Lawrence Livermore National Laboratory

Science & Technology REVIEW

June 2013

Innovative Energy Solutions

Also in this issue:

Meeting the Certification Challenge

A Friendly Competition for Improved Software

About the Cover

High-performance computing (HPC) systems have been a boon for defense- and national security–related research, allowing scientists and engineers to virtually test new processes, design prototypes, and analyze massive data collections. Making these powerful tools more readily available to industries could help address other important problems and foster innovations to enhance U.S. economic security. The article beginning on p. 4 describes the hpc4energy incubator, a pilot program that pairs Livermore computational scientists with industrial partners to apply HPC resources toward energy-related technology development. Beginning in 2012, this yearlong program provided six companies with computational time on the Laboratory's Sierra supercomputer and demonstrated how access to HPC resources and expertise can benefit U.S. industries. (Spray images courtesy of Computational Thermo-Fluids Laboratory, Cornell University.)

Cover design: Daniel S. Moore

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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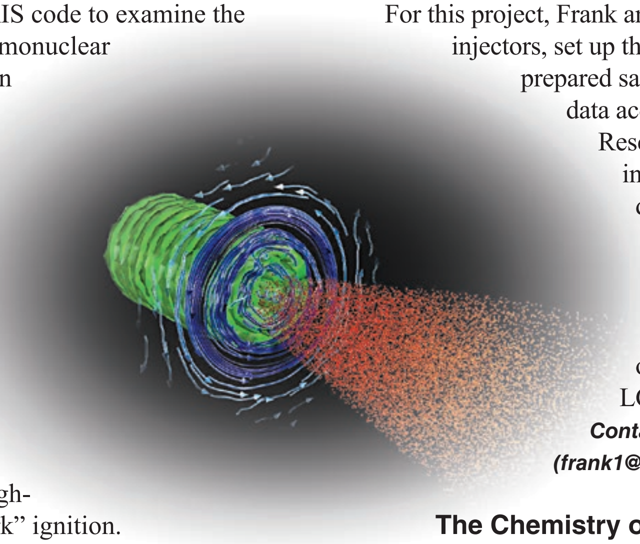
Record Simulations Conducted on Sequoia

In January 2013, Livermore researchers completed the largest particle-in-cell (PIC) simulations ever performed, using all 1,572,864 cores of the Sequoia supercomputing system. Sequoia is an IBM BlueGene/Q machine and the first supercomputer to exceed 1 million computational cores. At peak operation, it can process 20 quadrillion floating-point operations per second.

Frederico Fiuza, a Lawrence Fellow and physicist in the Laboratory's Physical and Life Sciences Directorate, led the simulation effort, which used the OSIRIS code to examine the fast-ignition approach to sustained thermonuclear burn and energy gain (simulation shown at right). In fast ignition, lasers deliver more than 1 petawatt (a million billion watts) of power in less than one-billionth of a second to heat compressed deuterium–tritium fuel to temperatures exceeding 50 million degrees Celsius.



Fast ignition differs from the central hot-spot approach used at the National Ignition Facility in which laser beams simultaneously compress and ignite a spherical fuel capsule. Instead, fast ignition adds a high-intensity, ultrashort-pulse laser to "spark" ignition.

OSIRIS has been developed over more than 10 years in a collaboration involving the University of California at Los Angeles and Instituto Superior Técnico in Portugal. In the record-setting simulations, the code demonstrated excellent scaling on the full Sequoia system. OSIRIS operated at 75-percent efficiency under "strong" scaling, in which a relatively small problem of fixed size is modeled with a large number of cores. It performed even better under "weak" scaling, achieving 97-percent efficiency when the total problem size was increased.

Fiuza notes that processing these large problems can take an entire year on a cluster of 4,000 cores, but Sequoia can produce results in one day. "We can also simulate problems 400 times greater in size in the same amount of time," he says. "Combining this unique supercomputer with the highly efficient and scalable OSIRIS code is allowing for transformative research."

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Breakthrough Research on a Deadly Parasite

An international collaboration involving Livermore physicist Matthias Frank and postdoctoral researcher Mark Hunter has determined the atomic-scale structure of a protein that is key to the survival of the single-celled parasite *Trypanosoma brucei*. *T. brucei* is responsible for African sleeping sickness, which kills 30,000 people each year and debilitates many more. The team's research appeared in the January 11, 2013, issue of *Science* and was recognized as one of the top 10 science breakthroughs in 2012.

Traditional x-ray diffraction studies could not fully characterize the propeptide, or precursor form, of this essential protein, because the enzyme's crystals were not large enough for analysis. The collaboration instead used the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory. In a technique called diffraction before destruction, individual nanometer-size crystals produced by the parasite are passed one by one through the LCLS x-ray beam. The resulting diffraction data on 178,875 nanocrystals were then "stacked" for analysis.

For this project, Frank and Hunter developed the nanoparticle injectors, set up the laser pump probe experiments, prepared samples, modeled damage, and monitored data acquisition during the LCLS experiments.

Researchers will use the structural information obtained in the study to develop drugs that mimic the propeptide, inhibiting the enzyme and thus killing the parasite. The team's achievement also demonstrates that diffraction before destruction is a viable approach for obtaining biomolecular information in LCLS experiments.

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The Chemistry of Boron at Room Temperature

Livermore researchers Tadashi Ogitsu and Eric Schwegler, along with Giulia Galli of the University of California at Davis, have for the first time characterized the element boron at room temperature. In the March 8, 2013, online edition of *Chemical Reviews*, the team describes the history of boron research and details the properties of beta boron—the element's stable form at room temperature—as inferred from experiments and theories.

Boron remains the only element purified in macroscopic quantities for which the ground-state geometry has not been completely determined by experiments. Theoretical progress over the last decade has revealed numerous properties of elemental boron, allowing researchers to thoroughly characterize its structure at ambient conditions as well as its electronic and thermodynamic properties.

Boron sits on the first row of the periodic table in a peculiar, transitional position. The only nonmetal in the third column of the table, it is flanked by metallic elements on its left and nonmetals on its right. The crystallographic structure and topology of beta boron are extremely complex. Beta boron is characterized by interconnecting icosahedra—a regular polyhedron with 20 identical equilateral triangular faces—and partially occupied sites. It also has more than 300 atoms per unit cell, an unusually large number. No other element on the periodic table shares these features.

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Commentary by Dona Crawford

Together, Great Minds and Advanced Computing Boost Innovation

IN an increasingly global marketplace, businesses that use high-performance computing (HPC) often gain a strategic advantage. As demonstrated in the defense, aerospace, and pharmaceutical industries, HPC greatly reduces the time and cost to design, develop, prototype, and deploy new products. A 2003 study by the Council on Competitiveness found that HPC is considered indispensable by nearly all businesses that have adopted it, including some of America's largest companies.

Governments throughout the world are also recognizing how HPC technology can foster industrial innovation and economic competitiveness, and they are thus making strategic, sustained investments in this area. For instance, the Japanese government has teamed with industry to develop computing applications for energy creation, life science studies, and drug discovery. The European Union also maintains strong partnerships with industries that focus on software development.

Through the Department of Energy's economic competitiveness initiatives, several U.S. HPC centers and laboratories—including Lawrence Livermore—are making these large-scale computing resources available to companies both large and small. Today, the Laboratory has established a solid record of successful industrial collaboration in the area of HPC.

Few institutions could hope to match Livermore's array of HPC resources, but our "special ingredient" is our people, who include both computer scientists with applications development, networking, storage, and analysis expertise and scientists and engineers adept at applying HPC to a range of scientific challenges. As described in the article beginning on p. 4, the Laboratory recently concluded a successful one-year collaborative program called the hpc4energy incubator. Six energy companies, chosen through a competition, were paired with talented computer scientists at Livermore to solve a problem or advance an energy-related research effort using the Sierra supercomputing system.

Many industrial firms are working on challenging computational problems, but many more struggle to justify the costs of acquiring large-scale HPC systems and simulation tools and of hiring the knowledge experts needed to effectively use those resources. Efforts such as the hpc4energy incubator are intended to accelerate partnerships with industry and help overcome the roadblocks to broader HPC usage. Energy-related HPC research collaborations, including the six incubator projects, hasten development of efficient and affordable energy solutions. In addition, they protect the country's economic, environmental, and energy security interests, thereby contributing to Livermore's national security mission.

By spurring U.S. companies to incorporate HPC into their workflow, the incubator and related efforts such as Livermore's HPC Innovation Center also serve to increase the user base for supercomputing systems. Expanding the market for existing advanced computing technologies makes it easier and more affordable for institutions such as Livermore to drive development of the next-generation hardware and software required to perform future mission-related work. Solving industrial problems allows us to test simulation tools and applications in a new environment, providing us with valuable feedback. It also widens the experience and skill set of our researchers.

In 2012, the Laboratory adopted a practice found in the computing industry and began holding a series of 24-hour programming competitions called ShipIt days. As described in the article starting on p. 16, these events allow computer scientists from different organizations and topical areas to work on a product of their choosing, provided that it fosters innovation, collaboration, or learning, or it advances a Laboratory mission. ShipIt days not only build camaraderie and encourage creativity, but they also can lead to new ideas for important projects while helping us retain our greatest asset—our people. Given the enthusiastic employee response to the inaugural event, we plan to hold up to four of these competitions in 2013.

Whether tapping their domain expertise to apply HPC to a technical problem, crafting detailed theoretical equations, or writing lines of code to improve a model's accuracy, Livermore engineers and scientists are helping to spur economic competitiveness and technological innovation through the use of advanced computing resources. Initiatives such as hpc4energy and ShipIt demonstrate what really drives innovation: an environment that encourages the cross-fertilization of ideas between disciplines and departments and among businesses, national laboratories, universities, and other research centers. These multidisciplinary research collaborations are a potent catalyst for change.

■ Dona Crawford is associate director for Computation.

Scaling Up Energy Innovation

Computer scientists Pythagoras Watson (left) and Teresa Kamakea work on Sierra, a high-performance computing (HPC) system that can process more than 260 trillion floating-point operations per second. Project teams supported by the hpc4energy incubator, a yearlong pilot program at Livermore, received time on this workhorse machine to accelerate development efforts on energy technologies.

through Advanced Computing

Collaborations through the hpc4energy incubator demonstrate how high-performance computing can help energy companies accelerate their research.

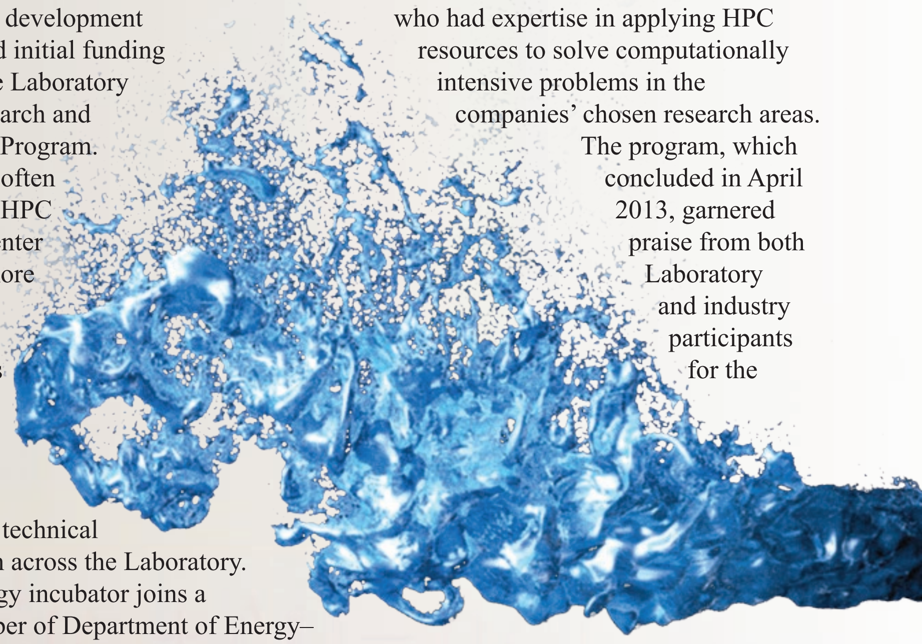
HIGH-PERFORMANCE computing (HPC) systems and software have already changed how science is done. Industry is its next frontier. With HPC, computing systems with millions of processors run calculations simultaneously—in parallel—instead of sequentially, often slashing run times from weeks to hours or minutes. This massive increase in computational power and speed has allowed scientists to explore research problems that, because of scale or complexity, have previously been impossible to model.

Despite the promise of HPC for innovation, dedicated and experienced industrial users remain a relatively small group. Large communities of researchers and technology developers within both the public and private sectors use desktop workstations exclusively, and as a result, they have complex problems that remain unsolved. Many segments of the energy sector, for instance, rely solely on experiments and physical prototypes for product development. (See *S&TR*, December 2011, pp. 4–11.) Trillions of calculations per second may sound impressive, but companies want further proof that HPC modeling and simulation will benefit their business model before they move beyond what commercial software and a modest in-house computer cluster can offer.

Lawrence Livermore's hpc4energy incubator (see *S&TR*, June 2012, pp. 24–25) has demonstrated how national laboratories and companies might partner to expand the adoption of HPC, a tool capable of addressing such national grand challenges as energy security, economic prosperity, and scientific leadership. The one-year pilot program was designed to exhibit the benefits of incorporating HPC modeling and simulation into energy technology development.

The hpc4energy incubator is part of Livermore's broader industrial outreach and economic development initiatives, and initial funding came from the Laboratory Directed Research and Development Program. Project teams often worked at the HPC Innovation Center on the Livermore Valley Open Campus, which provides industrial clients with access to computing resources and technical expertise from across the Laboratory. The hpc4energy incubator joins a growing number of Department of Energy–sponsored partnerships that are helping to connect energy businesses with HPC resources and meet the nation's carbon emission and energy security goals.

The six industrial participants, selected through a competition, differ in their level of HPC experience and the problems they want to examine, but they share one commonality. "These are all forward-thinking companies willing to embrace new technologies and research tools," says former Livermore engineer Clara Smith, who managed the incubator program. Each company was granted time on Sierra, a supercomputing system that can perform more than 260 trillion floating-point operations per second. Project teams were matched with Livermore staff members who had expertise in applying HPC resources to solve computationally intensive problems in the companies' chosen research areas. The program, which concluded in April 2013, garnered praise from both Laboratory and industry participants for the



GE Global Research and Livermore coupled sophisticated numerical methods and high-performance computing (HPC) to create a high-resolution simulation of liquid fuel spray. This research effort focused on reducing the number of design iterations needed to create advanced fuel injectors. (Courtesy of Computational Thermo-Fluids Laboratory, Cornell University.)

exposure to new research tools, methods, and collaborators.

John Grosh, deputy associate director for Computation Programs, says, "I was pleased to see how enthusiastic and committed the six companies were to our collaboration. They knew the program was a unique opportunity, and they were intellectually engaged and responsive."

Whether the goal was designing a more efficient combustion engine, simulating complex energy networks to improve planning and scheduling, refining a new geothermal drilling technology, or analyzing energy use in buildings, the partners concurred that Livermore supercomputers and expertise accelerated the cycle for product and service development. The incubator project encouraged them to approach research problems in a new way. "When you have computing capabilities you didn't have before, you think differently about problems," says Eugene Litvinov, the senior director for Business Architecture and Technology at ISO New England. "You can ask questions you didn't think of asking before."

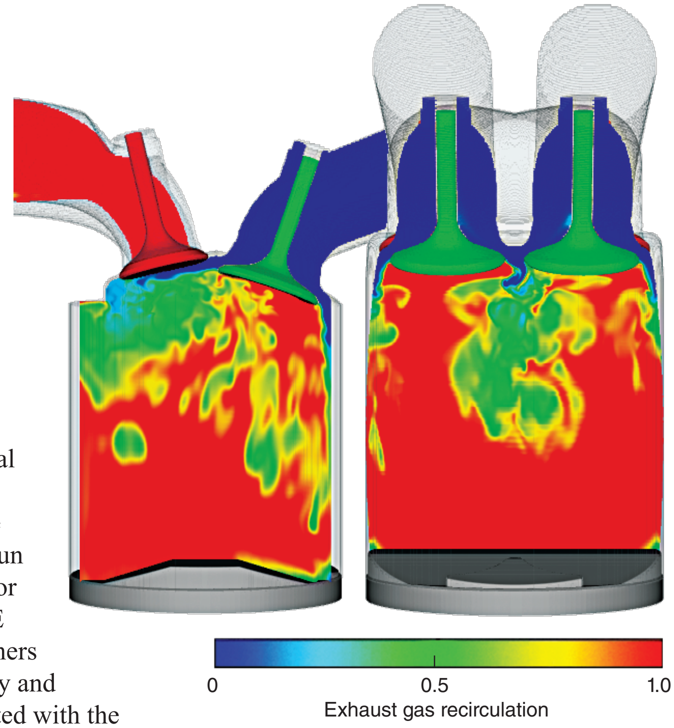
Injecting HPC into Fuel Simulation

Aircraft and automobile manufacturers are interested in developing more-efficient engines that last longer and generate less pollution, but the current engine optimization cycle of prototype design, fabrication, and laboratory testing is onerous. Designers cannot see inside or measure many engine systems during laboratory experiments. Conducting a series of tests that replicate the full range of potential operating conditions is impractical. As a result, the current prototyping and testing process can be expensive and inefficient. Two hpc4energy participants, GE Global Research and Robert Bosch, LLC, are augmenting laboratory measurements with modeling and simulation to better understand combustion, turbulence, and other processes that affect engine performance.

An engine's overall performance hinges in part on how well the injected liquid fuel disperses into a turbulent spray of droplets that mix with an oxidizer and burn. Scientific understanding of turbulence has improved in recent years, largely because of new high-fidelity numerical techniques, but industry researchers often do not have the computational power to run the software. For the incubator effort, jet engine designer GE Global Research and researchers from Arizona State University and Cornell University collaborated with the Laboratory to deploy numerical methods developed by the universities on an HPC machine. Using these codes on Sierra, team members simulated turbulent spray breakup in three dimensions and, with those results, evaluated two designs for fuel-injector engines.

For the test simulation, the incubator team examined liquid fuel entering the combustion chamber to determine how the shape of the opening affects spray breakup as fuel droplets intersect with a turbulent cross-flowing current of air. Both numerical codes simulated the problem at a range of resolutions, in some cases with droplets as small as 20 micrometers in diameter. These simulations used nearly 16 million core-hours of computing time on Sierra, by far the largest demand for HPC resources among the incubator projects. A typical run took more than 3 days of continuous computing on more than 11,000 cores.

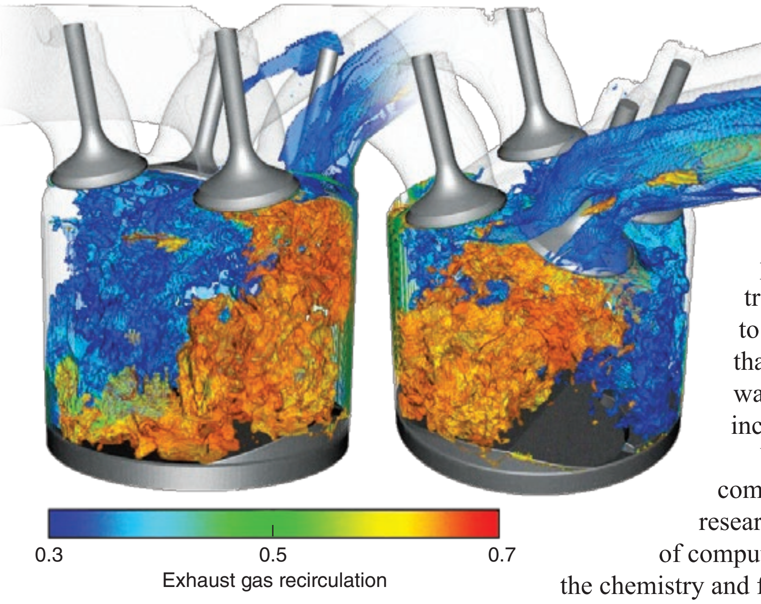
Postprocessing analysis of the simulation data sets and comparison with existing experimental measurements are ongoing, but the initial findings have been encouraging. For instance, results showed that Cornell's NGA code effectively captures the shape and distribution of fuel droplets as the fuel and air mix. The simulations also



Researchers at Robert Bosch, LLC, have developed a three-dimensional numerical code to simulate how exhaust gas recirculates in the combustion chamber of a new engine design. Calculations run on the Bosch in-house computing cluster show fresh air (blue) entering the combustion chamber and interacting with leftover combustion products from the previous cycle.

indicated that experimentally drawn conclusions accurately describe how the injector pipe's shape affects fuel droplet size, speed, distribution, and shape. These factors are important because they influence the efficiency, durability, reliability, and safety of engine operation.

Livermore computational physicist Gregory Burton observes, "The fidelity of the simulations has been astonishing. The work provides an unprecedented opportunity to delve deeply into the physical processes governing droplet formation and ultimately learn how to control these processes to develop higher-performance engines." Gary Leonard, the global technology director at GE Global Research, adds that through the incubator effort, "We've started to learn about some



In their hpc4energy project, Bosch researchers worked with Laboratory computer scientists to scale the Bosch code to run efficiently on Livermore's Sierra supercomputer. They reduced the calculation time for each engine cycle by 70 percent and improved the model resolution, allowing them to examine combustion in greater detail than the Bosch computer system can produce.

of the physics going on in our jet engines that we didn't know about. And we've been building jet engines for 60 years."

Combustion Switches Gears

Certain advanced combustion technologies in automobile engines could reduce fuel consumption by more than 30 percent in low- to moderate-load driving conditions, such as while idling or cruising at a steady speed. Unfortunately, these technologies cannot provide the same performance level as conventional combustion in high-load circumstances, for example, when merging onto a highway or starting from a complete stop. Engines currently under development combine the two combustion modes to optimize performance and fuel efficiency. Switching between modes, however, will require advanced control algorithms. Before those calculations can be developed, researchers must better understand the complex chemistry and physics involved in the transition from one mode to the other—a problem that Bosch collaborators wanted to evaluate in their incubator project.

Using their in-house computer cluster, Bosch researchers needed two weeks of computational time to calculate the chemistry and flow through one engine cycle. Understanding how a set of timing parameters affects the transition from conventional to high-efficiency combustion requires modeling 10 four-stroke engine cycles: two cycles in conventional mode, followed by eight in high-efficiency mode. Processing those calculations on the Bosch system would require 20 weeks of uninterrupted computational time—much too slow to make meaningful progress.

For the incubator project, the collaborators scaled the sophisticated Bosch codes to run efficiently on the Laboratory's computing system. The team reduced the calculation time for each cycle by 70 percent, making it possible for the first time to simulate the full transition process. Expedited processing times also enabled the team to complete multiple sets of test cycles and vary parameters such as the fuel-injection method to more thoroughly validate the combustion model.

Livermore mechanical engineer Dan Flowers says, "Combustion is one of the hardest processes to model because events are occurring at a wide range of size and timescales simultaneously." Capturing the fine-scale effects of combustion was the most important factor in this study, so the team focused its effort on computationally expensive simulations at extremely high resolutions. The researchers observed some unusual and possibly significant physical behaviors, such as high-frequency pressure wave effects, that would rarely if ever appear in the results of less-detailed simulations.

Through the hpc4energy collaborations, GE Global Research and Bosch had access to far more computing power than is available to either group internally, allowing their researchers to perform multiple tests and study complex physical phenomena with more precision than they could have otherwise. The insights these teams gained into spray breakup and combustion modes will help the companies improve the models they use for engine design and testing.

Livermore researchers emerged with a better understanding of the engineering and simulation problems that most concern these two participants and similar energy companies. Laboratory scientists also gained first-hand experience with two advanced numerical techniques developed by GE Global Research to examine spray breakup problems. In addition, the GE codes will now be available for use in other research projects through the new Turbulence Analysis and Simulation Center at Livermore.

Anticipating Changes in the Grid

In its 2003 book *A Century of Innovation: Twenty Engineering Achievements That Transformed Our Lives*, the National Academy of Engineering identified the U.S. electric power grid as the greatest engineering achievement of the 20th century. Modernizing the grid's infrastructure and tools to meet 21st-century needs poses a significant challenge. New, "smart" grids incorporate more sensors and automated controls to operate efficiently and better prevent interruptions.

However, many organizations involved in grid planning and scheduling have found that the accompanying increases in data volume and system complexity are straining available processor performance.

In addition, integrating intermittent power sources such as wind and solar energy into the grid can confound planning efforts. To address these issues, two incubator teams examined how HPC could improve energy-grid modeling and planning for complex networks.

In many parts of the world, electricity is now a dependable and vital resource. If a power line is damaged by a falling tree or a connection is offline for maintenance, electricity must keep flowing or quickly be restored to customers. Utility planners often use the GE Positive Sequence Load Flow (PSLF) software to predict how a system's events might affect energy transmission. PSLF analyzes the systemwide effects of failed components for a given grid configuration and pinpoints configurations that will continue to operate in the event of such failures.

When calculations are made on a desktop computer, the contingency analyses, or what-if scenarios, must be examined consecutively. Completing the calculations for larger grid systems can take hours or days. To reduce the turnaround time, planners may lean on their expertise. For example, they might identify the most-likely failures and simulate only those scenarios. However, this type of selective testing increases the chance of overlooking a critical failure point.

The PSLF developer, GE Energy Consulting, wanted to scale up the software model while reducing the computational load. Through the incubator program, GE Energy could run the software on more powerful computing systems and simulate extremely large networks, many times the size of those previously simulated on the company's computing cluster. The collaboration also enabled GE Energy scientists to perform more contingency analyses than they could process in-house. Livermore computer scientist Steve Smith says, "By running a more comprehensive simulation on our machines, the GE team increased confidence in the results produced by PSLF."

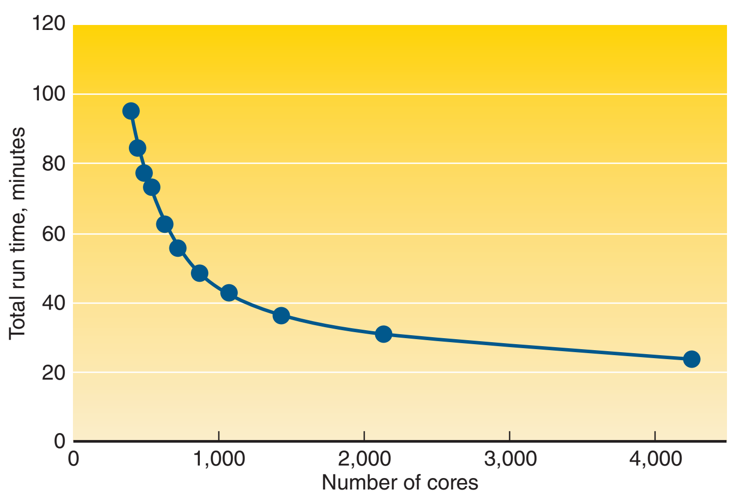
Laboratory researchers optimized the PSLF code to run in parallel on Sierra, thereby reducing the run time for all contingencies to the time required to solve the longest running contingency. In a study of 4,217 contingencies, the total calculation time on Sierra was only 23 minutes. Processing this number of analyses consecutively would have required an estimated 23.5 days. Devin Van Zandt, software products manager for GE Energy Consulting, says, "Working with the Laboratory team to improve the performance of our code was a great opportunity. Their experience in solving problems similar to ours coupled with the HPC infrastructure at Livermore helped us understand the potential of our code base."

After the successful Sierra test, GE Energy worked with Livermore experts to speed up the processing on individual contingency analyses. GE Energy researchers are now studying how to incorporate these scaling and performance improvements into a new version of PSLF.

Tomorrow's Forecast for Energy

In scheduling electric grid operations, system operators evaluate the supply and demand, or load conditions, forecast for the following day and, through a process called unit commitment, determine which power generators will be used. If the day's forecast is inaccurate—say, for example, the amount of wind energy available is significantly below projections—operators may not be able to start up the uncommitted power sources quickly enough to alleviate the shortfall. Traditional models for unit commitment are thus designed to generate conservative estimates, an approach that is neither very cost effective nor efficient in its use of renewable resources.

ISO New England, the company responsible for power generation and transmission throughout that region, enlisted Livermore's help in comparing this point forecast approach with a new method that accommodates a range of uncertainty. A preliminary experiment by ISO New England indicated that the newer technique, termed robust unit commitment, could substantially reduce dispatch costs and improve reliability. Assessing the operational and economic benefits of robust commitment required generating day-ahead forecast ranges for projected electric load and renewable power generation. These ranges were then used to identify an optimal unit commitment schedule for



GE Energy performs contingency analysis to determine the stability of an electric grid when a connection is removed from the system, for example, for required maintenance or because of a damaged power line. With the increased computational power provided by Sierra, GE Energy could simulate all of the contingencies for a large network simultaneously rather than in sequence, producing more rapid and thorough results.

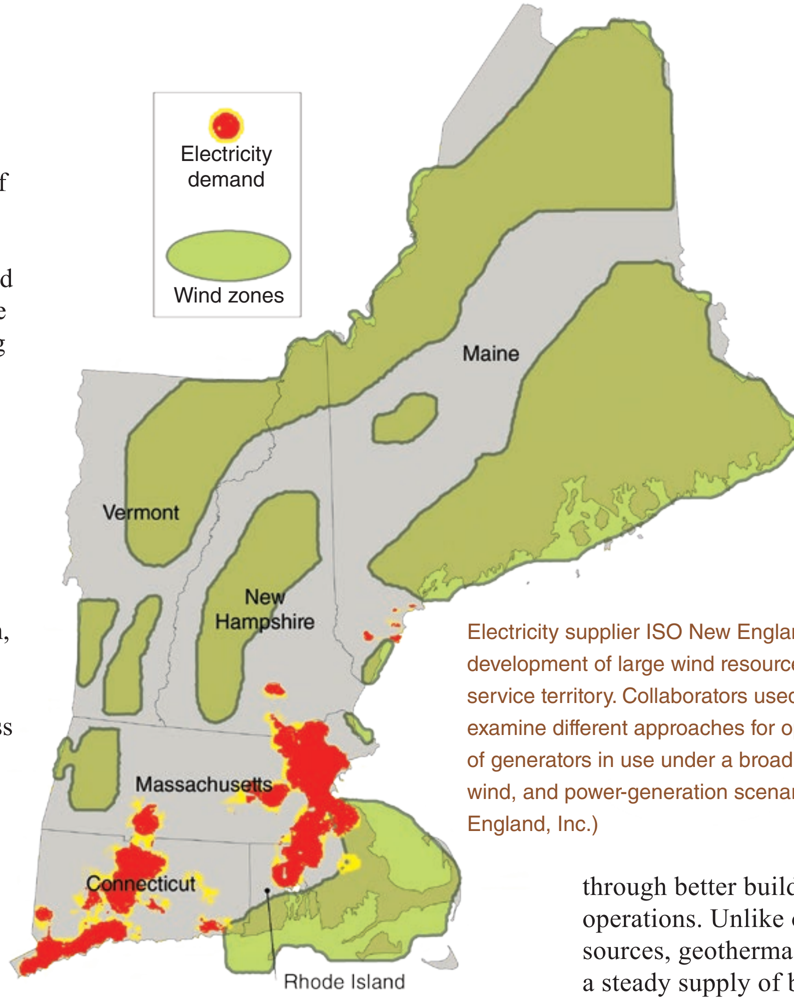
the day. The final step was testing the system dispatch over that day for each of many possible realizations of load and renewable power generation.

Since each unit on the grid is scheduled to be either on or off, optimizing schedule scenarios is a computationally demanding mathematical problem that leads to millions of possible combinations. For a set of 1,600 robust unit commitment configurations, for example, solving each scenario takes about 30 minutes, or 800 hours of processing time on one desktop computer. Up to 10,000 dispatch problems, each one taking 15 seconds, must be answered for every configuration, for a total dispatch-solving time of 67,000 hours on a desktop.

By parallelizing the software to process the robust problem set and running it on 1,600 core processors, the hpc4energy collaboration reduced the calculation time from 800 hours to 90 minutes. After demonstrating that the optimized code could efficiently process such a large number of scenarios, the team completed more than 10,000 simulations using Monte Carlo sampling based on historical load and wind-generation data combined with a Livermore-developed statistical model of this behavior. The team also evaluated the optimal size of the uncertainty range for the robust approach.

Processing thousands of occurrences at once provided researchers with a more comprehensive evaluation of the next day's schedule and allowed them to assess the effectiveness of the robust unit commitment approach under a broad range of energy use, wind, and power-generation scenarios. "We can't explore all of the possibilities because it would cause what is appropriately called combinatory explosion," says Livermore computer scientist Barry Rountree. "But we can look at thousands more scenarios than ISO New England could with their in-house computing resources."

The Livermore team's greatest contribution in the ISO New England project was in statistical modeling and visualization. Laboratory researchers helped frame the problem and prepared a statistical model to simulate wind and load for the Sierra calculations. In the GE Energy effort, the Laboratory team provided a third-party evaluation of the GE application and demonstrated how larger-scale HPC resources could benefit that work. Using Sierra to efficiently run thousands of simulations, the two energy companies gathered statistically significant results that they can use to evaluate and develop sophisticated scheduling and contingency analysis software.

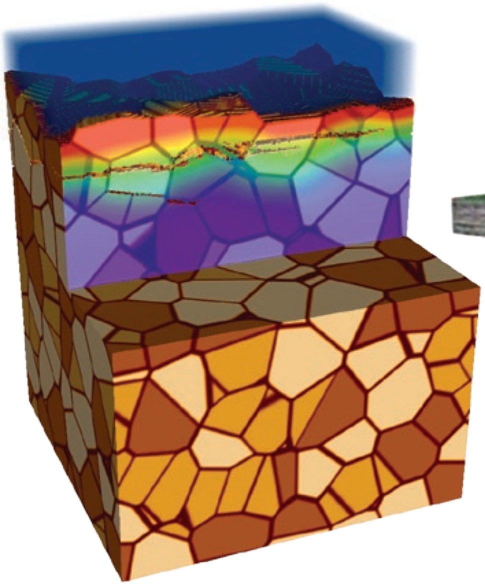


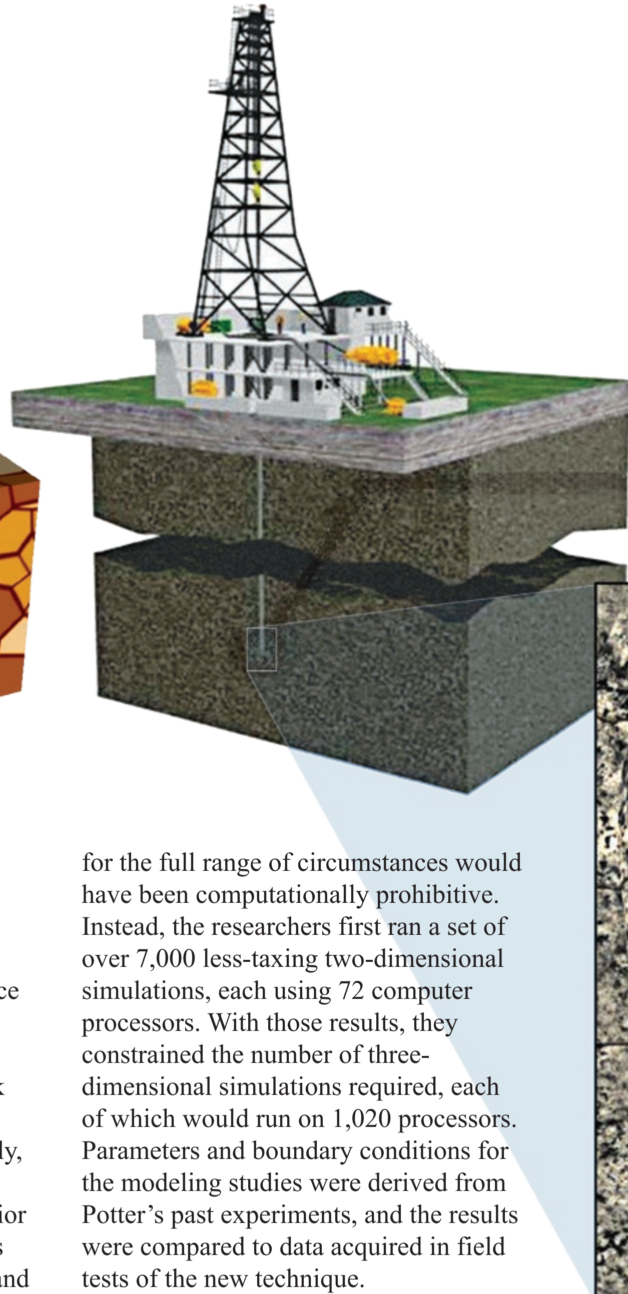
Electricity supplier ISO New England is studying future development of large wind resources throughout the company's service territory. Collaborators used the hpc4energy project to examine different approaches for optimizing the daily schedule of generators in use under a broad range of energy use, wind, and power-generation scenarios. (Courtesy of ISO New England, Inc.)

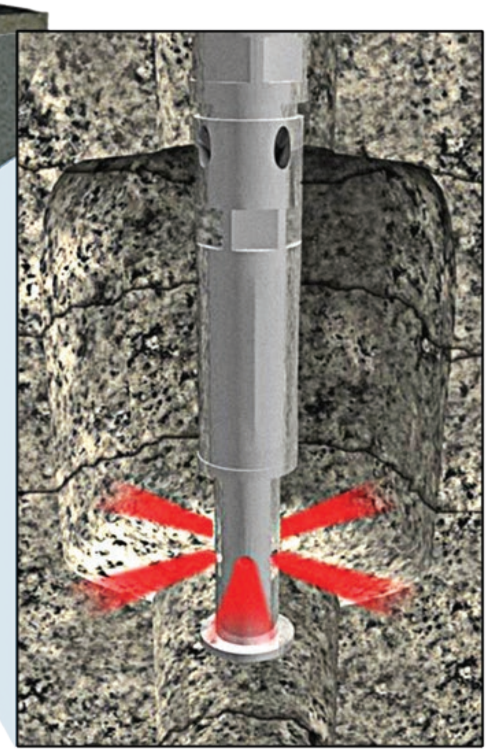
Modeling a New Drilling Technique

The final two incubator efforts focused on making a clean energy source more cost competitive and on saving energy through better building design and operations. Unlike other renewable power sources, geothermal resources generate a steady supply of base-load energy without the need for storage or power-grid modifications. However, capital costs and potential economic risk have deterred investors. Geothermal wells are drilled up to 6 kilometers underground in hard rock formations such as granite, which have a high heat capacity. Because of the depths involved and the difficulties associated with penetrating hard rock, mechanically drilling the wells is expensive.

Potter Drilling, a small start-up company, has developed a technology called hydrothermal spallation drilling that could reduce drilling time and cost and make existing wells twice as productive. Thermal spallation uses a jet of superheated water to penetrate granite at two or more times the rate of conventional technologies, without the drill bit ever contacting the rock. Livermore mathematician Stuart Walsh notes that once a well location is determined, "The economics of drilling a well is the time







Potter Drilling worked with Laboratory researchers to create a grain-scale model (shown at far left on a 1-centimeter cube of granite slab) of hydrothermal spallation drilling, a new technique (below) that efficiently removes rock from a well bore. Hydrothermal spallation could reduce the time and cost for drilling deep geothermal wells and could make existing wells more productive.

involved. If you have a technology that allows you to drill faster or replace drill bits less frequently, then you gain a competitive advantage."

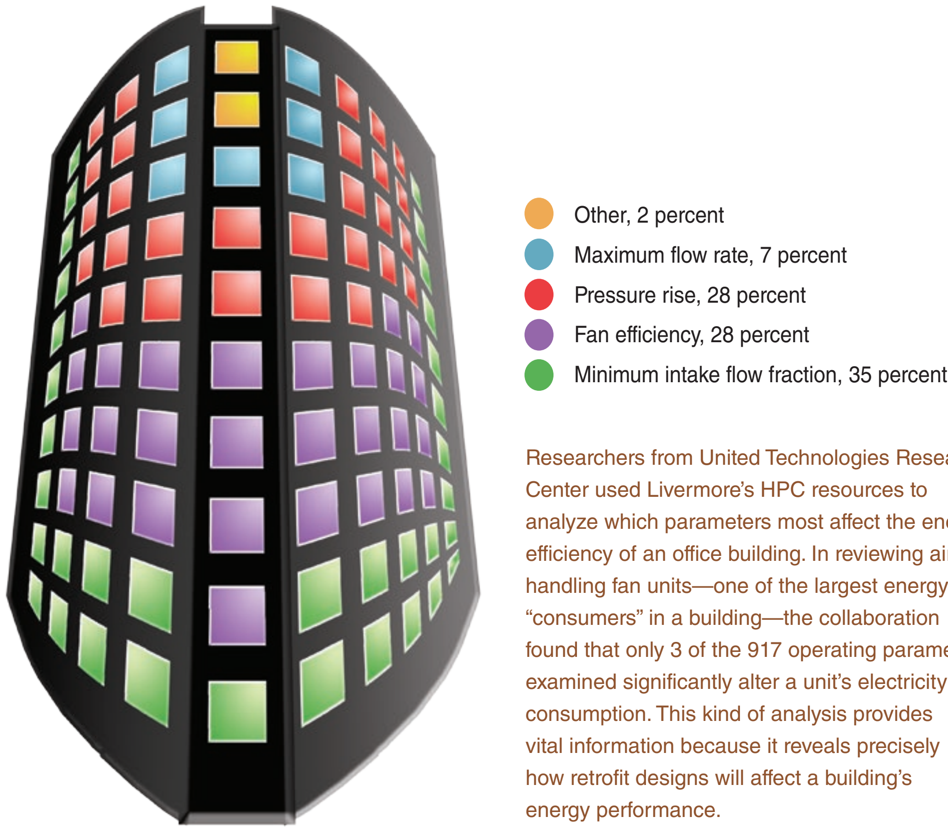
Before its collaboration with Lawrence Livermore, Potter Drilling relied on laboratory experiments and field testing. Unfortunately, most of the relevant work occurs in deep boreholes where it is impossible to monitor the process directly, making system optimization difficult, slow, and expensive. In the two years prior to the incubator project, Potter engineers completed 15 field trials and 30 design and process changes. Through the hpc4energy collaboration, the company conceptually tested operations under a broad range of conditions, such as encountering different rock types or drilling in deeper wells with higher pressure than could be experimentally simulated.

The incubator team developed a model to study hydrothermal spallation drilling at the mineral grain scale and combined it with Livermore's GEODYN and PSUADE codes to determine how about two dozen model parameters affect the drilling process. Even with the computational support provided through the incubator, completing three-dimensional simulations for the full range of circumstances would have been computationally prohibitive. Instead, the researchers first ran a set of over 7,000 less-taxing two-dimensional simulations, each using 72 computer processors. With those results, they constrained the number of three-dimensional simulations required, each of which would run on 1,020 processors. Parameters and boundary conditions for the modeling studies were derived from Potter's past experiments, and the results were compared to data acquired in field tests of the new technique.

Jared Potter, cofounder of Potter Drilling, says, "Initial results of the Livermore modeling studies have shown a good replication of the key features thought to occur during the spallation process, including the initiation of spalls and movement of the damaged zone into the rock with time. Future collaborative work could lead to predictive capabilities and the ability to change drilling tool operating conditions, depending on such parameters as rock type or drilling depth." Working with the 19-employee company was a valuable experience for Livermore participants, highlighting the needs and concerns of start-up companies, whose core business can rapidly evolve. The collaboration also produced software tools that will be valuable to future energy and drilling research efforts at the Laboratory.

Factoring in Uncertainty

Commercial and residential buildings account for more than 40 percent of U.S. energy consumption. Making buildings more energy efficient could thus generate substantial savings in operational costs and energy use while reducing carbon emissions. Predicting a building's efficiency requires engineers and planners



Researchers from United Technologies Research Center used Livermore's HPC resources to analyze which parameters most affect the energy efficiency of an office building. In reviewing air-handling fan units—one of the largest energy "consumers" in a building—the collaboration found that only 3 of the 917 operating parameters examined significantly alter a unit's electricity consumption. This kind of analysis provides vital information because it reveals precisely how retrofit designs will affect a building's energy performance.

to quantify uncertainties in the parameters they use to estimate energy consumption for a building's lifecycle, from design and construction to operations and maintenance. The actual energy usage for a building is often up to 30 percent greater than originally projected because of variability in building materials, occupant behavior, weather, and maintenance. If the primary factors causing uncertainty can be identified and analyzed through simulation, an accurate risk assessment can be made prior to investing in a building retrofit, making energy-efficient designs and remodeling more attractive to investors.

Through the incubator program, United Technologies Research Center (UTRC) identified key operational variables for predicting building energy performance and estimated some effects of such uncertainty. UTRC researchers will use this information to validate and calibrate the company's models and to advise builders and building operators on a facility's use patterns and areas to target for improvement. "For existing facilities, the operations staff can determine a sustainable or wasteful path for building use," says Livermore engineer Noah Goldstein. "The people who run these buildings are really starting to understand the value HPC can add to operations."

UTRC researchers had incorporated parallel computing into their analysis process prior to the incubator project, reducing the turnaround time for whole-building analysis from 2 weeks to less than 24 hours. But their analysis was somewhat limited in scope. With the Livermore collaboration, they expanded their optimization effort to run the simulations in a massively parallel form. Working with an energy use model of an office building located in the Philadelphia Navy Yard, the incubator team tested variations in more than 900 operating parameters, including such factors as the performance of heating and air-conditioning equipment, energy used by lighting fixtures and appliances, insulation properties of different walls and windows, weather changes, and occupant activities in the building. On Sierra, operating with 1,000 computer cores per simulation, calculation time was reduced by a factor of 60, permitting UTRC to efficiently complete 10,000 simulations and accelerate uncertainty modeling. Analysis turnaround time was reduced from days to only hours.

Goldstein notes that collaborating with UTRC helped Laboratory scientists better understand how to simulate the energy consumption of a building. It also allowed them to compare approaches of uncertainty quantification to Livermore-developed methods.

The company is now comparing the model results and sensitivity levels from the incubator project with a year's worth of data on energy usage and occupant behavior from the Philadelphia building. The UTRC analysis indicates that, for simulating a typical building, only a small number of parameters has the greatest effect when modeling energy use. Variations in all other parameters have a negligible effect. One such example is the electricity consumption of a building air-handling system. Results from the HPC models suggest that the system's performance depends primarily on only three parameters, while the combined effect of all other parameters is less than 10 percent. This finding, if proven accurate, would simplify a building retrofit design, because it gives clear guidance to the engineers regarding where to focus their effort and resources.

In the project's final months, the incubator team began designing a more efficient refrigeration system to meet the needs of certain commercial building users. HPC has rarely been used to consider heating and air-conditioning designs because such computations cost more than the retail price of the system. The incubator collaborations are thus helping address a wider range of engineering problems.

Although UTRC is already an HPC user, the company benefited from working with researchers who had an established HPC-based workflow for building analysis and were experienced in quantifying uncertainty. Both the Potter Drilling and UTRC efforts show how advanced computing can enable companies to quickly narrow the list of significant variables, freeing up time and resources to focus on optimizing the factors that will likely yield the greatest improvements.

Problems on a Whole New Scale

The Laboratory's hpc4energy incubator helped demonstrate that businesses of all sizes can benefit from applying HPC to reduce risk and optimize designs. Through the pilot program, energy companies observed new details about the physical processes involved, modeled problems with extremely fine resolution, and captured the variability in the systems they were evaluating. Livermore participants learned about the energy industry's requirements and goals. In the process, they helped solve new problems, worked with unfamiliar algorithms and methods, and expanded their computational skills.

Initiatives such as the hpc4energy incubator support the Laboratory's mandate to transfer technology and expertise to the private sector. At a November 2012 workshop, Laboratory Director Penrose (Parney) Albright noted, "The Lab's culture is about bringing together multidisciplinary teams to work on problems of national importance. Now, we want to take some of the capabilities we've developed and put them in the service of the U.S. economy."

In addition, fostering wider adoption of and demand for HPC drives down hardware and software costs, which benefits Lawrence Livermore and its mission work. "Broadening the HPC user base makes it easier and more affordable to push the cutting edge," says Livermore computer scientist Rob Neely. "Everyone wins."

With an effective template for industry engagement in place, the Laboratory's HPC leaders are considering which other research areas to "incubate." Several industrial sectors with urgent research problems have yet to fully embrace HPC and could benefit from Livermore's computational expertise. For instance, an HPC incubator for bioinformatics and pharmaceutical design could expand the traditional "number-crunching" capabilities of HPC simulation by marrying it with the Laboratory's strengths in molecular dynamics and big data analysis. (See *S&TR*, January/February 2013, pp. 4–11.) Such collaborations have the potential to produce highly precise results and reduce the need for laboratory testing.

The competitive nature of business often makes companies reluctant to share their HPC success stories. An effort such as hpc4energy can strengthen the case for investing in this technology and can teach prospective users to think differently about problem solving. "Because of limited computational resources, many researchers have gotten used to constraining their models in resolution and scale," says Goldstein. "We've shown them that they can model a whole system, do full-scenario planning, or even do real-time modeling. The hpc4energy incubator has helped crack open the box of what simulation and modeling can do. It's not just faster—it's about thinking on different scales."

—Rose Hansen

Key Words: clean energy technology, contingency analysis, fuel-injection engine, high-efficiency combustion, high-performance computing (HPC), hpc4energy incubator, HPC Innovation Center, hydrothermal spallation drilling, parallel computing, smart electric grid, turbulence, uncertainty quantification, unit commitment.

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Ready to Respond to Chemical Weapons

Livermore scientist Sarah Chinn works in the nuclear magnetic resonance (NMR) laboratory at Livermore's Forensic Science Center (FSC).

LAWRENCE Livermore's Forensic Science Center (FSC) is one of just two U.S. laboratories accredited by the Organisation for the Prohibition of Chemical Weapons (OPCW) to analyze samples from suspected chemical weapon production facilities. Maintaining accreditation requires the successful completion of complex, fast-turnaround proficiency tests to identify the contents of samples spiked with unknown chemical compounds. Staying on top of this game—in which the tests get more difficult with every passing year—pushes the FSC staff to continually extend the center's capabilities in analytical chemistry.

In force since 1997, the Chemical Weapons Convention (CWC) has been ratified by 188 countries, including the U.S., and is administered by OPCW in The Hague, Netherlands. The CWC prohibits the development, production, acquisition, stockpiling, and use of chemical weapons as well as the transfer of chemical weapon–related technologies.

Chemical weapons are easily and affordably manufactured and provide a route to inflict mass casualties. In 1988, Saddam Hussein infamously killed 5,000 Iraqi citizens with chemical weapons, and in 1995, the Japanese cult Aum Shinrikyo released the nerve gas sarin in a Tokyo subway, killing 13 people and sickening nearly 5,000.

When the U.S. Senate ratified the CWC in 1997, the only OPCW-designated laboratory in the U.S. at the time was Edgewood Chemical Biological Center at the Aberdeen Proving Ground in Maryland. In 2000, Livermore's FSC proposed to the Department of Energy that it become the second U.S. OPCW-designated laboratory.

The Challenge of Certification

Years before the CWC was ratified, the international community began to develop procedures that could be used to verify the presence of chemical weapon agents. A series of round-robin tests in the 1980s and 1990s, involving Lawrence Livermore, Edgewood, and laboratories in other countries, served to determine such protocols as how to size samples, how much to spike them, appropriate testing criteria, and chain-of-custody requirements. Livermore scientists prepared the samples for one round-robin in 1993. Chemist Armando Alcaraz, who has led the Laboratory's OPCW work for many years, says, "Once the community was confident in its procedures, proficiency tests could begin. They began even before the treaty was ratified."

Today, proficiency tests are held semiannually. The tests that led to FSC's initial accreditation in 2003 occurred in November 2001, April 2002, and October 2002. To maintain certification, all OPCW-designated laboratories must maintain a three-year rolling minimum average of at least two "A" and one "B" grades.

To date, the samples examined by certified laboratories have been those prepared specifically for proficiency tests and exercises. No samples have been officially collected from an actual or suspected chemical weapon site. The proficiency tests involve analyzing and characterizing environmental samples that contain extremely dilute amounts of chemical warfare agents, precursor chemicals, and degradation materials. Other substances are always included to complicate the analysis. For each test, one OPCW-designated laboratory formulates the test samples, and another certified laboratory grades the findings. "The laboratory preparing the samples often makes the problem as difficult as possible," says Brian Mayer, a Livermore expert in nuclear magnetic resonance (NMR) spectroscopy.

A test begins when OPCW announces a scenario. Each laboratory then has 15 days from receipt of the samples to complete the test. Samples may include soil, water, laboratory residues, or other material containing evidence of chemical weapon–related activity. "Just to make things interesting," says Mayer, "a sample may or may not contain any evidence at all. We also cannot make any assumptions about the contents of the samples based on the scenario."

Sarah Chinn, another NMR expert at the Laboratory, says that all other FSC activities essentially shut down for the duration of a test. A conference room is turned into a "war room." Documentation and chain-of-custody requirements are rigorous. In the short time available, the team must execute all analyses quickly, flawlessly, and with perfect documentation.

However, the process does not always go as planned. In 2010, the FSC team received a "C" on a proficiency test. The grade was not because the team's analysis was wrong but because of document-reporting errors, procedural problems that the team quickly corrected. However, the center's certification was suspended for a time. Alcaraz notes that only 8 of the 22 designated laboratories have never been suspended, and just one laboratory, in Finland, has consistently received "A" grades. After passing three tests—in October 2011, April 2012, and October 2012—with "A's," Livermore's FSC was recertified in early 2013.

Analytical Chemistry Solves the Mystery

When the 15-day countdown for a test begins, FSC chemists first divide the samples into dozens of individual batches, many of which are further processed using classical chemical techniques such as solvent extraction or chemical derivatization. "Preparing the samples for analysis concentrates the targeted compounds without obscuring or destroying them," says Alcaraz. The prepared samples are then analyzed with an array of instruments and techniques to identify and semi-quantify their compounds. Some of these techniques are the same ones used by other facilities to detect performance-enhancing drugs in urine and pesticides in nutritional supplements.

Gas and liquid chromatography (GC and LC) coupled to various element-specific detectors are the workhorses for chemical separation and suspect-compound screening. GC and LC coupled to a mass spectrometer can detect ultratrace quantities of organic compounds weighing one-billionth of a gram or less. Because of their trace sensitivity and associated searchable chemical databases, GC and LC mass spectrometry are typically used as the initial tools to identify some of the suspect compounds.

OPCW requires that at least two analytical techniques be used for positive identification. However, the Livermore team strives to obtain confirmation from three or four methods, which may include GC mass spectrometry with chemical ionization, GC infrared spectroscopy, or NMR spectroscopy. Each instrument provides a unique set of data about the sample.

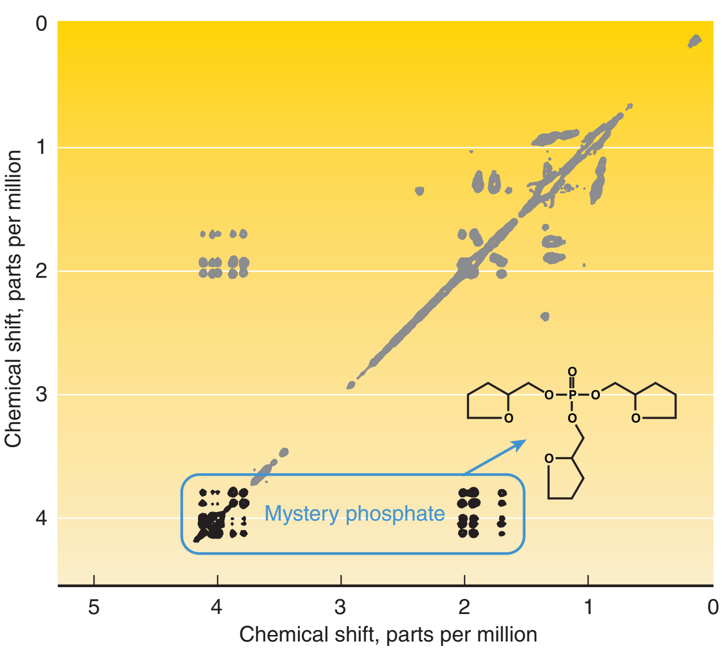
Until recently, the FSC team used NMR primarily to screen for the presence of common spiking chemicals. During the April 2012 test, the researchers were challenged when they could not identify a phosphorous-containing molecule found in the test sample. The unusual molecule did not show up in any of the GC or LC databases. Phosphates frequently appear during OPCW tests because many of the identified chemical weapon agents, including VX, soman, and sarin, are organophosphorus compounds or close relatives.

Solving this mystery required the researchers to use more sophisticated analytical technologies, and FSC's recently purchased, top-of-the-line NMR instrument proved its mettle. It is significantly more sensitive than existing NMR instrumentation. Finding a solution with earlier equipment would have proven considerably more difficult in the required short time frame.

The team discovered that the test sample was loaded with a "red herring" phosphate molecule, which obscured the OPCW-reportable phosphorous compounds. "The sample contained almost 10 times more of the red herring than of the reportable substances," says Mayer.

"Sometimes the instrumentation does not provide a solution," says Alcaraz. "Then we fall back on 'old-school' know-how. At these times, intuition based on years of analytical experience often solves the puzzle."

Once the FSC scientists are satisfied with every detail of a test, they must prove that the sample contains what they claim by cross-referencing their data against data from reference materials. The team purchases the reference compounds commercially, if they are available. If not, FSC's organic chemists synthesize the precursors, pure toxin, red herrings, or degradation products, as necessary—all within the 15-day test period.



FSC scientists use complex NMR spectra such as the one shown here to identify unknown compounds in test samples. This spectrum highlights the structure of tris(tetrahydrofurfuryl) phosphate and one piece of chemical data used to characterize a mystery compound during the Laboratory's proficiency test for recertification by the Organisation for the Prohibition of Chemical Weapons.

Improving Methodology, Advancing Capabilities

Because phosphate molecules appear so frequently during the tests, Mayer, Chinn, and other Laboratory scientists have made NMR even more valuable by developing a new method to zero in on organophosphorus compounds. It combines two techniques—heteronuclear single quantum coherence (HSQC) and diffusion-ordered spectroscopy (DOSY)—to edit out all proton signals except those coupled to phosphorous nuclei. A direct relationship is then established between the remaining resonances and their respective diffusivities. HSQC–DOSY has been used for carbon-13 analysis, and HSQC and DOSY have been applied individually to phosphorus-31. However, FSC is the first to combine the two techniques to not only isolate molecules containing organosphorus groups but also identify unknown degradation products. In the OPCW tests, identifying a compound's degradation products is required as well as identifying the agent itself.

FSC scientists are also exploiting their analytical techniques for other chemical forensics programs. For example, NMR was recently applied to a proof-of-concept experiment for using cyclodextrin molecules as a means to capture tetramethylenedisulfotetramine, or TETS. This lethal neurotoxin is commonly used in China as a rodenticide. Accidental poisonings have caused hundreds of human deaths in China. TETS can be easily manufactured and is persistent in the environment, which could make it attractive for illicit activities. FSC scientists Mayer and Carlos Valdez used NMR spectroscopy to identify the real-time interactions between TETS and cyclodextrin. According to Mayer, "Our research establishes a methodology for assessing cyclodextrin candidates as a potentially powerful tool for removing TETS from a contaminated water source."

The OPCW-certified laboratories want to be sure they have the full range of analytical capabilities that might be needed should a chemical attack occur. All of the tests to date have been on environmental samples such as soil and water. "However, if a chemical attack were suspected to have occurred, we would want the capability to test the victims' blood or urine," says Alcaraz. "The OPCW will need proof that an attack actually happened." The certified laboratories, including FSC, are working together to develop appropriate protocols applicable to clinical samples, just as they did for environmental samples before the CWC was ratified. Preparedness is key to prevention and deterrence of a chemical attack.

—Katie Walter

Key Words: chemical warfare, Chemical Weapons Convention (CWC), Forensic Science Center (FSC), nuclear magnetic resonance (NMR) spectroscopy, Organisation for the Prohibition of Chemical Weapons (OPCW), organophosphorus compounds.

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Software Developers Get Their Hack On

Livermore software developers (counterclockwise from left) Carolyn Albiston, Gary Laguna, and Anh Quach meet at the Livermore Valley Open Campus to discuss their project for a ShipIt day—a designated 24-hour period during which software developers are free to hack on code and explore new applications.

THE term “hacker” typically conjures up images of computer-savvy villains devilishly clicking and typing their way into unsuspecting victims’ computer systems. Within the software development community, however, hacking has a more positive purpose. “To hack” is to innovate, test, and experiment with computer code to create new, purposeful software for various applications.

Livermore has taken a page from the software industry’s playbook, conducting special events during which computer scientists throughout the Laboratory have 24 hours in which to brainstorm, develop, and improve software products. This friendly competition, known as ShipIt days, provides an outlet for developers to explore different software languages and to collaborate with others in their field. “During ShipIt, employees have autonomy to work on software-related products that they find interesting without the added pressure of having to make the project succeed,” says Kyle Dickerson, a Livermore software engineer and ShipIt participant. “The opportunity to be creative with few restrictions helps boost employee morale, motivation, and ingenuity.” By providing a break from regular work activities, the events help employees reinvigorate their software-developing psyche.

ShipIt projects focus on either advancing a Laboratory mission or developing a relevant skill, and employees are free to evaluate a wide range of products that may or may not have immediate applicability to their work activities. “ShipIt events provide a venue for rapid code development,” says Katherine Lewis, a Livermore computer scientist and one of the event organizers. “They are a time for employees to indulge in inklings or interests that could potentially lead to programmatic applications.”

The ShipIt day name and format are derived from a similar program created by Atlassian, an Australian-based software development company. Two weeks before an event, organizers and participants meet to discuss the day’s schedule, suggest project ideas, form teams, and outline project goals. The actual event occurs over a 24-hour period, but teams are not required to participate the entire time. Toward the end of the day, teams present their results to fellow participants. Xinh Huynh, a former Livermore computer scientist and past event organizer, says, “It’s a little like being on ‘American Idol.’ After the final presentations, the audience votes for the best project. The judges are people we consider Computation ‘celebrities’—division leaders and other high-level managers.”

Nearly 80 Computation employees took part in the first three ShipIt days, working in their offices, conference rooms, or the High-Performance Computing Innovation Center (see *S&TR*, September 2012, pp. 22–25), which is part of the Livermore Valley Open Campus. Events for Global Security and for Livermore Computing (LC) in the Computation Directorate were held August 24–25, 2012, with the competition beginning at noon one day and ending at noon the next. Computation's Applications, Simulations, and Quality Division held the third event on February 28 and March 1, 2013.

Future ShipIt days will be interdepartmental, encouraging an even broader range of ideas. Outstanding projects from the first competitions include a mobile Android application for counterproliferation efforts; a portlet for viewing computer simulation results via a Web browser; and a widget for LabBook, the Laboratory's internal social network.

A Mobile Tool for Counterproliferation

Software engineers in Global Security are devising applications to navigate and analyze the massive amounts of data acquired in support of counterproliferation efforts. One such application is Element Centric (EleCent), a component in the Laboratory's Counterproliferation Analysis and Planning System. (See *S&TR*, December 2011, pp. 19–21.) EleCent allows users to store, update, retrieve, and analyze critical data, including the location and type of hazardous materials housed at facilities worldwide. It combines an enormous database with Web-based tools for viewing results in various formats, from tabular lists to geospatial maps. A Google Earth plug-in summarizes data in a geospatial display.

Dickerson and two colleagues used ShipIt time to develop an app that displays EleCent data on an Android device, such as a tablet or phone. "The GPS component of mobile systems makes an EleCent app appealing," says Dickerson. "It would allow users to get information specific to their exact location, such as what facilities and materials are nearby that they need to be aware of." He adds that this type of tool has potential for defense applications and for humanitarian efforts. "Someone working in an active emergency response zone, for example, would be able to identify the locations of facilities in the area and the types of hazards they present."

For ShipIt, team members configured their desktop computers to run Google's software development kit for Android apps and divided project tasks among members. "Prior to the event, we were not allowed to write any code," says Dickerson. Over the next several hours, they overcame coding, database, and interface issues to deliver a simple working prototype for their final presentation. "We created a working model that retrieves actual data and displays the results on a mobile device."

More extensive work would be needed before the tool could be deployed for defense applications, but the EleCent mobile app prototype shows what is possible. "We've demonstrated that the technology fits nicely into our programmatic work," says Dickerson. "It offers real potential for our customers."

Going a Different Direction

Project teams are much freer to experiment when they are less concerned about an idea failing. A project by Global Security software engineers Tim Bender and Josh Oakgrove demonstrates how a ShipIt team can change direction and still yield fruitful results. "We started working on a neural network framework for Java that could be used for space situational awareness," says Bender. (See *S&TR*, July/August 2009, pp. 4–11.) "The framework would help users determine the difference between the estimated and actual elliptical drift of an object around Earth."

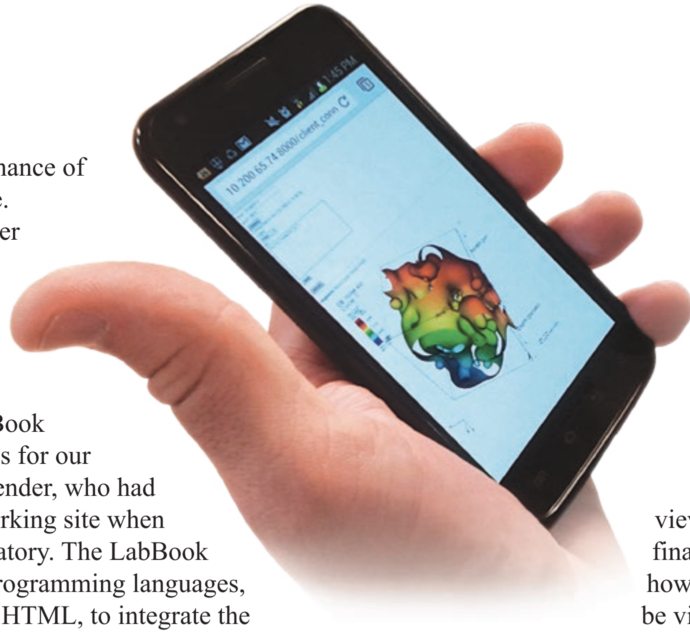
After finding open-source software for the application, the engineers hacked on that code for several hours until they realized they did not have enough time to produce results with their data set. At midnight, they abandoned their initial idea and started a completely different project: developing a Klout score component to LabBook. With only 12 hours remaining for ShipIt, they decided the Klout

The Element Centric (EleCent) mobile app enables users to search EleCent data by geographic area and topic of interest using a handheld device such as an Android phone (left). In the results display (right), icons denote "hits" in the selected geographic area. Touching an icon produces summary information about that site, including the organization, address, and types of materials housed at the facility.

score project had a better chance of success in such a short time.

Klout scores measure user engagement and activity on social networking sites based on several factors, including number of subscribers. "We had to remap the LabBook data model to obtain metrics for our ShipIt application," says Bender, who had worked on the social networking site when he first started at the Laboratory. The LabBook developers used multiple programming languages, such as SQL and PHP with HTML, to integrate the existing LabBook with the new model. "By the end of ShipIt, we had a full beta version of the application." One month later, the application was added to LabBook as part of a routine upgrade, allowing users to view scores that rank their influence on the site.

Bender sees the benefits of ShipIt from both an employee standpoint and that of the institution. "These types of events engage employees and motivate them to do something they wouldn't normally have considered, and that could potentially help Laboratory missions," he says. The team is already looking to improve the current version of the application, for example, by providing percentile rankings among users.



A prototype of the VisIt portlet on a mobile device allows users to control a remote instance of the application and visualize simulation results.

Improving Access to Simulation Results

Lawrence Livermore is renowned for its high-performance computing environment and is home to some of the world's fastest supercomputers and sophisticated software that optimizes these machines. For another ShipIt event, Cyrus Harrison, Brad Whitlock, and Ming Jiang collaborated with Harinarayan Krishnan from Lawrence Berkeley National Laboratory to improve how LC customers access the results of simulations run on the Laboratory's systems.

LC users have access to a personalized Web portal called MyLC that provides a wealth of information on their accounts, such as bank and disk usage, quotas, and active jobs on LC systems. Another application developed at Livermore is VisIt, a visualization tool for viewing and analyzing meshes produced by large-scale simulations. "VisIt is an existing software framework and is quite complex. For ShipIt, our team wanted to expand the accessibility of VisIt by attempting to expose the application in the context of a Web browser," says Harrison.

The team developed a prototype of a MyLC portlet that helps users execute VisIt scripts and receive rendered or interactive views of data sets via a Web browser. For their final presentation, the software developers showed how simulation data rendered with VisIt could be viewed from a mobile phone. "Our proof of concept demonstrates that a VisIt Web browser tool is viable and could be made available to all LC customers," says Harrison. A production-ready version of the tool, including quality assurance testing and debugging, would require additional time and resources outside the scope of ShipIt. However, the researchers agree that ShipIt allowed them to gain experience with a technology they had yet to work with.

Harrison adds that another benefit to ShipIt is the project management aspect. "By having to assemble teams and develop a project schedule, participants get experience in project planning and organization," he says. The event also provides an avenue for participants to present their ideas to peers, helping employees enhance their presentation skills. Says Harrison, "From my perspective, the ShipIt experience overall is very positive. It provides a venue for employee development and allows participants to innovate to produce software products that have real applicability."

The first three ShipIt events have been a success for both the Laboratory and its employees. "The feedback has been very positive," says Lewis, adding that Livermore plans to host events two to four times a year. "Support and interest for the 'hack-a-thons' continues to grow." By giving software developers time to engage in projects that tap their inner creativity, Lawrence Livermore is continuing its tradition of fostering innovation.

—Caryn Meissner

Key Words: Element Centric (EleCent), hacker, high-performance computing, Klout score, LabBook, Livermore Computing (LC), mobile app, MyLC, ShipIt day, social media, software application, VisIt.

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Sorting, Amplification, Detection, and Identification of Nucleic Acid Subsequences in a Complex Mixture

Neil R. Beer, Benjamin J. Hindson, Billy W. Colson, Jr., Joseph P. Fitch
U.S. Patent 8,338,166 B2
December 25, 2012
This apparatus can identify all the known and unknown pathogenic or nonpathogenic organisms in a sample. A droplet generator creates droplets from the sample. These droplets constitute subnanoliter volume reactors containing the organism-size particles. A lysis device releases the organisms' nucleic acids. An amplifier amplifies the nucleic acids, and a fractionator releases the nucleic acids from the droplets. A parallel analyzer then identifies all of the known and unknown pathogenic or nonpathogenic organisms.

Thermal Oxidation of Single Crystal Aluminum Antimonide and Materials Having the Same

John William Sherohman, Jick Hong Yee, Arthur William Coombs, III, Kuang Jen J. Wu
U.S. Patent 8,338,916 B2
December 25, 2012
In one method for forming a nonconductive crystalline oxide layer on an aluminum antimonide (AlSb) crystal, the crystal is heat-treated in a partial vacuum. The vacuum temperature is conducive for air-adsorbed molecules to desorb, surface-molecule groups to decompose, and elemental antimony to evaporate from the crystal's surface. When the crystal is exposed to oxygen, a crystalline oxide layer forms on its surface. In another method, an AlSb crystal is heat-treated in a nonoxidizing atmosphere at a temperature conducive for decomposing an amorphous oxidized surface layer and evaporating elemental antimony from the crystal's surface. Stable oxides of aluminum and antimony are then formed from residual surface oxygen, which results in a crystalline oxide layer on the crystal's surface.

Sensor-Guided Threat Countermeasure System

Brent C. Stuart, Lloyd A. Hackel, Mark R. Hermann, James P. Armstrong
U.S. Patent 8,339,580 B2
December 25, 2012
This countermeasure system can protect a target from an incoming sensor-guided threat. It includes a laser system for producing a broadband beam and a means for directing the broadband beam from the target to the threat. The incoming sensor-guided threat is then blinded or confused.

Dual Waveband Compact Catadioptric Imaging Spectrometer

Michael P. Chrisp
U.S. Patent 8,339,600 B2
December 25, 2012
A catadioptric dual-waveband spectrometer images visible through shortwave infrared light and the midwave infrared spectral regions. The instrument disperses visible through shortwave infrared light with a zinc selenide grating and midwave infrared light with a sapphire prism. The grating and prism are at the cold-stop position, enabling the pupil to be split between them. The spectra for both wavebands are focused onto the relevant sections of a single, dual-waveband detector. Spatial keystone distortion is controlled to less than one-tenth of a pixel over the full wavelength range, facilitating the matching of the spectra in the midwave infrared and shorter wavelength regions.

Micro-Optical-Mechanical System Photoacoustic Spectrometer

Jack Kotovsky, William J. Benett, Angela C. Tooker, Jennifer B. Alameda
U.S. Patent 8,342,005 B2
January 1, 2013
All-optical photoacoustic spectrometer sensing (PASS) systems include the hardware needed to determine whether any of a variety of materials (solid, liquid, and gas) is present. Some all-optical PASS systems require only two optical fibers to communicate with the optoelectronic power and readout systems outside the material environment. These methods improve the signal-to-noise ratio and enable microscale systems.

Matrix-Assisted Energy Conversion in Nanostructured Piezoelectric Arrays

Donald J. Sirbuly, Xianying Wang, Yinmin Wang
U.S. Patent 8,344,597 B2
January 1, 2013
A nanoconverter can directly generate electricity through a nanostructure embedded in a polymer layer that experiences differential thermal expansion in a stress-transfer zone. Semiconductor nanowires or nanotubes with a high surface-to-volume ratio (such as zinc oxide, silicon, and carbon) are grown either aligned or substantially vertically aligned on a substrate. The resulting nanoforest is then embedded with the polymer layer, which transfers stress to the nanostructures in the stress-transfer zone. A nanostructure voltage output occurs as a result of the piezoelectric effect acting on the nanostructure. Electrodes attached at both ends of the nanostructure generate output power at densities of about 20 nanowatts per square centimeter with heating temperatures of about 65°C. Nanoconverters arrayed in a series parallel arrangement may be constructed in planar, stacked, or rolled arrays to supply power to nano- and microdevices without use of external batteries.

Phase-Sensitive X-Ray Imager

Kevin Louis Baker
U.S. Patent 8,351,569 B2
January 8, 2013
X-ray phase-sensitive wavefront sensor techniques can measure the entire two-dimensional x-ray electric field, both the amplitude and phase, with a single measurement. Hartmann and two-dimensional shear interferometry wavefront sensors do not require a temporally coherent source and are compatible with x-ray tubes and laser-produced or X-pinch x-ray sources.

Multiplex Detection of Agricultural Pathogens

Thomas R. Slezak, Shea Gardner, Clinton Torres, Elizabeth Vitalis, Raymond J. Lenhoff
U.S. Patent 8,354,514 B2
January 15, 2013
These kits can be used to detect agricultural pathogens. Genomic sequence data from agricultural pathogens are analyzed to identify signature sequences, such as polynucleotide sequences, and determine whether a pathogen is present in a sample. Primer and probe sets are optimized for use in a polymerase-chain-reaction–based, multiplexed Luminex assay to identify pathogens that are present in a sample.

UWB Transmitter
Gregory E. Dallum, Garth C. Pratt, Peter C. Haugen, Carlos E. Romero
U.S. Patent 8,355,453 B2
January 15, 2013
An ultrawideband (UWB) dual-impulse transmitter is made of a trigger-edge-selection circuit actuated by a single-trigger input pulse. A step recovery diode– (SRD-) based pulser connects to the trigger-edge-selection circuit to generate an initial impulse output. A second SRD-based pulser connects to the trigger-edge-selection circuit in parallel with the first pulser to generate a second impulse output, which has a selected delay from the first impulse output.

Slurried Solid Media for Simultaneous Water Purification and Carbon Dioxide Removal from Gas Mixtures
Roger D. Aines, William L. Bourcier, Brian Viani
U.S. Patent 8,361,195 B2
January 29, 2013
A slurried solid media simultaneously purifies water and removes carbon dioxide from gas mixtures. The gas mixture and carbon dioxide are dissolved in water, providing a gas–carbon dioxide–water mixture. A porous solid media is added to this mixture to form a slurry, which is then heated. Steam produced in the heating process is cooled, which yields purified water and carbon dioxide.

Imaging Mass Spectrometer with Mass Tags
James S. Felton, Kuang Jen J. Wu, Mark G. Knize, Kristen S. Kulp, Joe W. Gray
U.S. Patent 8,362,415 B2
January 29, 2013
This method for analyzing biological material exposes the material to a recognition element that is coupled to a mass tag element. A mass-spectrometer ion beam directed toward the biological material interrogates at least one region of interest, producing data that can then be distributed in plots.

Sensor and Transmitter System for Communication in Pipelines
John F. Cooper, Alan K. Burnham
U.S. Patent 8,362,919 B2
January 29, 2013
This system is designed for sensing and communicating in a pipeline that contains a fluid. An acoustic signal with information about one of the fluid properties is produced in the pipeline and transmitted through it. The signal with the relevant information is received and used by a control.

Laser Heating of Aqueous Samples on a Micro-Optical-Electro-Mechanical System
Neil Reginald Beer, Ian Kennedy
U.S. Patent 8,367,976 B2
February 5, 2013
In this system for heating a sample on a microchip, the sample is positioned within a microchannel flow channel, and a laser beam is directed onto the sample to heat it. A wall section in the microchannel receives the laser beam and allows the beam to pass through without the microchannel being appreciably heated by the beam. A carrier fluid in the microchannel moves the sample such that the fluid is not appreciably heated by the laser beam.

Awards

Lawrence Fellow **Frederico Fiuza**, who works in Livermore's Physical and Life Sciences Directorate, is one of three recipients of the **2013 Ph.D. Research Award** from the **European Physical Society** (EPS) **Plasma Physics Division**. Fiuza received the award for his doctoral thesis, "Multi-Scale PIC Simulations of High Energy Density Scenarios: From Laboratory to Astrophysics." His research spanned several different topics, including multiscale particle-in-cell simulations of the fast-ignition approach to fusion burn and energy gain—work based on a hybrid algorithm proposed by Livermore physicist Bruce Cohen. (See the news brief on p. 2.) He has also studied collisionless shocks and particle acceleration from laser–plasma interactions under laboratory conditions as well as Raman amplification of lasers in plasmas.

The Ph.D. Research Award honors work of exceptional quality in plasma physics by a graduate student in an EPS member state. The award is a key element of the Plasma Physics Division's activities to recognize outstanding research by young scientists.

Dave Trombino, a nuclear engineer in the Global Security Principal Directorate, was honored with a **certificate of appreciation** from the **U.S. Coast Guard** for his efforts to develop radiation detection capabilities for law-enforcement agencies that patrol the San Francisco Bay. The award citation reads, "Your efforts facilitated the adoption of the region's concept of operations plan for Preventative Radiation and Nuclear Detection, making the San Francisco Bay area law enforcement agencies among the first in the nation to use radiological source detection equipment for routine operations."

Trombino was one of about a dozen members of the 40-member Northern California Area Maritime Security Committee honored for his work. The committee includes representatives from law-enforcement agencies; the ports of Oakland, San Francisco, and Stockton; industry; harbor pilots; and Bay Area ferry operators.

Abstract

Scaling Up Energy Innovation through Advanced Computing

Modeling and simulation using high-performance computing (HPC) systems allow scientists and engineers to analyze massive amounts of data and test new processes or design prototypes in virtual space. Global industry has only recently begun to adopt this powerful set of tools to answer its most challenging questions. As a leading user of HPC for both scientific and defense applications, the Laboratory embarked on a pilot program to accelerate the adoption of HPC in pursuit of technological innovations for discovering, delivering, and using various energy resources. Designed to enhance U.S. economic competitiveness and energy security, the yearlong hpc4energy incubator provided six companies with access to the Laboratory's Sierra supercomputer, simulation software, and subject-matter experts. These projects demonstrate how U.S. industries can use HPC resources to efficiently solve some of their most challenging problems.

Contact: John Grosh (925) 424-6520 (grosh1@llnl.gov).

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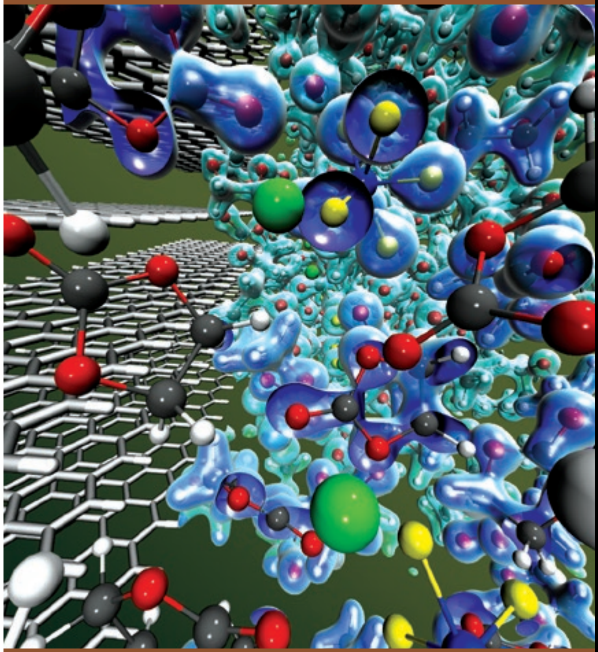
Coming Next Issue

Reaching for New Computational Heights



Years of planning and partnership yield dividends as Sequoia, Livermore's newest supercomputer, assumes its role in support of stockpile stewardship.

Also in July/August

• In January 2013, the Laboratory celebrated the life and contributions of Johnny Foster, one of its greatest leaders, in honor of his 90th birthday.

• Laser experiments at the National Ignition Facility reveal new characteristics of diamond when compressed to extremely high pressures.

• Simulations of and experiments on the dense plasma focus Z-pinch, a configuration that previously was not well understood, are producing intriguing results.

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