard M. Nixon until 1973, when he became a vice-president of TRW, Inc.

After retirement in 1988, he joined the boards of directors of a number of corporations. Today, Foster is a member of several defense-related advisory committees and task forces. He also remains active as a national security consultant and continues to advise the Laboratory’s senior leadership and technical workforce. He has won many awards for service to the nation, among them the E. O. Lawrence Award, the James Forrestal Memorial Award, three Department of Defense Distinguished Public Service Medals, the
Contributions of Johnny Foster

Founders Award from the National Academy of Engineering, the Enrico Fermi Award, and the Department of Defense Eugene G. Fubini Award.

Celebration Comprised Two Main Events

The first event of the day began with a roundtable discussion of technical challenges for Livermore’s early nuclear weapons program and current national security challenges. (See the box on p. 17.) A second afternoon event honored Foster’s lifetime of leadership with notable speakers that included Ellen Tauscher, former congressional representative and Under Secretary of State for Arms Control and International Security; Harold Agnew, former director of Los Alamos National Laboratory; Miriam John, former vice president of Sandia National Laboratories; and Mike May, Bruce Tarter, and George Miller, former directors of Livermore. A prerecorded tribute by U.S. Air Force General (Retired) Larry Welch of the Department of Defense was also played. Finally, Foster discussed his experiences as scientist, Laboratory director, and adviser and shared his thoughts about the Laboratory’s and the nation’s future. Between the morning and afternoon events, Foster met with young Livermore weapons scientists.

“Johnny was instrumental in shaping the Laboratory as we know it today,” said Miller. “He helped create the focus on technical excellence, innovation, and critical thinking that characterizes the culture of the Laboratory.” This culture, Miller suggested, reflected what Foster learned at Berkeley under Professor Lawrence. They worked on technically risky but highly important programs and “established an informal management

Foster recalled the formation of a Livermore branch of the University of California Radiation Laboratory in Berkeley. (The Radiation Laboratory was later renamed the Ernest O. Lawrence Radiation Laboratory after the death of Lawrence in 1959.) In the background is a photo of a historically significant 1962 visit to the Berkeley site by President John F. Kennedy. The visit included (from left) Norris Bradbury, director of the laboratory in Los Alamos; Foster, director of the Livermore site; Edwin McMillan, director of the Berkeley site; Glenn Seaborg, chairman of the Atomic Energy Commission; President Kennedy; Edward Teller, cofounder and former director of Livermore; Secretary of Defense Robert McNamara; and Harold Brown, director of Defense Research and Engineering (not shown).
Miller pointed to Foster’s “extraordinarily broad” national security interests and noted that under Foster’s directorship, the Laboratory’s inertial confinement fusion, biology, and intelligence programs were born. “The breadth of his knowledge and his expertise in the national security arena have made him an invaluable asset to policy makers in Washington, led to his appointment to leadership positions in the Department of Defense, and later recruitment by industry,” Miller said. “His technical accomplishments are remarkable, and his words ring as true to me today as they did more than 40 years ago. He continues to be an inspiration to all of us.”

May said, “Johnny and his colleagues essentially revolutionized the way the U.S. stockpile would look from then on, in particular the SLBM [submarine-launched ballistic missile].” May noted that B Division always remained “Johnny’s pride and joy. I learned more about leadership from Johnny than I have from anyone else. He knew how to motivate people so they contributed more than they ever knew they could contribute. Above all, he has never lost his faith and his belief in the Lab’s mission and its importance.”

Competing with Los Alamos

Agnew declared, “The best thing that ever happened to LANL [Los Alamos National Laboratory] was the founding of Livermore.” He explained, “We were fat and sassy. We thought we knew everything. All of a sudden, we realized we didn’t when Livermore, Johnny, and his compatriots started to compete.”

Agnew recalled a historic meeting in 1956 to discuss the U.S. Navy’s desire to arm its submarines with ballistic missiles but of a much smaller size than land-based missiles. At the meeting, both Los Alamos and Livermore leaders gave presentations on what they considered possible for meeting the Navy’s requirements. Livermore cofounder Edward Teller presented an imaginative solution that Los Alamos scientists did not consider feasible. However, Foster, along with his A Division counterpart and future Laboratory Director Harold Brown, helped turn Teller’s concept into reality by leading an intense development effort at the young laboratory that produced a warhead suitable for the Navy’s Polaris submarine fleet.

“That was the beginning of the Navy’s nuclear deterrent program,” said Agnew. “It was Johnny who ran with the ball, and that really shook up things at Los Alamos and changed the attitude there about how one would design future warheads.”

John noted that Foster was instrumental in starting Sandia’s California facility. In the mid-1950s, Foster was making regular 12- to 15-hour trips to Sandia’s headquarters in Albuquerque, New Mexico. He suggested as an efficiency measure that managers
send some Sandia people to Livermore where they could use the empty barracks across the street from Lawrence Livermore as an “initial base camp.” Within three years, the first contingent of about a dozen Sandia people had grown to 1,000 people working in Livermore.

**Never Stopped Learning**

In a videotaped message, General Welsh recounted his first meeting with Foster 45 years ago, when Welsh was a young major. In discussing a proposed aircraft development program with Foster, Welsh said, “I probably learned more in 1 hour than in the previous 10 years.” He also noted, “Foster was relentless about the need to examine your assumptions, look at programs to see what you had missed and what could go wrong that you hadn’t thought of.” Over the years, Foster became the “go-to person” for difficult defense-related problems. “He never stopped learning, he never stopped digging, and he never stopped giving great advice. Dr. Johnny Foster is a great American. He’s a great leader, and he’s a great friend.”

Calling him “the world’s greatest single-person red team [experts providing an impartial review of a system or strategy],” Tarter described Foster’s arguments as “always persuasive, often forceful, but never strident and never apocalyptic.” Tarter, who led the planning for the event, wrote in an invitation to employees, “To understand where we’re going and understand the enduring spirit of the Lab, it is important to know where we came from. Johnny

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**Reuniting B Division Leaders**

The morning session celebrating Johnny Foster featured a roundtable that reunited 9 of Livermore’s 10 living B Division leaders. (See the photo at right.) The wide-ranging discussion covered key weapon-design challenges during Livermore’s formative years as well as issues current scientists face in keeping the nation’s aging nuclear forces reliable, safe, and secure. Bruce Goodwin called Foster “my number one technical hero.” He added, “There were three technical ideas that transformed nuclear weapons, that miniaturized nuclear weapons, and they came from this Laboratory, and Johnny wrote those papers.”

The impact of those papers, said Michael Anastasio, was “the validation of Lawrence Livermore as a real nuclear weapons institution.” What’s more, all the modern features of nuclear weapons were invented, developed, and demonstrated by “Johnny and his team” in the early to mid-1950s. “If you think of the tools they had available to them, it was pretty remarkable they were able to achieve what they did, but the inspiration came from Johnny himself,” Anastasio said.

Participants also credited Foster for inspiring efforts to develop safety features into warhead designs that make it nearly impossible for a nuclear detonation to occur if a weapon is dropped or fired on. Anastasio added that one of Foster’s greatest achievements was mentoring several generations of weapons scientists and leaders, and he counted himself one of Foster’s many disciples.

In later reflections on the day honoring Foster, Mike Dunning noted that at the age of 90, Foster still consults on special projects for Livermore’s Weapons and Complex Integration Principal Directorate and B Division. “It’s like he’s part of our team,” he said. “Johnny remains a very inspirational figure.” As an example, during the day Foster found time to meet with early-career weapons scientists, who “came out of the meeting glowing,” Dunning reported.
Foster is emblematic of the spirit that put Livermore on the global map. We owe him a debt of gratitude.”

In 2008, Tarter was a member of a group charged by then Congresswoman Tauscher, chair of the Strategic Subcommittee of the House Armed Services Committee, to write a report on the future of the nation’s strategic weapons. Tarter recalled that Foster was instrumental in helping the politically divided group reach consensus.

For her part, Tauscher called Foster “Indispensable Johnny on the Spot.” She said, “You and your name have become synonymous with credibility, honesty, integrity, and just being the best.” Tauscher also recalled Foster’s key role in working across partisan lines to produce the strategic future report, which served as a “primer” for the most recent Department of Defense Nuclear Posture Review.

**Belonging to the “Lawrence Family”**

Clearly moved by the day of accolades and warm thanks for a career spanning seven decades, Foster remarked, “The day has been total immersion for me, and I’m humbled, and I don’t know how to handle it.”

Following military service in World War II, where he worked on radar countermeasures, Foster joined the UC Radiation Laboratory (now Lawrence Berkeley National Laboratory) as a graduate student under Professor Lawrence. At the Radiation Laboratory, he spent most of his time building accelerators used to discover new subatomic particles, nuclear isotopes, and nuclear interactions. “These folks were shaking the tree of knowledge, and the isotopes were falling down in droves,” he said.

Foster recalled the Radiation Laboratory employees as being “one big family.” As head of the family, Professor Lawrence noticed one day that Foster was riding a motorcycle and ordered him to get rid of it because he had gone “too many mean free paths [the average distance a moving particle or molecule travels between collisions].” Foster said that many of the characteristics that make Lawrence Livermore unique, such as following the matrix management approach (forming collaborative teams of physicists, chemists, engineers, and others), were inherited from Lawrence and his Berkeley laboratory.

The decision to start a second nuclear weapons lab had followed several years of controversy over whether to have a competitive weapons laboratory. Lawrence and Teller decided to site such a lab at an abandoned naval air base in Livermore and organize it as a branch of the Radiation Laboratory in Berkeley. In 1952, Foster was among the first group of scientists to arrive from Berkeley. The fledgling scientific group, which included first Laboratory Director Herb York, May, Teller, and others, was charged with taking nuclear design approaches different from those adopted by Los Alamos.

Foster said, “The Livermore Lab was established in the midst of a heated political and military controversy and always faced the threat of being shut down, and that helped provide the incentive to perform so well.” In fact, the first two tests of a Livermore warhead, a novel but risky design, were embarrassing failures. However, within a few years, the new laboratory was deemed a worthy competitor to Los Alamos, and many of Livermore’s design breakthroughs are still reflected in the current U.S. strategic arsenal. Foster refused to take major credit for those successes. “A lot of people had a hand in those projects, and their successful execution was because of the hard work of dozens and in some cases thousands of people.”

In discussing the Laboratory’s pioneering contributions to the nation over the past half-century, Foster mentioned advances in many fields of science and technology. As examples, he cited controlled thermonuclear reactors, the magnetic mirror concept for fusion energy, ballistic missile defense, defensive weapons using high-energy particle beams, x-ray lasers (the only weapon condemned by a Russian leader, he noted), Brilliant Pebbles (the center of the Strategic Defense Initiative that helped lead to the Soviet Union breakdown), the Clementine mission to the moon, Project Plowshare (clean thermonuclear explosives for civilian applications), ultrahigh-power and energy lasers, communication with submerged submarines, computer modeling of Earth’s weather patterns, supercomputer efforts, underground nuclear power reactors, and computer-aided design.

Looking to the future, Foster said, “It should be the responsibility of the leaders of this Lab to accept the burden of the initiative to stimulate the Laboratory to come up with game-changing innovations in science, technology, processes, and products.” He commented, “Life is tough. But we all remember what the tough characteristically do when the going isn’t easy. It’s up to you to help the folks in Washington, D.C., to improve processes and see the relevance of what we do for national security.” He added, “The Lab must use its record of accomplishments to continue attracting the best and the brightest.”

—Arnie Heller

**Key Words:** B Division, Ernest. O. Lawrence, Johnny Stuart Foster, Jr., Lawrence Radiation Laboratory, Los Alamos National Laboratory, Nuclear Posture Review, nuclear weapons, Sandia National Laboratories, University of California (UC) Radiation Laboratory.

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We know that diamond is the hardest, strongest form of carbon on Earth. However, under extreme pressures—similar to those deep inside giant planets such as Saturn or Jupiter—diamond becomes something quite different. In recent experiments, a team of scientists from Lawrence Livermore, Princeton University, and the University of California at Berkeley compressed diamond samples to a density greater than lead at ambient conditions. The team’s experimental results access a previously unexplored region of carbon’s phase diagram.

The research team, led by Livermore physicist Ray Smith, performed its unprecedented experiments at the National Ignition Facility (NIF), which houses the world’s largest, most powerful laser. The researchers used a relatively new technique called laser ramp compression to apply extraordinarily high pressures, up to 5 terapascals, or 50 million times ambient air pressure, to the diamond samples and compress them to almost 4 times their normal density.

Keeping Cool at High Pressures
Laser ramp compression joins two other methods for applying very high pressures to materials. One uses tiny anvils of diamond to very slowly compress a substance. Diamond-anvil-cell experiments can achieve pressures of 300 gigapascals,
Four sample thicknesses of synthetic diamond are mounted on the outside of a hohlraum capsule in ramped compression experiments at NIF. The layered diamond target absorbs x-ray energy emitted when laser beams converge inside the hohlraum. The x rays ablate the initial diamond layer, which induces ramp compression throughout the stepped sample. Measuring the speed at which each sample thickness moves during the experiment (as shown in the graph) helps researchers better understand material behavior at high pressure.

Shock experiments have for years been the standard method for studying the interplay of pressure, density, and temperature, which describes a material’s equation of state (EOS). Every model that explains how a material deforms at high pressures—which occurs in planetary interiors and during explosions—assumes an understanding of the material’s EOS.

However, a model of a planet’s interior cannot be based on EOS data gathered at high temperature. Compression in these bodies occurs from gravitational force over long periods. Those processes are inherently shock free, and thus, the matter remains much cooler than in shock compression experiments. Expanding EOS data into this realm of high pressures and low temperatures requires laser ramp compression, in which researchers carefully control the laser pulse shape to avoid shocking the material and thereby maintain its solid phase.

**Ramping without Shock**

In previous experiments to study other materials at lower pressures, Smith’s team used the OMEGA laser at the University of Rochester’s Laboratory for Laser Energetics and the Janus laser at Lawrence Livermore. (See S&TR, June 2009, pp. 22–23.) The NIF laser offers unique advantages for performing ramp-compression experiments. NIF allows scientists to arbitrarily control the laser’s energy to customize the pressure wave exerted on the sample and deliver very high-pressure, shock-free compression.

In the NIF experiments, 176 of the laser’s 192 beams converge in the target chamber on a tiny cylindrical hohlraum, creating powerful x rays that ablate the back side of a synthetic
diamond target placed outside the hohlraum. The ablation process drives a compression wave through the target. The front of the diamond target is “stepped” to create four thicknesses, ranging from 140 to 172.5 micrometers, to generate multiple data points. The Livermore team used the diagnostic tool VISAR (Velocity Interferometer System for Any Reflector) to record the compression wave’s arrival time and its speed at each step. Iterative Lagrangian analysis of the collected data revealed the stress, density, and sound speed of the diamond at high pressures.

The team had developed a playbook for the laser shots based on detailed modeling using LASNEX, a radiation hydrodynamics code that models the full geometry of the hohlraum, capsule, and interacting laser light during an experiment. However, shots would be occurring in an entirely new realm of pressures and densities. Although considerable experimental data are available up to about 1 terapascal, less information exists above that pressure, and virtually none beyond 2 terapascals.

In four shots, or individual experiments, the team systematically increased the ramp-compression drive from 2.2 to 5 terapascals. The pulse shape used for the first shot at 2.2 terapascals produced some shock in the diamond target. A modified pulse shape eliminated the shock and achieved higher pressures of 2.7 terapascals. The third and fourth shots also did not produce shocks and took pressures even higher to 3.7 and 5 terapascals, which is somewhat higher than the expected core pressure of Saturn. Future experiments are planned to exert pressures on diamond to 7 terapascals, which scientists believe to be the pressure in the deep center of Jupiter.

The Livermore researchers demonstrated that diamond is compressed 3.7-fold at a peak pressure of 5 terapascals. Their findings provided the first experimental data above 3 terapascals for use by theorists and in planet evolution models. The NIF experiments also provided data to improve the predictions of the LASNEX code. In preliminary experiments performed before the final four, scientists determined that LASNEX overpredicted the ablation rate and peak pressure as a function of peak laser power. “The samples did not become as dense as we expected,” says Smith. “They were surprisingly stiff and resistant to being compressed.”

Solving the Mystery

In the summer of 2013, a novel x-ray diffraction capability will be used to probe the samples to reveal the changes in their crystal structure at these unprecedented high pressures. The experiments may explain why the ramped samples were less compressible than expected. Furthermore, with measurements of specific changes at various pressures, scientists can begin to develop an EOS for carbon under previously unexplored conditions relevant to those found within planetary interiors.

—Katie Walter

Key Words: carbon, diamond, equation of state (EOS), laser ramp compression, National Ignition Facility (NIF), planetary interiors, Velocity Interferometer System for Any Reflector (VISAR).

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Coming Through in a Pinch
Z-Pinch Plasma Heralds Novel Accelerator Designs

(right) Vincent Tang and Andréa Schmidt work on Livermore’s dense plasma focus Z-pinch device. (above) The plasma forms and the Z-pinch occurs in the gun (shown here detached from the device).
ARTICLE accelerators are a fundamental tool of modern science for advancing high-energy and nuclear physics, understanding the workings of stars, and creating new elements. The machines produce high electric fields that accelerate particles for use in applications such as cancer radiotherapy, nondestructive evaluation, industrial processing, and biomedical research. The steeper the change in voltage—that is, the more the voltage varies from one location to another—the more an accelerator can “push” particles to ever-higher energies in a short distance.

With current accelerator technologies, electric-field gradients for ion accelerators are limited to approximately 30 megavolts per meter and low peak currents. However, all that may change, thanks to research conducted by Livermore’s Vincent Tang, Andréa Schmidt, Jennifer Ellsworth, Steve Falabella, and Brian Rusnak to better understand the acceleration mechanisms in Z-pinch machines. Scientists may eventually be able to use Z-pinches created from dense plasma foci for compact, scalable particle accelerators and radiation-source applications. With this simple technology, electric-field gradients greater than 100 megavolts per meter and with kiloampere-class peak currents may be possible.

Bringing Z-Pinch into Focus

In its simplest form, a Z-pinch device uses the electric current in a plasma to generate a magnetic field that compresses the plasma, or “pinches it down.” The “Z” designation refers to the direction of the current in the device: the z axis in an x, y, z (three-dimensional) coordinate space. “This simple plasma configuration was the first one to be identified,” says Tang, an engineer who led the Z-pinch research. He explains that the static spark one gets between a doorknob and a finger is a type of Z-pinch plasma in nature. “In a basic laboratory setup,” says Tang, “one runs a current through two plates, the current ionizes a gas and forms a plasma, and the plasma then self-pinches.” In a Z-pinch machine, a cylinder of plasma (ionized gas) collapses on itself, momentarily producing extremely high temperatures and pressures at the center of the cylinder as well as very high electric fields.

Z-pinches have been a subject of interest since the 1950s, when they were explored as a possible avenue for creating fusion power. At that time, research with pinch devices in the United Kingdom and U.S. proliferated. However, instabilities in the plasma led to this effort being abandoned. “Still,” says Tang, “the experiments created neutrons—a classic signal of fusion. It just wasn’t thermonuclear fusion, which is what scientists thought was needed to achieve energy gain.”

Nuclear fusion was one of Tang’s interests in graduate school, so he had Z-pinch devices in mind when, in 2007, he was working on research involving compact directional neutron sources at Livermore. “I had just read a few papers on the high-electric-field gradients produced in Z-pinch devices. In the past, most people weren’t interested in specifically using the electric fields produced in a Z-pinch. The fields were considered a by-product and a nuisance, because most researchers were focused on using the devices for thermonuclear fusion. I brought up the possibility of using these fields for some of our accelerator applications to my colleague Brian Rusnak.” However, such machines were not well enough understood to harness the electric-field gradients they produced. “It was essentially a wide-open field of inquiry, with many unknowns,” says Tang.

Put the Pinch under the Microscope

In the fall of 2010, Tang obtained Laboratory Directed Research and Development (LDRD) funding to better understand fast Z-pinches and demonstrate that they could
accelerate particles such as protons and deuterons. Tang and his team combined new simulation and experimental approaches in their research. They concentrated their efforts on Z-pinches generated by dense plasma focus (DPF) devices. These devices have high-electric-field gradients, are technologically simple, and have open geometries that allow for beam injection and extraction.

A DPF Z-pinch consists of two coaxially located electrodes with a high-voltage source connected between them, typically a capacitor bank. When the high-voltage source is energized with a low-pressure gas in the chamber, a plasma sheath forms at one end of the device. In the “run down” phase, the plasma sheath is pushed down the outside length of the inner electrode, ionizing and sweeping up neutral gas as it accelerates. “One can think of it as essentially a plasma rail gun,” Tang explains. When the plasma sheath reaches the end of the electrode, it begins to collapse radially inward during the “run in” phase. In the final pinch phase, the plasma implodes, creating a high-density region that typically emits high-energy electron and ion beams, x rays, and neutrons.

For the simulation side of the research, the team turned to a fully kinetic, particle-scale simulation, using the commercially available LSP code for modeling a DPF device. LSP is a three-dimensional, electromagnetic particle-in-a-cell code designed specifically for large-scale plasma simulations. The code calculates the interaction between charged particles and external and self-generated electric and magnetic fields.

Schmidt, who leads the simulation effort, explains, “We had to use the more computationally intensive particle approach instead of a fluid approach because the plasma distribution functions are not Maxwellian. The ions form beams when they accelerate, and high electric fields are created partially through kinetic electron instabilities that are not modeled in a fluid code. Until recently, though, we just didn’t have the computing power or the tools to model a plasma particle by particle.”

With LSP running on 256 processors for a full week on Livermore’s Hera machine, the team became the first to model what happens in the pinch process at the particle scale. The results of the simulations reproduced experimental neutron yields on the order of $10^7$ and megaelectronvolt-scale high-energy ion beams. “No previous, self-consistent simulations of DPF pinch have predicted megaelectronvolt ions, even though ion energies up to 8 megaelectronvolts have been measured on kilojoule-class DPF devices,” notes Schmidt.

The team also compared its results with those from simulations performed with fluid codes and with hybrid codes that combine aspects of kinetic and fluid codes. “The fluid simulations predicted zero neutrons and were not capable of predicting ion beams, says Schmidt. The hybrid simulations underpredicted the experimental neutron yield by a factor of 100 and did not predict ions with energies above 200 kiloelectronvolts. The more complex, fully kinetic simulation was necessary to get the physics right.”

The team also designed, fabricated, and assembled a tabletop DPF experiment to directly measure the acceleration gradients inside the Z-pinch. The first gradient recorded was a time-of-flight measurement of the DPF’s self-generated ion beam using a Faraday cup. “These measurements, made during subkilojoule DPF operation, now hold the record for the highest measured DPF gradient in that energy class,” says Ellsworth.

A second and more sophisticated measurement of the gradient is now under way. The team has refurbished a radio-frequency-quadrupole accelerator to make an ion probe beam for the pinch plasma. (See the figure on p. 25.) The accelerator produces a 200-picosecond, 4-megaelectronvolt ion probe beam, which

Deuterium ion density is shown inside this first fully kinetic simulation of a dense plasma focus Z-pinch. The pinch occurs on axis where the density is highest (red). The cross section of a cylindrical hollow anode is shown in gray.
An artist’s rendering shows the formation of a plasma sheath (purple) and Z-pinch (white), along with the injection and acceleration of a probe beam (green) through the pinch plasma. (Rendering by Kwei-Yu Chu.)

is injected into the hollow center of the DPF gun just as the pinch occurs. The researchers will use this tool to measure the acceleration of the probe beam through the Z-pinch. From that, they will deduce the acceleration gradient of the plasma and demonstrate the possibility of using the Z-pinch as an acceleration stage. “The probe-beam experiments will directly measure for the first time the particle acceleration gradients in the pinch,” says Tang.

Accelerating into a Bright Future

The initial measurements of beam energies, accelerating fields, and neutron yields are promising, matching well with simulation results. “The device is producing high gradients,” says Tang, “and we’re proving that one can use Z-pinches to accelerate injected beams. This research opens a world of possibilities for Z-pinch systems.”

The most advanced application would be the use of Z-pinch devices as acceleration stages for particle accelerators. In addition to being compact, the devices are technologically simple, which means less cost and potentially less to go wrong. They also produce gradients much higher than those obtained with today’s standard radio-frequency stages. Some near-term applications might include using Z-pinch devices to produce well-defined particle beams for nuclear forensics, radiography, oil exploration, and detection of special nuclear materials.

With the LDRD phase of DPF Z-pinch research coming to a close, Tang and his team are exploring various uses of a Z-pinch device with agencies in the U.S. departments of Energy, Defense, and Homeland Security. “It’s a very exciting time for us,” Tang says. “We now have a predictive capability for this phenomenon. As a result, we have a better idea of what happens in a Z-pinch plasma configuration. We hope to apply this discovery to future generations of accelerators and other areas of research. It’s a fundamental discovery and a contribution to basic science understanding. With this new simulation capability and the ramping up of the probe-beam experiments, we see an exciting future ahead.”

—Ann Parker

Key Words: accelerator, dense plasma focus (DPF) device, LSP code, particle beam, Z-pinch.

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Dual Isotope Notch Observer for Isotope Identification, Assay and Imaging with Mono-Energetic Gamma-Ray Sources

Christopher P. J. Barty
U.S. Patent 8,369,480 B2
February 5, 2013

A dual isotope notch observer for isotope identification, assay, and imaging with monoenergetic gamma-ray sources includes a detector arrangement with three detectors downstream from the object under observation. The third detector, which operates as a beam monitor, is an integrating detector that monitors the total beam power arriving at its surface. The first and second detectors each include an integrating detector surrounding a foil. The foils of these two detectors are made of the same atomic material, but each foil is a different isotope. For example, the first foil may comprise uranium-235, and a second foil may comprise uranium-238. The integrating detectors surrounding these pieces of foil measure the total power scattered from the foil and can be similar in composition to the final beam monitor. Nonresonant photons will, after calibration, scatter equally from both foils.

Method and Computer Program Product for Maintenance and Modernization Backlogging

Bernard G. Mattimore, Paul E. Reynolds, Jill M. Farrell
U.S. Patent 8,360,550 B2
February 19, 2013

In one embodiment, this computer program for determining future facility conditions includes a computer-readable medium with a computer-readable program code. The code will calculate a time-period-specific maintenance cost, modernization factor, and backlog factor. Future facility conditions equal the time-period-specific maintenance cost plus modernization factor plus backlog factor. In another embodiment, a computer-implemented method calculates a time-period-specific maintenance cost, modernization factor, and backlog factor. Future facility conditions equal the time-period-specific maintenance cost plus modernization factor plus backlog factor. Other embodiments are also presented.

Diagnosis and Assessment of Skeletal Related Disease Using Calcium-41

Darren J. Hillegonds, John S. Vogel, Robert L. Fitzgerald, Leonard J. Deftos, David Herold, Douglas W. Burton
U.S. Patent 8,388,930 B2
March 5, 2013

A method of determining calcium metabolism in a patient comprises the steps of administering the radioactive isotope calcium-41 to the patient and allowing time to elapse sufficient for dissemination and reaction of the calcium-41 by the patient. A sample of the calcium-41 is then obtained from the patient, and its calcium content is isolated in a form suitable for precise measurement of isotopic calcium concentrations. Finally, the calcium content is measured to determine parameters of calcium metabolism in the patient.

Method and System for Laser-Based Formation of Micro-Shapes in Surfaces of Optical Elements

Isaac Louis Bass, Gabriel Mark Guss
U.S. Patent 8,389,889 B2
March 5, 2013

A method of forming a surface feature extending into a sample includes providing a laser to emit an output beam and modulating the output beam to form a pulse train with a plurality of pulses. The method also includes (a) directing the pulse train along an optical path intersecting an exposed portion of the sample at a position i, and (b) focusing a first portion of the plurality of pulses to impinge on the sample at the position i. Each pulse is characterized by a spot size at the sample. The method further includes (c) ablating at least a portion of the sample at the position i to form a portion of the surface feature, and (d) incrementing counter i. The method includes (e) repeating steps (a) through (d) to form the surface feature. The sample is free of a rim surrounding the surface feature.

Method and System for Assembling Miniaturized Devices

Richard C. Montesanti, Jeffrey L. Klingmann, Richard M. Seugling
U.S. Patent 8,393,066 B2
March 12, 2013

An apparatus for assembling a miniaturized device includes a manipulator system with six manipulators to position and orient components of the miniaturized device with submicrometer precision and micrometer-level accuracy. The manipulator system includes a first plurality of motorized axes, a second plurality of manual axes, and force and torque sensors. Each of the six manipulators includes at least one translation stage, at least one rotation stage, tooling attached to at least one translation stage or one rotation stage, and a mechanism disposed at a distal end of the tooling for attaching at least a portion of the miniaturized device to the tooling. The apparatus also includes an optical coordinate-measuring machine (OCMM) including a machine-vision system, a laser-based distance-measuring probe, and a touch probe. The apparatus also includes an operator control system coupled to the manipulator system and OCMM.

Catalyst Functionalized Buffer Sorbent Pebbles for Rapid Separation of Carbon Dioxide from Gas Mixtures

Roger D. Aines
U.S. Patent 8,394,351 B2
March 12, 2013

A method for separating carbon dioxide from gas mixtures uses a slurried media impregnated with buffer compounds. The solid media is coated with a catalyst or enzyme that promotes the transformation of carbon dioxide to carbonic acid. Buffer sorbent pebbles with a catalyst or enzyme coating are used for rapid separation of carbon dioxide from gas mixtures.

Synthesis of Triazole-Based and Imidazole-Based Zinc Catalysts

Carlos A. Valdez, Joe H. Satcher, Jr., Roger D. Aines, Sarah E. Baker
U.S. Patent 8,394,351 B2
March 12, 2013

Various methods are described herein related to a zinc-centered catalyst for removing carbon dioxide from atmospheric or aqueous environments. According to one embodiment, a method for creating a tris(triazolyl) pentaerythritol molecule includes connecting a pentaerythritol molecule with a propargyl halide molecule to create a trialkyne molecule, and connecting the trialkyne molecule with an azide molecule to create the tris(triazolyl)pentaerythritol molecule. In another embodiment, a method for creating a tris(imidazolyl)pentaerythritol molecule includes alkylating an imidazolyl 2-carbaldehyde molecule to create a monoalkylated aldehyde molecule, reducing the monoalkylated aldehyde molecule to create an alcohol molecule, converting the alcohol molecule to create an alkyl halide molecule using thionyl halide, and reacting the alkyl halide molecule with a pentaerythritol molecule to create a tris(imidazolyl)pentaerythritol molecule. In another embodiment, zinc is bound to the tris(triazolyl)pentaerythritol molecule to create a zinc-centered tris(triazolyl)pentaerythritol catalyst for removing carbon dioxide from atmospheric or aqueous environments.
Method and System for High Power Reflective Optical Elements
Stavros G. Demos, Alexander M. Rubenchik, Raluca A. Negres
U.S. Patent 8,395,079 B2
March 12, 2013
A method of repairing damage in an optical element includes a laser system with at least one optical element. The element has a coating layer with an incident light surface. A pulse from the laser system is directed to impinge on the incident light surface. The method also includes sustaining damage to a portion of the incident light surface and melting this portion and a region adjacent to the damaged portion. The method further includes flowing material from the adjacent region to the damaged portion and solidifying the material in the damaged portion and the region adjacent to it.

Passive Blast Pressure Sensor
Michael J. King, Roberto J. Sanchez, William C. Moss
U.S. Patent 8,397,551 B2
March 19, 2013
A passive blast-pressure sensor detects blast overpressures of a predetermined minimum threshold pressure. The blast-pressure sensor includes a piston–cylinder arrangement. One end of the piston has a detection surface exposed to a blast-event-monitored medium through one end of the cylinder. The other end of the piston has a striker surface positioned to impact a contact-stress-sensitive film. The film is positioned against a strike surface of a rigid body, such as a backing plate. The contact-stress-sensitive film changes color in response to a predetermined minimum contact stress that is defined as a product of the predetermined minimum threshold pressure and an amplification factor of the piston. In this way, a color change in the film arises from the impact of the piston accelerated by the blast event, providing visual indication that a blast overpressure encountered from the blast event was more than the predetermined minimum threshold pressure.

Capacitive De-Ionization Electrode
William D. Daily, III
U.S. Patent 8,398,840 B2
March 19, 2013
An electrode cell used in a capacitive deionization reactor consists of the electrode support structure, a nonreactive conductive material, the electrode accommodation or substrate, and a flow-through screen separator. These “layers” are repeated, and the electrodes are sealed together with gaskets between two end plates to create stacked sets of alternating anode and cathode electrodes.

Aerial Vehicle with Paint for Detection of Radiological and Chemical Warfare Agents
Joseph C. Farmer, James L. Brunk, S. Daniel Day
U.S. Patent 8,409,524 B2
April 2, 2013
This paint is used to detect radiological or chemical substances. The paint is connected to a surface, and a material carried by the paint indicates when a radiological or chemical substance is detected. A thermoactivation material is also carried by the paint. In one embodiment, a surface is painted with an indicator material, and the surface is monitored for indications of a radiological or chemical substance. In another embodiment, the paint is connected to a vehicle, and a material carried by the paint indicates the presence of a radiological or chemical substance.
Awards

Lawrence Livermore was recently recognized by the National Safety Council for its strong and improving safety performance in 2012. The Laboratory exceeded 2 million work hours without a lost-time injury during the period February 15 through April 18. The Laboratory also was recognized for an overall significant improvement in safety performance in 2012 by reducing its lost-work-day frequency rate by more than 25 percent.

Allen Grayson, an environmental scientist in the Environment, Safety, and Health Directorate, was named Person of the Year by the Pretreatment, Pollution Prevention, and Storm Water Committee of the California Water Environment Association (CWEA) at the association’s annual conference in April 2013. Awards in more than 20 categories were presented to agencies and individuals recognized as leaders in the water and wastewater field. Established in 1929, CWEA’s awards program recognizes and honors California water environment professionals, collection systems, and treatment plants.

Grayson has been responsible for water pretreatment issues at Livermore for the past 23 years. He also has been actively involved in CWEA for more than 25 years, serving in numerous leadership positions. In addition, Grayson has been instrumental in conducting outreach efforts among elementary and high school students to help develop an early interest in water treatment careers.

Livermore physicist Yuan Ping was awarded $2.5 million in funding through the Department of Energy’s (DOE’s) Early Career Research Program. The DOE program is designed to bolster the nation’s scientific workforce by providing support to exceptional researchers during the crucial early career years, when many scientists do their most formative work.

“I am very honored and grateful for this great opportunity to do more high-quality work,” says Ping. Her project, selected by the Office of Fusion Research, aims to provide data on critical energy transport properties of high-energy-density (HED) matter. Transport processes, such as thermal and electrical conduction, determine the mechanisms and rates of energy transfer and redistribution within HED matter. A suite of recently developed novel x-ray and optical techniques makes it possible to obtain these challenging measurements.
Reaching for New Computational Heights with Sequoia

Sequoia, Lawrence Livermore’s newest and largest supercomputer, was developed in collaboration with IBM and Argonne National Laboratory. With Sequoia, the Laboratory once again demonstrates its leadership and expertise in the design, commissioning, and application of high-performance computing systems. To enable Sequoia to execute highly complex physics simulations for the National Nuclear Security Administration’s stockpile stewardship mission, IBM and national laboratory experts incorporated software innovations, such as new ways of parallelizing code, and hardware functions, such as transactional memory. As a first-of-its-kind advanced technology machine, Sequoia proved a challenge to install and debug, but the Laboratory and IBM working together systematically addressed the issues encountered. Now that Sequoia has been accepted, researchers are busy putting its incredible power to use. Unclassified simulations produced insights on the electrophysiology of the human heart and turbulent exhaust from jet engines. Going forward, Sequoia will serve primarily as a tool for improving weapons science models, understanding the sources and magnitude of error in weapons studies, and exploring and preparing for exascale, the next great milestone in computing.

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Livermore’s award-winning dynamic transmission electron microscope quickly captures irreversible material processes with nanometer-scale resolution.

Also in September

• With experiments at the National Ignition Facility, scientists can measure the shock effects of a simulated nuclear blast.

• A tabletop device gathers information that cannot be directly measured about neutrons and neutrinos emitted by radioactive nuclei.

• Gravity detectors under development have the potential to spot the heavy shielding that prevents traditional radiological detectors from finding illicit nuclear materials.