Lawrence Livermore National Laboratory

July/August 2011

Science & Technology Review

Also in this issue:

Simulations on a Grand Scale

Enhancing Raman Spectroscopy

Microbe Activity Revealed

About the Cover

As the article beginning on p. 4 describes, LIFE (Laser Inertial Fusion Energy) power plants could help the nation meet the increased demand for an environmentally sustainable, secure, and commercially attractive source of baseload electricity. The U.S. energy situation will become particularly acute in the period leading up to the middle part of this century, when the current fleet of nuclear and coal power plants will need to be replaced. Commercial LIFE plants driven by laser fusion could deliver 25 percent of U.S. electrical generation by 2050.

Cover design: Amy E. Henke

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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Contents

S&TR Staff

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Feature

Research Highlights

Departments

Mitigating Traumatic Brain Injury

In an effort to better protect soldiers against impact and blast injuries caused by improvised explosive devices (IEDs), the U.S. Army and the Joint IED Defeat Organization (JIEDDO) funded Livermore researchers to perform a one-year study during which the effectiveness of various military and football helmet pads was compared. Mechanical engineer Michael King and physicist William Moss used a combination of experiments and computational simulations to study the response of the various pad systems to battlefield-relevant impacts to gain an understanding of how helmet pads provide protection.

Five types of pad systems were studied: those currently and previously used by the Army, two used in National Football League helmets, and one used in other protective sports equipment. "For each of the pads, we performed experiments to characterize the material properties of the individual foam components as well as the response of the complete pad system to a range of impact velocities," says King. "Then we did a large number of computational simulations examining how various parameters such as foam material, pad thickness, pad area, and trapped air affect the overall impact response." The simulations made use of the PARADYN finite-element analysis software, a parallel version of the DYNA3D software developed by Livermore in the 1970s and 1980s to model the deformation of solid structures under impact.

Moss and King found that increasing the current 19-millimeter-thick military pad by an additional 3 to 6 millimeters could make a large difference in reducing the accelerations imparted to the head from blunt impacts. Implementing such a change would require no "system reconfiguration" but simply the use of a helmet one size larger with correspondingly thicker pads.

The researchers' findings appeared in the April 26, 2011, edition of the *Proceedings of the National Academy of Sciences*. "Our methods and results also are applicable to the civilian sector, particularly contact sports helmet design," says King. The National Football League, as well as college and youth sports organizations, have increased efforts to find better ways to protect their athletes from head trauma.

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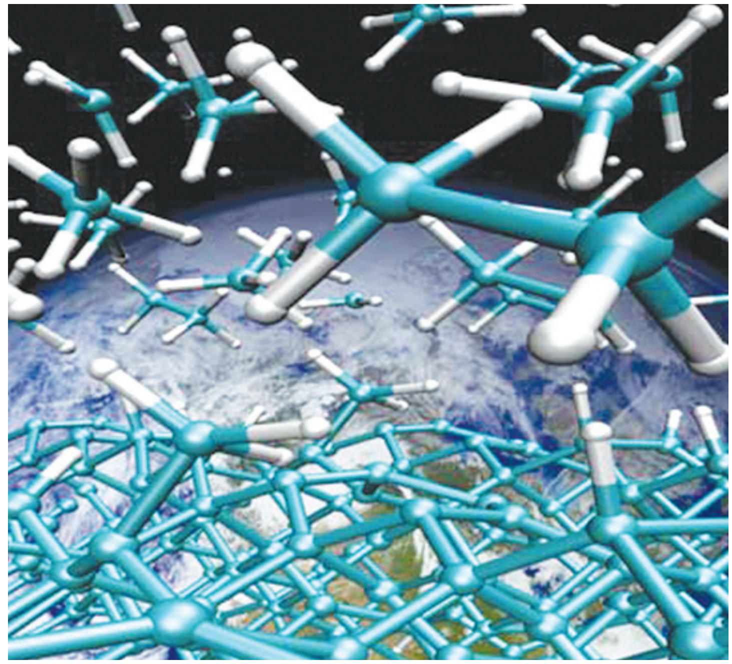
Hydrocarbons in the Deep Earth

A computational study by Livermore's Eric Schwegler and colleagues at the University of California (UC) at Davis, Shell Projects and Technology, and the Max Planck Institute in Meinz, Germany, has revealed how hydrocarbons (shown in the simulation above right) may be formed from methane in deep Earth at extreme pressures and temperatures. The thermodynamic and kinetic properties of hydrocarbons at high pressures and temperatures are important for understanding the behavior of carbon in underground reservoirs.



Hydrocarbons are the main building block of crude oil and natural gas, and they contribute to the global carbon cycle. Geologists and geochemists believe that nearly all (more than 99 percent) of the hydrocarbons in commercially produced crude oil and natural gas are formed by the decomposition of the remains of living organisms buried under layers of sediments in Earth's crust, a region to a depth of about 8 to 16 kilometers below the surface. However, hydrocarbons of purely chemical deep-crustal or mantle origin could occur in some geologic settings, such as rifts or subduction zones, according to former Livermore researcher Giulia Galli of UC Davis.

Galli and colleagues used the Mako computer cluster at UC Berkeley and computers at Livermore to simulate the behavior of carbon and hydrogen atoms at the enormous pressures and temperatures found 64 to 153 kilometers below Earth's surface. They used sophisticated techniques based on first principles and the computer software system Qbox, developed at UC Davis and Livermore.

The scientists found that hydrocarbons with multiple carbon atoms can form from methane (a molecule with one carbon and four hydrogen atoms) at temperatures greater than 1,500 kelvins and pressures 50,000 times those at Earth's surface (conditions found about 113 kilometers deep). "In the simulation, interactions with metal or carbon surfaces allowed the process to occur faster," says Leonardo Spanu of UC Davis. The research appeared in the April 26, 2011, edition of the *Proceedings of the National Academy of Sciences*.

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(*continued on p. 28*)

Commentary by Mike Dunne

An Energy Revolution Needs LIFE

SINCE its founding in 1952, Lawrence Livermore has successfully harnessed the creative powers of science and technology to meet critical national security challenges. Our accomplishments have been based on innovative approaches that combine the expertise of many scientific and engineering disciplines and a systems approach to design optimization and project delivery. Today, the national security challenge of ensuring abundant supplies of clean, safe, sustainable, and cost-effective energy requires our creativity, innovation, and multidisciplinary skills.

As the article beginning on p. 4 describes, we are leading a national effort to address this challenge of delivering an enduring energy solution capable of meeting the global need. The Laser Inertial Fusion Energy (LIFE) effort aims to change the paradigm for fusion by tackling these long-standing challenges. This effort takes advantage of Livermore's world-class expertise in lasers, fusion, materials science, large-scale supercomputer simulation, and experience from the National Ignition Facility (NIF). It is a challenge ideally suited to the capability, character, and history of the Laboratory.

Development of LIFE began more than 50 years ago. Shortly after the invention of the laser in 1960, several Laboratory scientists worked with early fusion design codes to study the possibility of using powerful laser pulses to compress and ignite a small quantity of deuterium–tritium fuel to the point of achieving self-sustaining fusion burn, thereby creating a net source of energy. Since then, the U.S. government has made substantial investments in the field, culminating in the planned demonstration of fusion ignition and energy gain on NIF. Demonstration of ignition will provide the required basis for applying laser fusion to commercial power generation.

Experiments to date on NIF give us confidence that we will demonstrate ignition conditions in deuterium–tritium targets in the near future. The next step is an integrated technology development program leading to the construction of a demonstration plant in the 2020s. This demonstration plant would be capable of well over 1-gigawatt thermal power output and would provide the foundation for the subsequent rollout of a commercial fleet.

The design of the LIFE power plant has been developed in close consultation with the electric utility industry, a wide range of vendors, licensing experts, environmental groups, and our national and international technical partners. It adopts a highly modular design concept that allows for off-site factory manufacture of principal subsystems and an operational model that can deliver high plant availability. The design takes advantage of substantial prior development of key technologies by other industries, such as the semiconductor market. Importantly, the system architecture allows for the use of conventional materials, and NIF provides full-scale performance data for the fusion engine. Together, these attributes significantly reduce technical risks and mean that decades can be saved compared to other approaches to fusion. By adopting pragmatic solutions using known technologies, the LIFE approach allows fusion energy to be delivered soon enough to make a difference to the world's energy and environmental challenges.

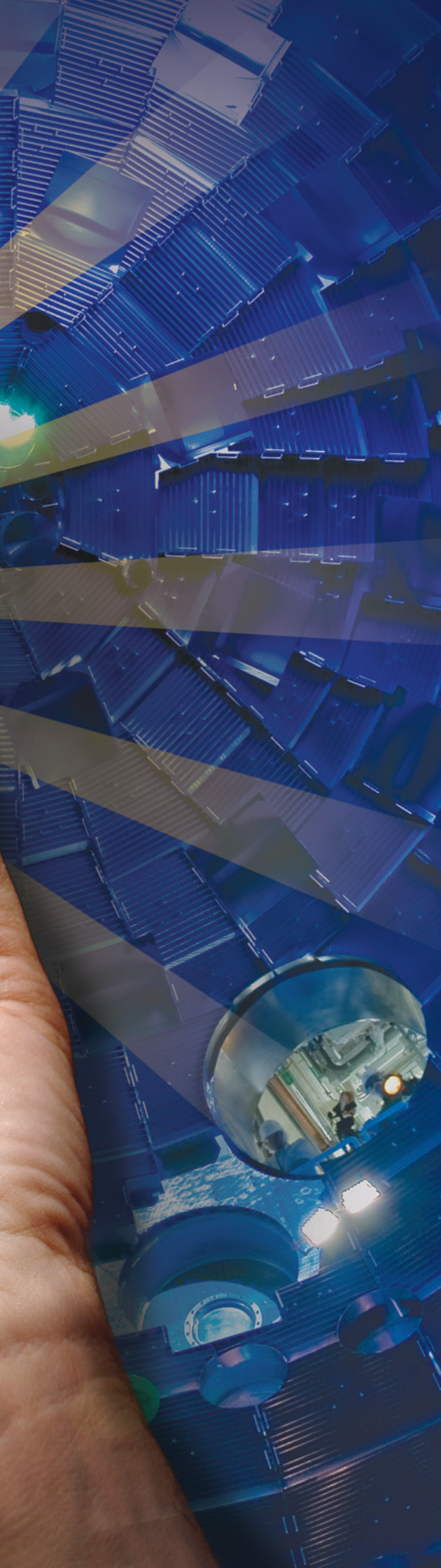
The benefits of a fusion energy economy have been well known for many years. Following the successful demonstration of ignition and plant operations, LIFE could provide a substantial contribution to meeting the demand for an environmentally sustainable, secure, and commercially attractive source of baseload electricity. The plants would produce no carbon-based or other noxious emissions. In addition, the LIFE design addresses key drawbacks of fission-powered plants, such as nuclear proliferation concerns, the need for nuclear fuel enrichment and reprocessing, and the generation and storage of high-level, long-lived nuclear waste. With LIFE, no possibility would exist of a runaway reaction or a core meltdown because the engine contains only tiny amounts of fuel at any given time.

LIFE is about transforming our energy future. We are poised to deliver a profound solution based on the capabilities of the Laboratory and its partners. These are exciting times.

■ Mike Dunne is program director for Laser Fusion Energy.

Igniting Our Energy Future

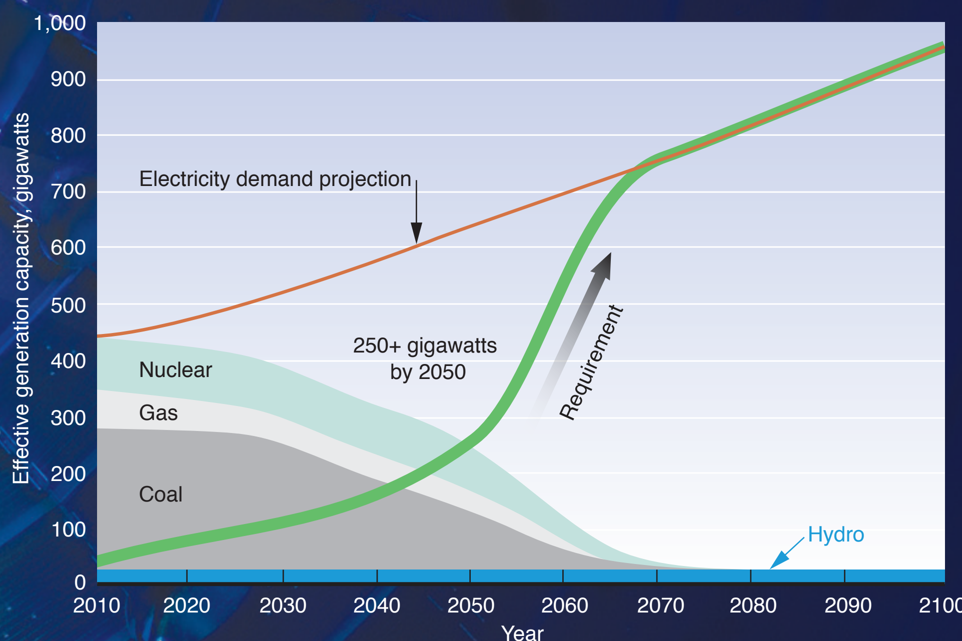
Livermore researchers are forging a commercial pathway for a revolutionary power plant called LIFE.



MEETING the nation's—and the world's—growing demand for electricity is one of the most urgent challenges facing society and the scientific community. Even with improvements in energy efficiency and conservation, a critical need exists to reduce dependence on imported fuels, decrease emissions, and stabilize greenhouse gas concentrations. Safe, environmentally sustainable, commercially attractive sources of baseload electricity are needed with an inherent security of supply and the capacity to meet the level of demand. Renewable sources such as solar, wind, and hydro will play an increasingly important role, but they are not expected to meet the majority of global baseload electricity needs.

The main alternative to burning fossil fuels is nuclear energy. Although attractive on many counts (no carbon emissions, for example), conventional nuclear fission plants face significant challenges such as cost to build; time to license; safety and proliferation issues associated with operations; enrichment; reprocessing; and high-level, long-lived nuclear waste.

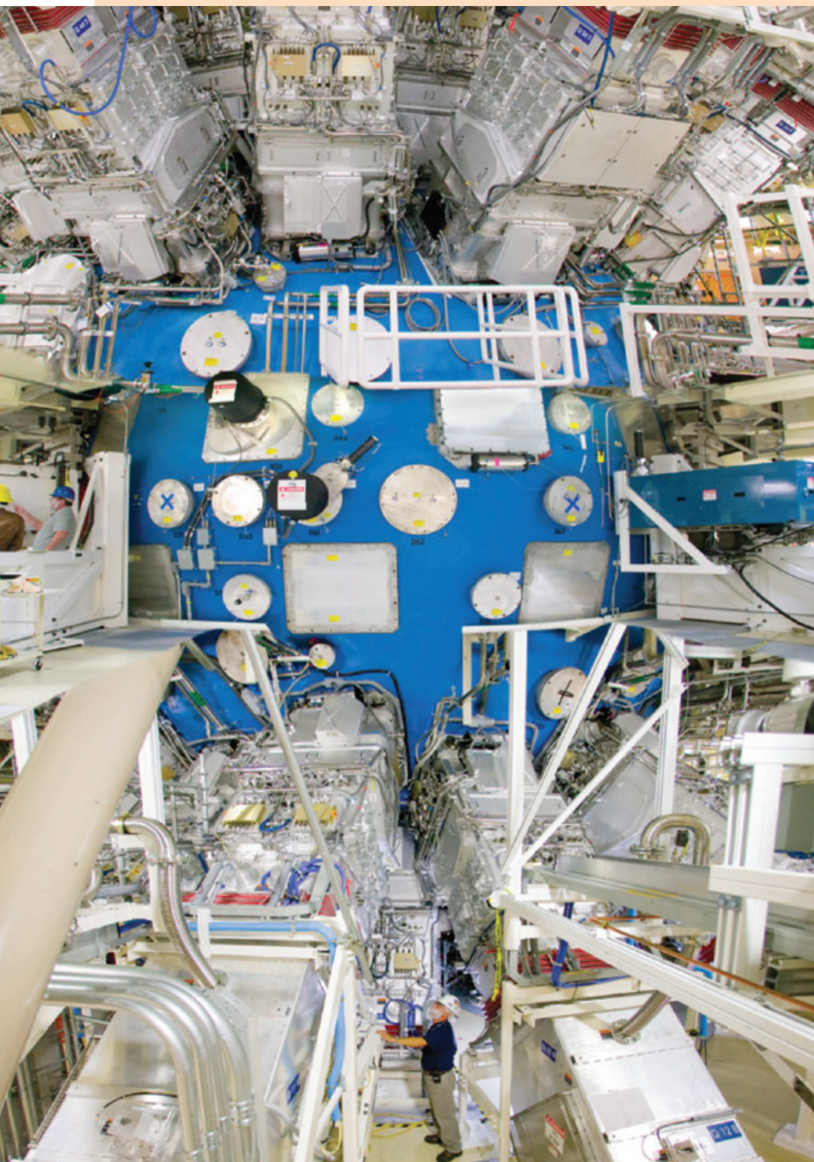
The U.S. energy situation becomes particularly acute in the period leading up to the middle part of this century, when the current fleet of nuclear and coal power plants will need to be replaced. "As a national lab, we must respond to the requirement to transform the energy landscape and do so soon enough to make a difference," says physicist Mike Dunne,



Experts predict the U.S. energy situation will become particularly acute in the middle part of this century, when the current fleet of nuclear and coal power plants will need to be replaced (source: U.S. Energy Information Agency's Annual Energy Outlook, 2009). Based on these power plant retirement curves, a LIFE fleet, beginning with an initial plant in the 2020s, could comprise 25 percent of newly built U.S. electrical generation plants by 2050 and a significantly greater fraction thereafter. Estimates of LIFE's capital and operational costs are strongly competitive with other baseload power plants.

Making History with the National Ignition Facility

The LIFE plant design builds on the geometry and performance of the National Ignition Facility (NIF) located at Lawrence Livermore. Completed in 2009, NIF is the largest scientific project ever built by the Department of Energy. NIF's 192 laser beams are capable of directing nearly 2 million joules of ultraviolet laser energy in billionths of a second to a fusion target.



NIF is designed to deliver net energy gain (more fusion energy out than the laser beams deliver). The experimental program to achieve fusion and energy gain, known as the National Ignition Campaign, is a partnership between Lawrence Livermore, the Laboratory for Laser Energetics at the University of Rochester, Los Alamos and Sandia national laboratories, and General Atomics, along with collaborators such as Massachusetts Institute of Technology, Atomic Weapons Establishment in the United Kingdom, and Commissariat à l'Energie Atomique in France.

The National Ignition Campaign began experiments in 2009. On September 29, 2010, an experiment successfully demonstrated the integration of all the complex systems required for the laser to ignite fusion fuel. In the test, NIF fired 1 megajoule of laser energy into its first cryogenically layered capsule. Then, on November 2, the team fired 1.3 megajoules of ultraviolet light into a cryogenically cooled cylinder called a hohlraum containing a surrogate fusion target known as a symmetry capsule. This experiment was the highest-energy laser shot in history and the first test of hohlraum temperature and capsule symmetry under conditions designed to produce ignition and energy gain.

"From both a system integration and a physics point of view, the results from these early experiments are extremely encouraging," says Ed Moses, principal associate director of NIF and Photon Science. "They give us increasing confidence that we will be able to achieve ignition conditions in deuterium–tritium fusion targets."

NIF ignition experiments will use a centimeter-size hohlraum containing a millimeter-size, thin-walled plastic or beryllium capsule filled with a mix of deuterium and tritium (hydrogen isotopes) gas. Compression of the capsule by the radiation field in the ignition hohlraum will drive the deuterium–tritium fuel to conditions under which it will ignite and burn, liberating more energy than is required to initiate the fusion reaction. Energy gain has been the goal of the ignition program since NIF was first conceived.

NIF's ability to create extraordinarily high pressures, temperatures, and densities—as much as 100 million gigapascals, 100 million kelvins, and 1,000 grams per cubic centimeter density—will enable major fundamental advances in support of the Department of Energy's national security, energy security, and fundamental science missions. A cornerstone of the Stockpile Stewardship Program, NIF will execute the science experiments necessary to ensure a safe, secure, and reliable nuclear weapon stockpile without underground nuclear testing.

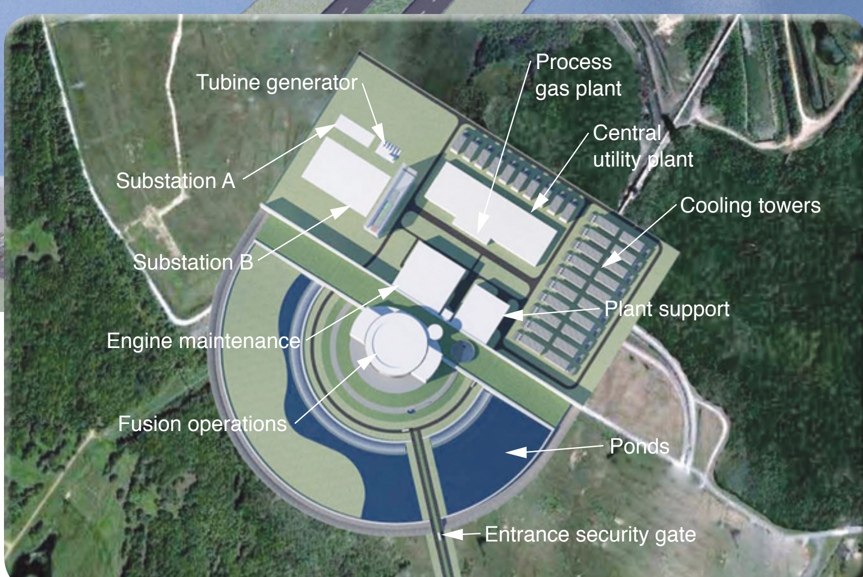
A scientist (bottom center) stands outside the National Ignition Facility's (NIF's) target chamber (blue), where 192 laser beams, in bundles of four, converge at the top and bottom of the target chamber and deposit their energy onto a BB-sized fuel capsule.

Livermore's program director for Laser Fusion Energy.

The Livermore-led effort to address the need for safe, secure, and sustainable energy is called Laser Inertial Fusion Energy, or LIFE. The development activities are headed by Dunne, with contributions by dozens of Livermore physicists, engineers, and materials scientists, along with major input from many other national laboratories, universities, and industry partners. LIFE draws on the success of the National Ignition Facility (NIF), the world's largest and most energetic laser system, and the sustained investment in inertial fusion energy by the Department of Energy and its predecessor agencies over the past five decades. Inertial fusion uses powerful lasers to compress and heat the hydrogen isotopes deuterium and tritium to the point of fusion and thereby liberate more energy than was required to ignite the reaction.

On the Brink of Ignition

NIF is designed to achieve the extreme conditions needed for fusion ignition, burn, and energy gain—the key milestone in the scientific pursuit of fusion energy as a source of electricity.



(above) An artist's rendering depicts a LIFE plant. (left) A plant could consist of a 100-meter-diameter main fusion operations building (circular building), an electrical generation building housing steam turbines, a tritium building for recovering fuel for new fusion targets, a maintenance bay for chamber refurbishment, and support facilities. At center right are forced-air cooling towers 14 meters tall that could replace the giant cooling towers used in many power plants.

"Demonstration of ignition will establish that the physics underpinning laser-driven fusion energy are fundamentally sound and ready to be exploited," says Dunne. "It will mark the culmination of over 50 years' work." Ignition would provide the basis for initiating a concerted LIFE development program to construct an electricity-producing demonstration plant by the 2020s. This first-of-a-kind power plant would provide the evidence required to allow rollout of a commercial fleet of power plants in the time period when many existing U.S. plants will be retiring. "The LIFE approach marks a dramatic shift from the conventional paradigm for fusion energy, which requires multiple intermediate facilities and much longer delivery timescales," says Dunne.

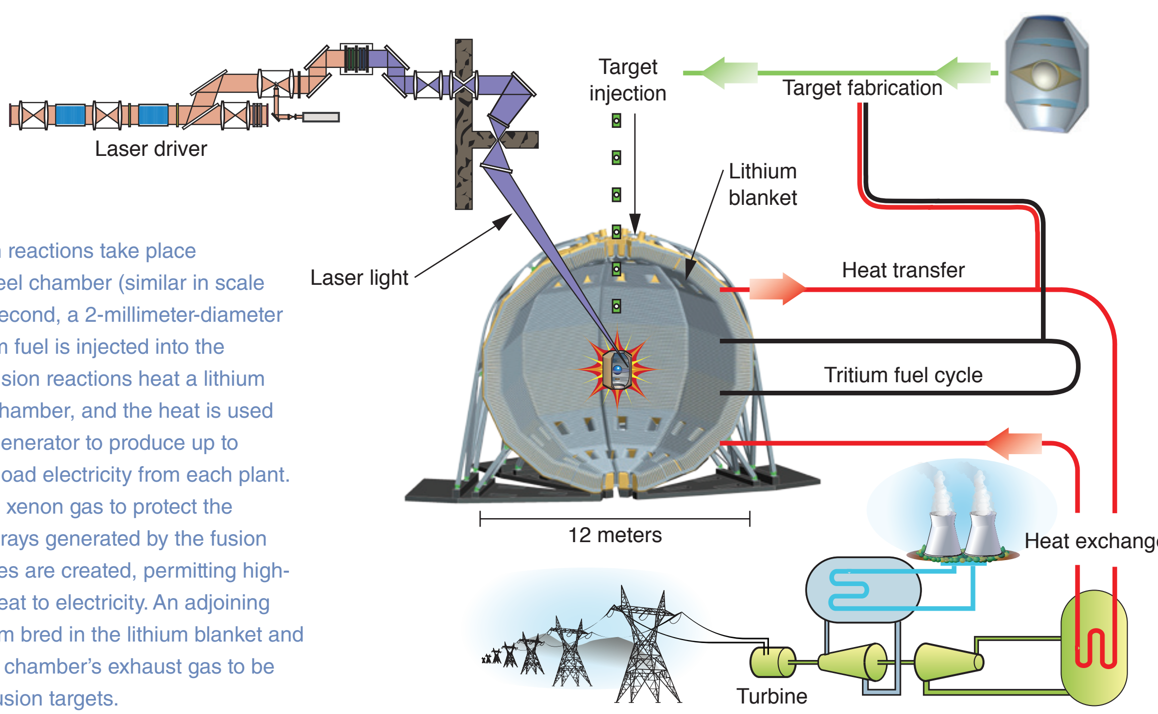
Deuterium and tritium, the fuels for LIFE, are derived from water and the metal lithium, abundant resources that can provide energy security across the globe. LIFE plants would produce no carbon-based or other harmful emissions. A principal benefit of a LIFE power plant is its intrinsic safety. No possibility would exist of a runaway reaction, a core meltdown, or the release of long-lived radionuclides. Decommissioning would only involve removal of steel and concrete structures for shallow land burial. When operations stop, the residual heat in the system does not require active cooling, so one can just walk away from the plant without any off-site consequences in the event of a natural disaster. The by-product of fusion is helium gas, which avoids the problem of spent-fuel storage.

The heart of LIFE is a laser fusion "engine," where 2-millimeter-diameter fuel capsules are injected into a chamber about 16 times every second (similar to the rate of an idling car engine). When the nuclei of deuterium and tritium fuse, the reaction creates a helium nucleus and releases a high-energy neutron. The repeated fusion reactions produce a steady stream of neutrons that heat a lithium blanket surrounding the chamber. The heat is used to drive a steam-turbine generator to produce up to 1,500 megawatts of baseload electricity from each plant.

Cost-Cutting Consciousness

The LIFE team is currently focused on meeting the required performance and costs for the dozens of systems and subsystems comprising a power plant. More than 30 vendors have been engaged from the semiconductor, optics, laser, construction, nuclear project delivery, and power-generation industries to assess component availability, performance, and cost. The team is taking advantage of marketplace advances for such components as laser diodes.

"LIFE economics will be strongly competitive with nuclear power plants and other low-carbon sources of electricity," says Dunne. The first LIFE power plant is being designed to generate a few hundred megawatts of electricity for the demonstration of continuous operation, high availability, and overall system reliability. Subsequent plants would likely



In the LIFE design, fusion reactions take place in a 12-meter-diameter steel chamber (similar in scale to NIF). Sixteen times a second, a 2-millimeter-diameter target of deuterium–tritium fuel is injected into the chamber. The repeated fusion reactions heat a lithium blanket surrounding the chamber, and the heat is used to drive a steam-turbine generator to produce up to 1,500 megawatts of baseload electricity from each plant. The chamber is filled with xenon gas to protect the chamber from ions and x rays generated by the fusion process. High temperatures are created, permitting high-efficiency conversion of heat to electricity. An adjoining tritium plant extracts tritium bred in the lithium blanket and unburned tritium from the chamber's exhaust gas to be used for producing new fusion targets.

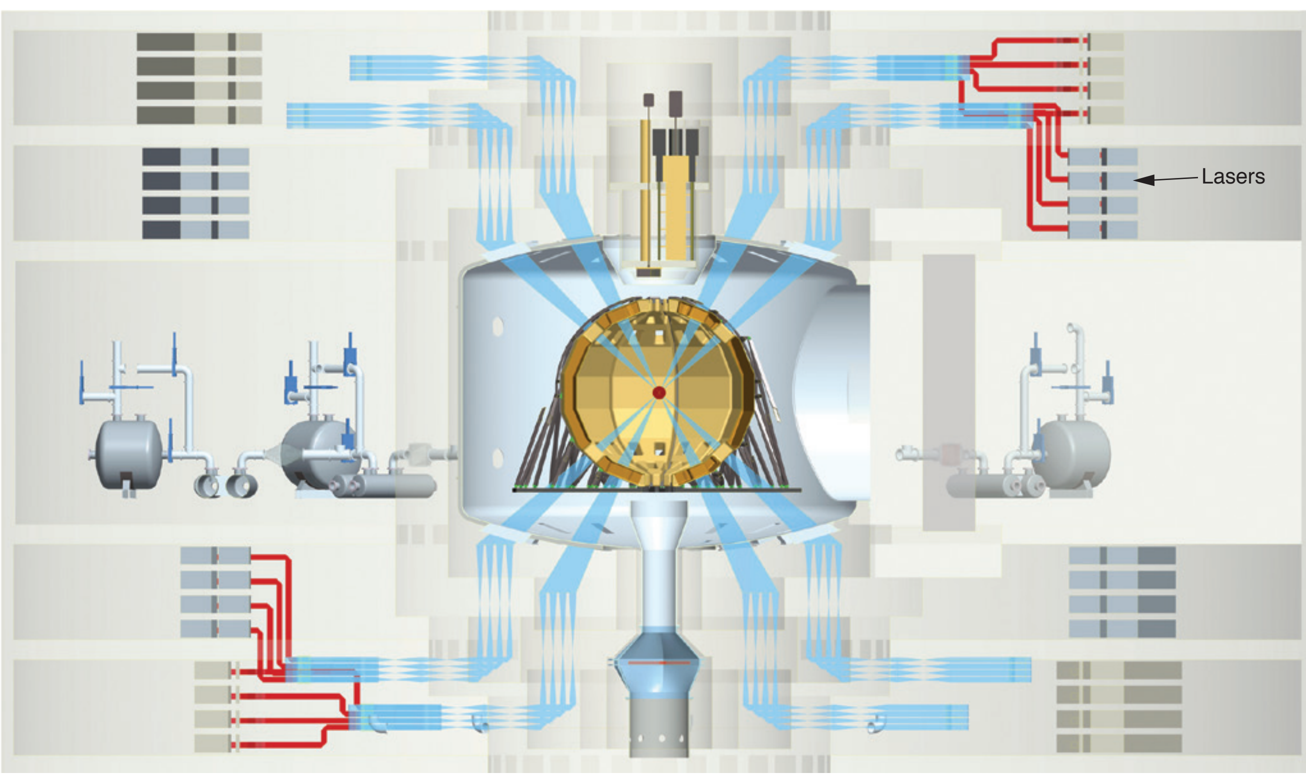
approach a gigawatt or more, benefiting from the significant economies of scale.

LIFE scientist Jeff Latkowski notes that the efficiency of the laser driver in converting energy supplied from the electrical power grid to the energy needed to compress the capsule, coupled with the energy "gain" of the capsule, must be sufficient to yield substantial net energy. The efficiency of the 2.2-megajoule laser driver is calculated to be 16 percent, coupled to a steel-blanket gain of 1.25, a thermoelectric conversion efficiency of 45 percent, and a fusion target gain of 60 (fusion energy divided by laser energy). This combination of efficiencies leads to a commercially acceptable overall plant gain of about 5.

Aiding cost efficiencies is the adoption of modular, line replaceable units (LRUs) throughout the plant. LRUs allow off-site factory construction and easy replacement of individual elements of the system, while maintaining plant operations. The LIFE strategy is to make components small, modular, and cost-effective. Modularity also permits improvements to be made throughout the lifetime of the plant, as long as the new technology fits in the same "box."

LRUs are used extensively on NIF and were previously instrumental in the atomic vapor laser isotope separation (AVLIS) project at Livermore. AVLIS used high-repetition-rate, multikilowatt lasers to separate isotopes of uranium. For more than 10 years, AVLIS demonstrated 24/7 operation with 99 percent availability. Several current LIFE and NIF managers have had experience running AVLIS. Ed Moses, principal associate director for NIF and Photon Science, for example, directed AVLIS operations for several years.

"Intense design, development, and review have led to enormous progress in the LIFE electrical power plant design over the past two years to meet performance and cost goals," says Moses. "LIFE will be based on the demonstration of fusion ignition at NIF and will use that facility's physics platform and architecture. However, the LIFE design has been transformed into a completely modular, factory-built laser system that can be put together and maintained using line replaceable units. An entire LIFE plant will be smaller than NIF and yet produce enough energy to power a city the size of San Francisco."



A cross-section of a LIFE power plant shows how it is based on the geometry of NIF. LIFE's 384 laser beamlines (twice the number as NIF) converge on a tiny target located inside the target chamber. The plant, optimized for high availability, features modular, factory-built components using existing materials and technologies.

A LIFE design team strategy session includes scientist Jeff Latkowski (standing, far left), Mike Dunne, program director for Laser Fusion Energy (standing, far right), and Ed Moses, principal associate director of NIF and Photon Science (seated below Dunne). Many Livermore physicists, engineers, and materials scientists are contributing to the LIFE design effort.

Listening to Utilities

The current LIFE power plant design is derived from the requirements of utilities, vendors, licensing bodies, and other stakeholders. "Rigorously addressing end-user requirements produces a very different design and delivery path than conventional approaches based on technical performance alone," says Dunne. This approach drives researchers to go beyond technical performance issues to take into account such factors as costs of construction and electricity production, licensing, reliability, availability (the amount of time the plant produces electricity), maintainability, inspectability, operability, urban environmental and safety standards, and public acceptability.

LIFE managers regularly confer with electric utility chief executive officers from across the U.S. and abroad. A group of utility executives recently formed an advisory committee to share industry expertise, experience, and insights with the LIFE development team. "When visitors from the power industry tour NIF, they realize a commercial plant could be viable soon enough to make a difference," says systems engineer Tom Anklam, who heads the effort to integrate LIFE's many systems.

"We've had a staggeringly positive response from the power industry," says Dunne. "But this is a hard-nosed industry that wants to know how we go from NIF's proof of principle to operating a commercial fleet of power plants. What matters to utilities is cost to build, cost to operate, reliability, and licensing pathways."

As a result of the advisory group meetings, LIFE designers took a long hard look at their approach. "We transformed a design that looked like an incremental adaptation of NIF into a commercially viable power plant," says Dunne. The new design emphasizes integrated coupling between every major system, an effort headed by Anklam.

Engineer Valerie Roberts, deputy principal associate director of NIF and Photon Science Operations, oversaw construction of NIF. Roberts is now working on the project delivery plan. "We want a plant that industry can build easily and reliably," she says. The LIFE design currently consists of a main fusion operation building, an electrical generation building housing steam turbines, a tritium building for recovering fuel for new fusion targets, a maintenance bay for chamber refurbishment, and all the required support facilities.

An earlier version of LIFE focused on a fusion–fission hybrid design that used waste from nuclear power plants as well as weapons-grade plutonium for fuel. (See *S&TR*, April/May 2009, pp. 6–15.) Although this option remains a possibility, the team is now focusing on a pure fusion option.

Instead of enormous cooling towers that characterize many existing power plants, LIFE features advanced forced-air cooling towers just 14 meters tall. Roberts says a LIFE plant could be placed in an urban setting on a site measuring 300,000 to 400,000 square meters (75 to 100 acres). It could also be sited at a retired coal or nuclear power plant to take advantage of much of the existing electrical grid infrastructure.

Fusion Reactions in LIFE Chamber

In the LIFE engine, fusion reactions occur in a 12-meter-diameter steel chamber similar in scale to the NIF system. The modular, factory-built first wall and blanket comprising the chamber is constructed from existing materials and rapidly replaced as needed every few years. A series of U-shaped steel tubes forms the first wall, backed by a thick blanket that allows the lithium to absorb the neutron energy and flow to a heat exchanger.

The chamber is constructed from eight modules that can be withdrawn on rails to a maintenance bay in isolation or as a complete unit. The chamber is housed inside a separate vacuum vessel, with connections only for cooling lines. By decoupling the chamber from the vacuum and optical systems, a relatively rapid exchange can be achieved.

The chamber will be filled with xenon gas to absorb ions and x rays given off by the fusion process, which otherwise would be damaging to the chamber wall materials. The gas does not interfere with the laser beam propagation or target injection.

The ability of a LIFE plant to generate high temperatures (typically 600°C) in the first wall and blanket permits high-efficiency conversion of heat to electricity. Liquid lithium running through both the first wall and blanket will capture the heat. Lithium was chosen as the LIFE coolant because when lithium atoms absorb the neutrons generated by the fusion reactions, the lithium is transmuted to tritium and helium. "A LIFE plant would breed all the tritium needed for the targets," explains Latkowski. The adjoining tritium plant would take tritium that has been bred in the lithium coolant and unburned tritium from the chamber exhaust gas for use in producing new fusion targets.

A typical LIFE plant will require up to 1.3 million targets daily. Techniques for the manufacture of large quantities of targets are being explored, along with methods to inject them accurately to the center of the target chamber at a velocity of 250 meters per second. A target factory alongside the fusion building will assemble targets from components manufactured off site. Independent analyses of target production factories show that mass production techniques should yield costs of $0.20 to $0.30 per target.

Each LIFE target will contain only about 0.7 milligrams of tritium. The site inventory of tritium will be low, with substantial segregation to ensure safe operations.

Diodes Transform Laser System

Engineer Robert Deri leads a team that is developing a compact, efficient, cost-effective laser system to drive the LIFE power plant. Deri notes that NIF's 192 beams were designed to fire simultaneously only once every few hours. After each shot, the laser glass must cool down to ensure that the optics operate correctly for the next shot. A LIFE plant, however, must operate at a much higher repetition rate (15 hertz). To achieve this, the team is taking advantage of recent advances in laser architecture and semiconductor technology that permit high-average-power operation.

Development of high-efficiency, high-repetition-rate, diode-pumped solid-state laser beamlines is under way for several international projects. In addition, technology and experience from Livermore's AVLIS and Mercury lasers and other high-average-power solid-state lasers is being incorporated into LIFE. Mercury can fire 10 shots a second over extended periods, using cooling technology that is being implemented at a larger scale in the LIFE laser design.

Whereas NIF uses 2-meter-long flashlamps to energize the neodymium atoms in the laser glass amplifiers, LIFE would rely on laser diodes. The diodes are 20 times more efficient than flashlamps, measure 10 to 12 times smaller, and give off substantially less waste heat. "Laser diodes give us the ability to fire 15 times a second, 24 hours, 7 days a week," says Deri.

More than 100 million diodes will be required for LIFE's 384 beamlines. "We're working closely with 14 laser-diode manufacturers to lower costs because diodes will account for a substantial fraction of the laser system's cost," says Deri. He compares the team's association with industry to the cadre of NIF scientists who worked closely with laser glass companies to manufacture affordable laser optics with unprecedented purity and performance.

Deri's team has designed an entire 1,053-nanometer wavelength infrared-light beamline that fits in one truck-transportable box—a "beamline in a box." (See the figure on p. 12.) Measuring less than 11 meters long, the beamline can be handled as an LRU. The compact size would allow for off-site manufacture, ease of maintenance during operation, and even changeover of individual beamlines while the plant remains operational. Beamlines would also have the ability to enhance their output to compensate for a failed neighboring beam. Optics outside the beam box would convert incoming laser light to 351-nanometer wavelength ultraviolet light for focusing on fusion targets. An important milestone during the intense component development phase will be construction of a "LIFElet," that is, a full-scale laser beamline for testing.

Demonstration Plant

The next step on the path to commercial LIFE plants would be a five- to seven-year technology development program, followed by a demonstration power plant generating about 400 megawatts of electricity. This plant, which could be operational by the mid-2020s, would demonstrate integrated operation of a commercial LIFE plant design. The demonstration plant would provide the required fusion environment for full-scale testing of materials, components, and systems; provide qualification and certification data for licensing of subsequent commercial plants; and drive vendor readiness for rollout of a commercial fleet.

"We aim to build a demonstration power plant. That's much different from a typical technology test facility," says Dunne. "By basing the design on evidence from NIF and using existing technology options, our strategy eliminates the costs and delays associated with a stepwise approach needed for other approaches to fusion. These approaches require multiple facilities to mitigate the risks arising from unproven physics, use of novel materials, and new technologies."

The team calculates that LIFE plants could deliver 25 percent of U.S.

electrical generation by 2050. Estimates of LIFE's capital and operational costs are highly competitive with other energy alternatives. Rollout of LIFE plants that would displace coal plants beginning in the 2030s could result in a decrease of 90 to 140 billion metric tons of carbon dioxide-equivalent emissions by the end of the century.

While LIFE researchers continue their design work, two national organizations are studying the cost effectiveness and scientific principles behind LIFE. The first study, by the Electric Power Research Institute, focuses on the best avenue toward a working fusion power plant. The second, by the National Research Council, is studying the technology goals, challenges, and path forward for inertial fusion energy.

Dunne believes that a strong national partnership among industry, national laboratories, government, nongovernmental organizations, and academia is required to deliver LIFE. Livermore researchers are already working closely with General Atomics on targets; Savannah River and Los Alamos national laboratories and Princeton Plasma Physics Laboratory on design of tritium systems; the University of Rochester's Laboratory for Laser Energetics on target and laser designs; the University of Wisconsin, University of California at San Diego, and University of Illinois on target chamber design; the Naval Postgraduate School on welding of specialty steels; and industry on all aspects of the power-generation technology.

"When ignition and gain are achieved on NIF, we will have a substantive delivery plan to take us to a commercial plant," says Dunne. "We will be ready to go."

—*Arnie Heller*

Key Words: deuterium, Electric Power Research Institute, electricity, flashlamp, inertial fusion, laser diode, Laser Inertial Fusion Energy (LIFE), lithium, National Ignition Facility (NIF), National Research Council, nuclear energy, power plant, tritium.

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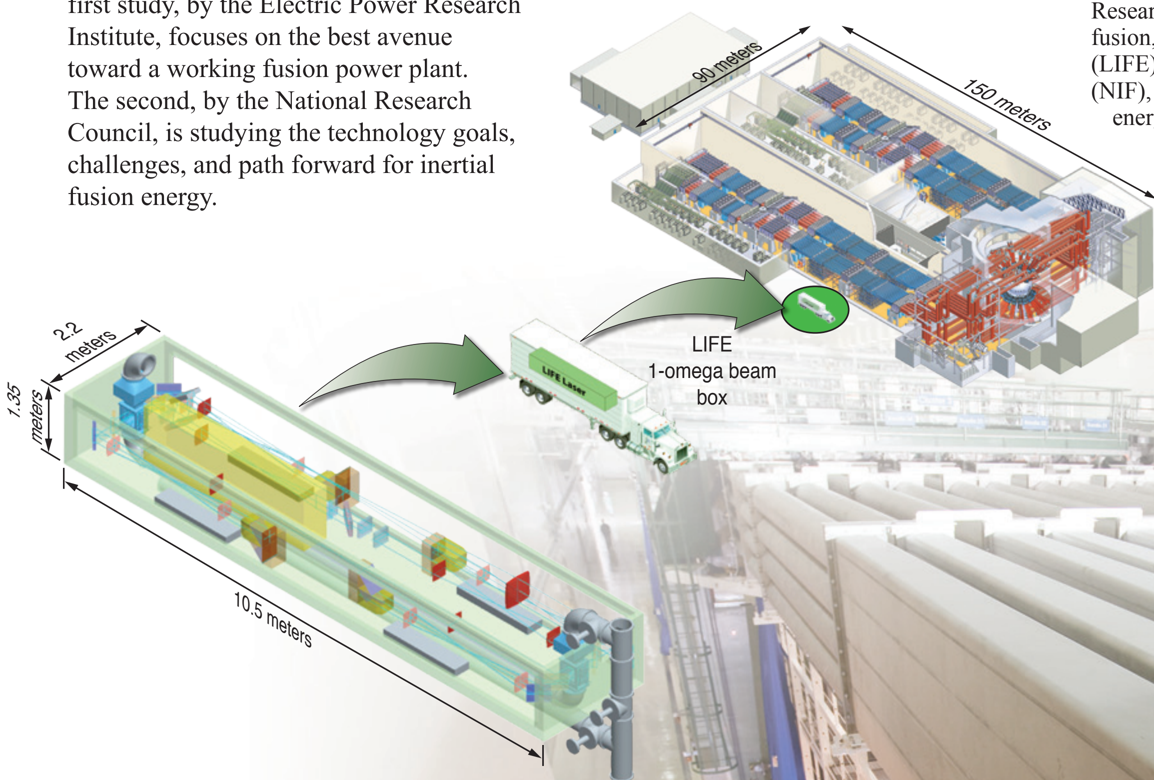


(above) This conceptual design shows how an entire 1,053-nanometer wavelength infrared-light laser beamline fits in a truck-transportable container. Because it measures less than 11 meters long, the beamline offers off-site manufacturing, ease of maintenance during operation, and even replacement while the plant remains operational. A truck holding a LIFE laser beamline is shown for size comparison next to NIF. (right) A mock-up of a LIFE "beam box" in the NIF laser bay shows the factor-of-10 size reduction compared to the NIF beamlines.

A "GRAND" WAY TO VISUALIZE SCIENCE

The Laboratory's high-performance computing machines allow researchers to push the frontiers of science.

WHETHER supercomputers are used for modeling the effects of climate change or the complex nature of molecular dynamics, they play a major role at Livermore in scientific discovery. The Laboratory's high-performance computing (HPC) machines consistently make headlines as some of the fastest, highest capability computers in the world, enabling simulations of physical processes that could not be investigated by experiment alone.

Livermore's HPC systems are predominantly dedicated to performing simulations in support of the National Nuclear Security Administration's Stockpile Stewardship Program for maintaining a safe, secure, and reliable nuclear deterrent. Time is also dedicated on these machines for other research that is important to the Laboratory's mission and programs, including projects funded through the Laboratory Directed Research and Development (LDRD) Program, which promotes potentially high-payoff projects.

In 2006, Livermore expanded access to its HPC resources to the broader Laboratory community through the Institutional Unclassified Computing Grand Challenge Awards. This program aims to further scientific innovation and at the same time advance supercomputing capabilities. "With Grand Challenge projects, we are looking to push the frontiers of computational science and to achieve scientific breakthroughs that would not be possible without HPC resources," says Fred Streitz, director of Livermore's Institute for Scientific Computing Research and chief computational scientist in the Laboratory's Physical and Life Sciences Directorate. "As a result of the Grand Challenge projects, we've seen teams develop new, more complex algorithms that enable them to substantially progress their research."

Last year, more than 400 million computing hours (number of processors times number of hours) were allocated to teams from across the Laboratory working on unclassified, mission-relevant projects that meet Grand Challenge objectives. In at typical year, 10 to 12 projects are given allocations for a one-year term, with more time provided to those projects that have greater Laboratory relevance and promise for maximum benefit from use of HPC machines. Says Streitz, "Projects awarded allocations are expected to receive high-level recognition from mission sponsors, the computing community, and the scientific community at large."

Divvying Up the Goods

Laboratory researchers apply for Grand Challenge allocations once a year during a formal call for proposals. Each proposal goes through a rigorous review process, which is managed by Streitz and Brian Carnes, director of Multiprogrammatic and Institutional Computing (M&IC). The M&IC program manages time allocations on all the Laboratory's unclassified supercomputers.

Streitz and Carnes spearhead the Institutional Grand Challenge Awards Committee, which arranges for each proposal to be peer-reviewed by internal and external subject-matter experts. Based on these experts' assessments and input from the committee, M&IC, and the Laboratory's Institutional Science and Technology Office, time allocations and priority are awarded. The projects are judged on five main criteria: quality and potential impact of proposed science or engineering; significance and potential impact of proposed computation; ability to effectively utilize a high-performance, institutional computing infrastructure; quality and extent of internal and external collaborations; and alignment with the Laboratory's science and technology strategic vision.

This article highlights five Tier 1 projects—those with the highest allocations—that were awarded in November 2010 to teams studying a wide range of high-energy-density (HED) physics topics. Simulations are run on the unclassified BlueGene/L and Sierra machines, both of which perform more than 200 trillion floating-point operations per second (teraflops). At the end of this year, award winners will formally present their work during a weeklong Laboratory colloquium.

A Universal Mystery

Understanding the origin and evolution of our universe has been a key scientific pursuit for nearly a century. The big bang theory suggests that in an instant no longer than a trillionth of a second occurring roughly 13.7 billion years ago, our universe began as a hot, dense plasma. Almost immediately, this primordial mixture rapidly expanded and cooled, producing the first elementary particles and their masses, and causing quarks and gluons—the building blocks of all nuclear material—to bind together into stable, nuclear particles, in particular, into protons and neutrons.

Billions of years later, exactly how these events unfolded still remains a mystery. In an attempt to help answer the tough questions associated with the origins of the universe, a team led by Livermore physicists Pavlos Vranas, Tom Luu, and Ron Soltz is using its Grand Challenge allocation to simulate the particle events that occurred shortly after the big bang. "We are performing numerical simulations to unravel the mechanism by which mass was created in the visible universe," says Vranas. "We are also calculating the transition and thermal properties of the quark–gluon plasma and the properties of the nuclear force as it emerges from the interactions of quarks and gluons."

Experimentally, particle accelerators, such as the Large Hadron Collider in Switzerland, the Tevatron at Fermi National Accelerator Laboratory (Fermilab), and the Relativistic Heavy Ion Collider at Brookhaven National Laboratory, create conditions similar to those that occurred after the big bang. Inside accelerators, particles are smashed together at extremely high energies, generating different particles that in turn provide details about the interaction itself. Simulations on supercomputers help explain current experimental findings and predict future results.

With the help of the unclassified BlueGene/L, the team, which also includes researchers at Yale University, University of California at Davis, Columbia University, University of Washington, Boston University, Fermilab, and Argonne and Los Alamos national laboratories, is modeling a technicolor theory in an attempt to simulate how nuclear particles obtain mass. (Technicolor theories are models of physics beyond the standard model that address the mechanism through which elementary particles acquire mass.)

The team is also modeling quantum chromodynamics (QCD), the theory that explains how quarks and gluons interact to form stable, nuclear particles. In both technicolor theories and QCD, particle interactions are modeled in a four-dimensional grid of points connected with links, known as a lattice. (See *S&TR*, January/February 2008, pp. 11–16.)

"For the first time, we have discovered strong evidence of mass generation in technicolor theories," says Vranas. "We've also begun incorporating our own lattice calculation of the QCD equation of state into a detailed, multistage model of a heavy-ion collision. This research is improving our understanding of how QCD manifests itself as nuclei and how these nuclei interact."

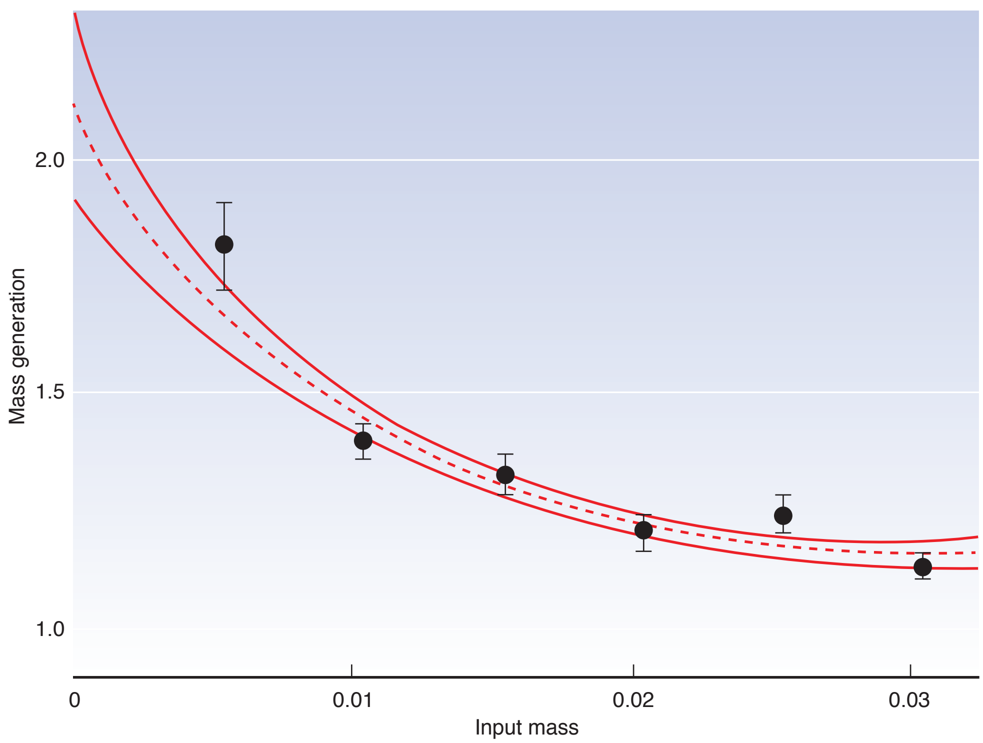
Ultimately, the team's research will help predict experimental results from the newest particle colliders. Vranas says, "High-performance computing may be the only way to understand the behavior of strongly interacting physics processes such as technicolor and QCD. It is an indispensable tool for probing deeper into the cosmic mysteries of our time."

A Carbon Conundrum

How matter began to form after the big bang is just one of the many secrets the universe holds. Another mystery that scientists have been sleuthing for decades involves the process by which stars, such as our Sun, and red giants, such as Betelgeuse, fuse helium particles to create all the carbon in the universe, including that on planet Earth. "The ability to know for certain how fusion happens in stars, especially carbon formation, is considered one of the Holy Grails in nuclear physics," says Livermore physicist Erich Ormand. Stars such as Betelgeuse are also responsible for the enigmatic process that results in helium and carbon fusing together to create oxygen.

To solve this fusion mystery, scientists must not only define the structure of light nuclei but also identify the exact mechanisms by which these particles interact. "We have used past Grand Challenge allocations to simulate the structure of these nuclei," says Ormand. "During this Grand Challenge cycle, we are attempting to simulate how the more realistically structured particles interact with each other." The work is being performed in collaboration with TRIUMF in Canada, University of Arizona, Iowa State University, San Diego State University, and Ohio State University.

At the heart of this research lies the need to develop a deeper understanding of nuclear properties, in particular, how nucleons interact and bind together to create atomic nuclei. For decades, scientists have sought to develop a first-principles approach to nuclear properties, but their efforts have been thwarted by a lack of adequate theory and the computational power necessary to run the calculations. Fortunately, over the last 10 years, significant advances have been made in both areas that could bring this goal to fruition. "With Livermore's supercomputers, we can simulate two- and three-body reactions, such as



A Grand Challenge team uses a technicolor theory to attempt to explain how elementary particles obtain their mass. The team's recent simulation results show that as the input mass is decreased to zero, nonzero particle masses are generated solely as a result of the inherent technicolor dynamics. That is, the inherent technicolor dynamics are capable of producing mass on their own without requiring theorists to set it in "by hand." Technicolor simulations may one day be able to explain why the electron has the mass we observe.

deuterium–tritium fusion, occurring at low energies," says Ormand. "Our research has already shown that pair-wise (two-body) interactions between nucleons are strongly augmented by triplet (three-body) interactions, which not only make nuclei more tightly bound but also alter their low-lying structure such as ground-state spin."

The team is using the no-core shell model combined with the resonating group method and state-of-the-art interaction codes to simulate the quantum states of particles involved in fusion processes. "Our approach is one of the few available today that is capable of simultaneously describing bound and scattered states in light nuclei based on first principles," says Ormand.

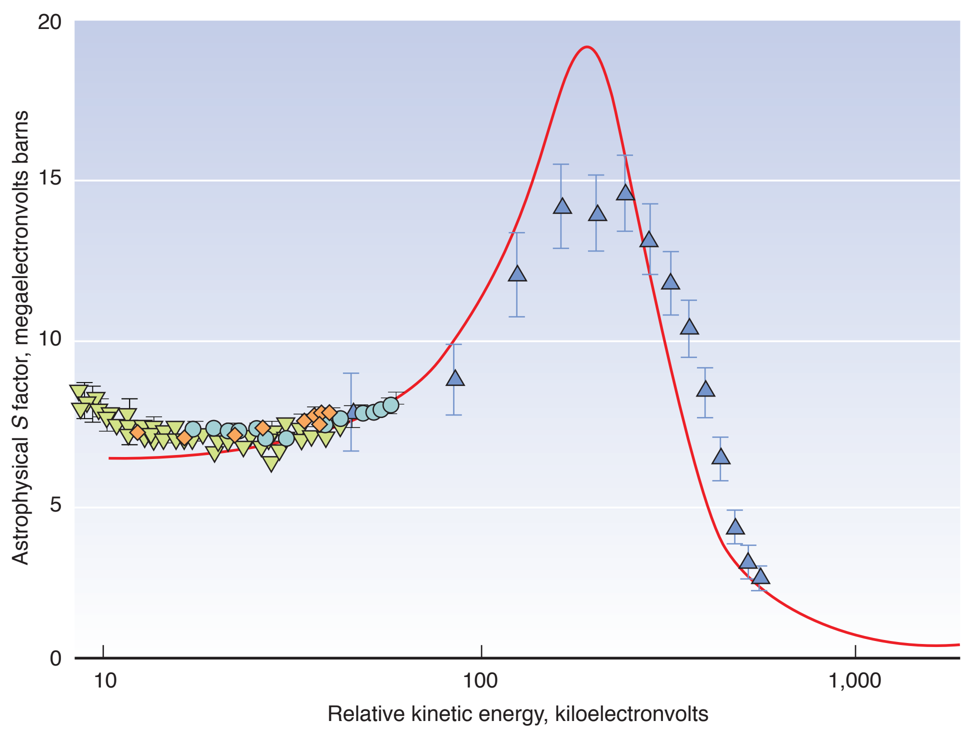
Current experiments are limited in their ability to create the right conditions for studying complex nuclear properties, but HPC machines coupled with advanced codes enable researchers to delve into never-before-seen physical processes. "With these simulations, we can model fusion reactions occurring at temperatures much lower than those that can be achieved in experiments," says Ormand. Ultimately, what the team discovers about nuclear properties will be instrumental in expanding scientific understanding of the complex physical processes involved in the universe, including the fusion reactions that occur in stars and in experiments performed at the Laboratory's National Ignition Facility (NIF).

Building a "Solid" Understanding

NIF–the world's most energetic laser—will be a hub for conducting the next generation of HED physics experiments and, as such, will provide scientists with a new, more powerful tool for studying materials under extreme temperatures, pressures, and strain rates. (See *S&TR*, April/May 2010, pp. 4–11.) Researchers will need supercomputers to analyze the atomic-level processes occurring within these experiments. Livermore physicist Robert Rudd says, "Simulations are like microscopes that allow us to see minute details that would not be visible by reviewing the experimental data." A team led by Rudd, along with collaborators from the University of Oxford, is simulating the extreme deformation of solid metals—tantalum and vanadium—under ramp-wave compression.

The team's research is directly correlated with a three-year LDRD strategic initiative led by Bruce Remington that is developing the capability on multibeam lasers, such as NIF, to both drive high-pressure ramp waves in solids and to generate x rays for in situ diffraction studies. X-ray diffraction techniques allow scientists to visualize the crystal lattice structure—the arrangement of atoms—within materials, which affects the material's behavior. "Using our Grand Challenge allocation, we can model what is happening in an experiment and account for every single atom in the simulated material," says Rudd. "Our goal is to predict the microscopic processes of plasticity that occur in laser-driven material experiments and to develop novel predictive simulations of plasticity in high-pressure ramp waves."

Understanding how ramp waves initiate phase changes in materials is of particular interest to scientists because unlike shock waves, ramp waves generate a relatively small amount of heat in materials during compression. As a result, materials remain in their solid state longer, enabling them to be compressed at much higher pressures. "With these experiments, we can test a material's behavior at relatively low temperatures," says Rudd. The ability to compress materials at lower temperatures and higher pressures is relevant to

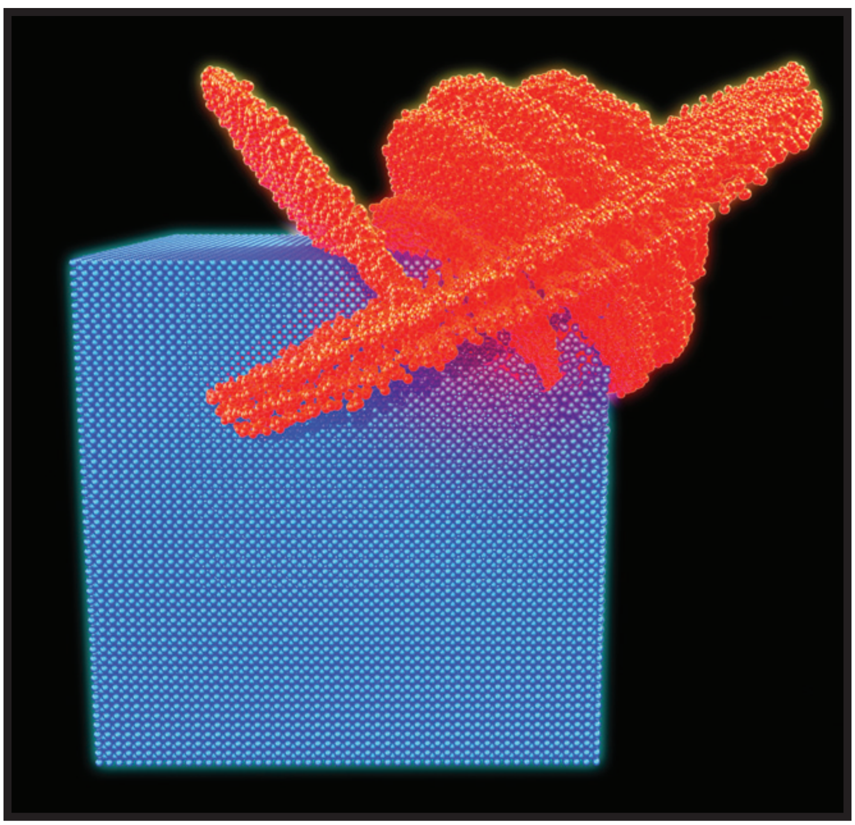


Another Grand Challenge team uses Livermore's supercomputers to simulate two- and three-body nuclear reactions occurring at low energies. This plot shows the first ab initio calculation (red line) of a deuterium–helium-3 fusion reaction as a function of energy for the incident deuterium nucleus compared with laboratory experimental data (points). Ab initio theories allow scientists to extrapolate data to the very low energies required for modeling stars.

many Laboratory missions including fusion research.

Modeling ramp waves requires more computational power than shock wave simulations because ramp wavefronts are less abrupt than shock waves. They also occur over larger temporal and spatial scales. Through its Grand Challenge allocation, the team now has access to more processors than before on the Laboratory's HPC machines. With the Livermore-developed molecular dynamics code dccMD, the researchers can use hundreds of thousands of processors at increased efficiency to model how atoms exert force on other atoms in a material. The code incorporates a modeling approach called generalized pseudopotential, which considers quantum mechanical bonding of the atoms. The latest version of dccMD handles the large density variations associated with dynamic compression. This upgraded code improves the quantitative predictive simulation of solid deformation for ramp-wave compression experiments.

In conjunction with the LDRD strategic initiative, these simulations will facilitate development of a new laser-based x-ray diagnostic for probing the lattice structure and properties of materials at ultrahigh pressures. "Through this Grand Challenge allocation," says Rudd, "we will simulate and interpret diffraction signals derived from next-generation HED experiments and provide an improved predictive modeling capability for Laboratory research."



As a solid material is compressed in a ramp wave, shear stresses can develop that are sufficiently strong to cause defects to form in the crystal lattice. Shown here is the nucleation of twins from a perfect single crystal of tantalum. The red spheres represent atoms in twin boundaries. Surrounding atoms are transparent to show the morphology of the twin. (Rendering by Kwei-Yu Chu.)

The Fast and the Curious

Achieving ignition at NIF is a key mission at Lawrence Livermore. The National Ignition Campaign, currently under way, is designed to demonstrate thermonuclear burn and energy gain for the first time in a laboratory. Although indirect-drive inertial confinement fusion is the predominant method by which NIF scientists are attempting to attain ignition, other methods are also being researched, including a technique called fast ignition. In this process, the target is first heated and compressed using the main laser, then a separate high-intensity, ultrashort-pulse laser ignites the fuel. Fast ignition has the potential to offer higher energy gains and has more relaxed requirements for implosion velocity and symmetry compared to conventional indirect-drive experiments.

For several years, Livermore physicist Andreas Kemp has been studying ultraintense laser–plasma interactions for fast ignition and for new types of HED physics experiments at NIF. To this end, Kemp has garnered multiple Grand Challenge allocations over the last five years. As part of earlier projects, Kemp helped develop a collisional particle-in-cell code called PSC that scales to thousands of processors for modeling short-pulse laser interaction with preformed plasma. This code has been further extended so that within a simulation, it can handle the orders-of-magnitude changes in plasma density found in experiments while achieving significantly improved efficiencies. Understanding laser–plasma interactions at ultrahigh intensities, and electron transport and velocity distribution, are paramount to making fast ignition a reality.

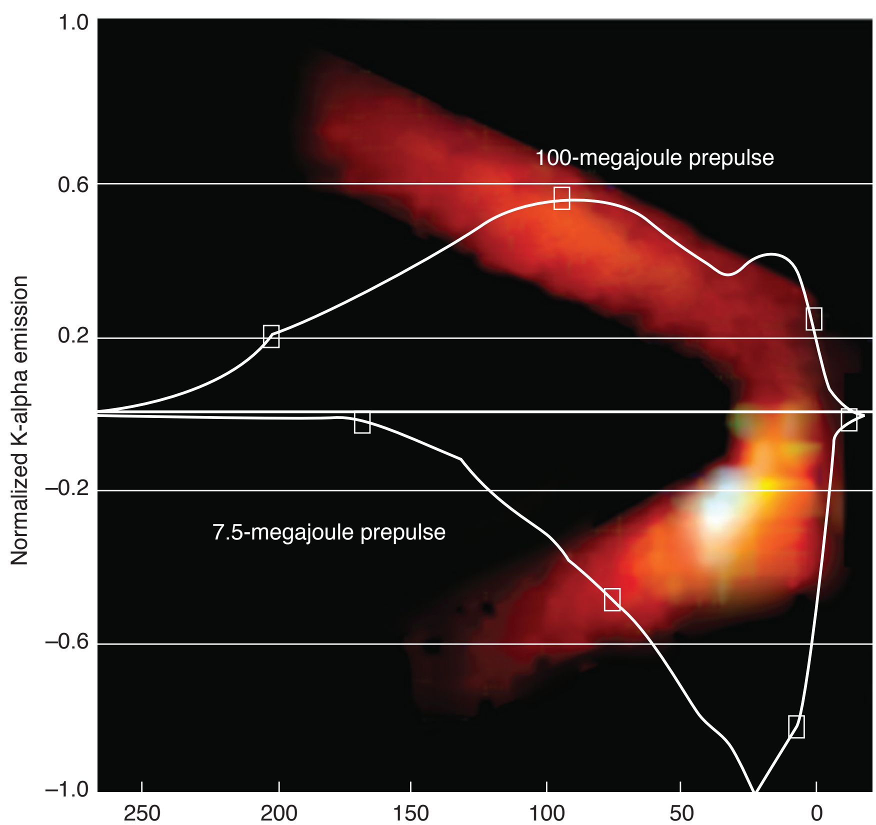
Most recently, Kemp has been working with colleagues at Livermore, the University of Nevada at Reno, and the University of Munich in Germany to further improve the PSC code. "We now propose to push the state of the art of short-pulse modeling by combining our particle-based hybrid algorithm with the radiation hydrodynamics code Hydra," says Kemp. The team will use this new version of the code to simulate the properties of solid-density plasmas. "We are able to model HED physics experiments on Livermore's Titan laser with almost quantitative accuracy. Our computational goal is to facilitate the first integrated simulation of a fast-ignition experiment that includes everything from the hydrodynamics of the capsule implosion to the high-power-laser interaction and heating of the dense core to ignition conditions," says Kemp. The simulations represent laser–plasma events occurring over picosecond timescales and will serve as a basis for designing targets for fast-ignition experiments.

"The sheer magnitude of the Grand Challenge computing allocations and the quality and consistency of the machines enable us to conduct simulations of the temporal and spatial domains found in actual experiments, which would not be possible with conventional allocations," says Kemp. "The work we are undertaking is ambitious, but with the Laboratory's supercomputers, we can create more realistic simulations that will eventually lead to a full-scale computer model of a fast-ignition experiment." Similar to the work done by Rudd, this research supports an LDRD strategic initiative for developing advanced inertial confinement fusion designs and diagnostics that will elucidate high-resolution details of HED experiments.

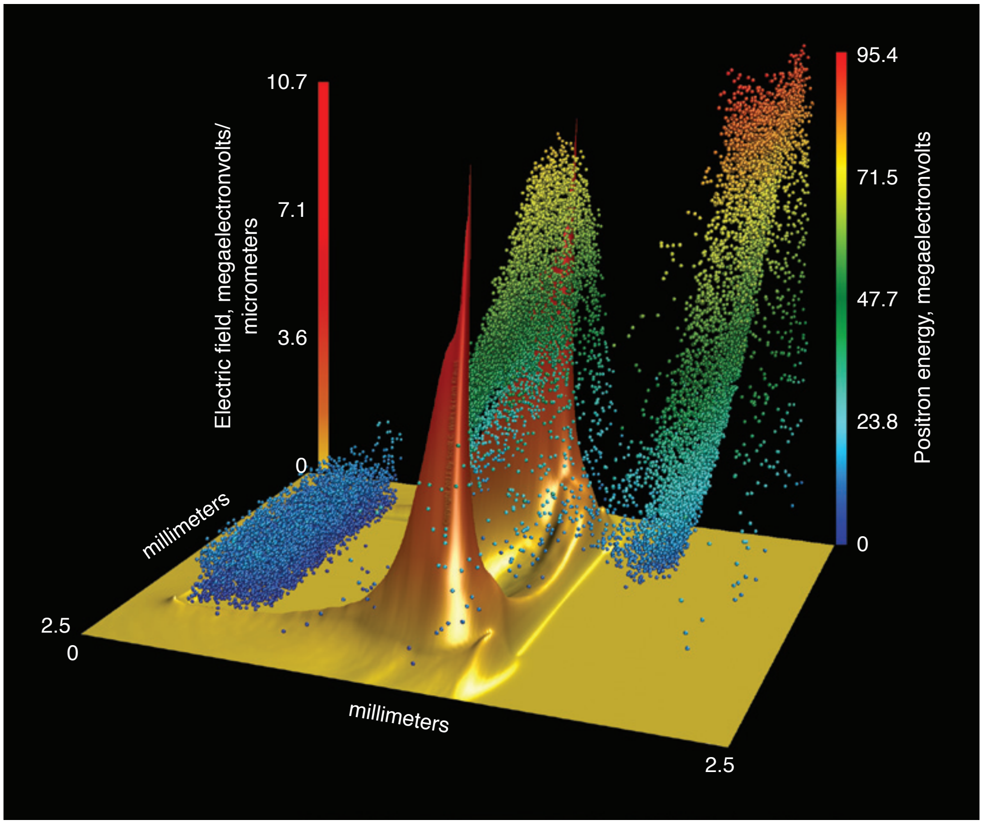
A Plethora of Particles

In 2009, Livermore scientists created the largest concentration of laser-generated positrons ever diagnosed in a laboratory setting by irradiating a millimeter-thick gold target with an ultrafast, high-energy laser. (See *S&TR*, January/February 2009, pp. 11–15.) Until that time, the prevailing belief was that more positrons could be effectively produced using ultrathin, foil targets a few micrometers in thickness. However, by simulating the laser–plasma–solid interaction on Livermore supercomputers, physicist Scott Wilks showed that thicker targets were a more efficient vehicle for generating positrons, thus increasing the yield by many times. LDRD funded the initial work on this project.

When a laser pulse hits the thicker target, a plasma is created on the surface of the material that contains electrons and ions. The strong electric field produced by the laser accelerates the electrons within the plasma, resulting in electrons with extremely high kinetic energies of more than 1 megaelectronvolt, the approximate threshold energy for electron–positron pair production. These hot electrons can interact with atoms in the target to either create electron–positron pairs directly, or instead create photons that in turn interact with other atoms in the solid to create a new electron–positron pair. Although adding the additional step of first creating photons may seem roundabout, it produces many more electron–positron pairs because the cross section for creating the pairs is about 100 times higher if one uses photons instead of electrons directly. These simulations coupled with experimental data proved that this process generated tens of billions



A Grand Challenge team is performing particle-in-cell simulations to explore the effect of preformed plasma in a fast-ignition target that uses a cone-shaped component to focus the laser into the dense core. In the results shown here, the two white lines indicate the 100-millijoule and 7.5-millijoule prepulses that were injected into the target before the main pulse during two separate simulations. The simulated K-alpha x-ray images compare well with experimental results.



A Grand Challenge allocation is allowing researchers to perform, for the first time, an integrated simulation that includes all the physical effects believed to occur in laser-generated electron–positron pair production and to see the connection between the escaping positrons and the hot electrons that created them. A superposition of the accelerating electric field (surface plot) on the rear of a millimeter-long target at the time positrons (colored dots) escape shows three "bunches" of positrons at three distinct times: inside the target (far left), exiting the target (middle, near peak of accelerating field), and after completely leaving the target (far right). The relative height of each bunch is a measure of the positrons' energy and indicates that the positrons gain several tens of megaelectronvolts as they exit the target.

of positrons in about a picosecond (a billionth of a second).

Using this year's Grand Challenge allocation, Wilks and collaborators from Ohio State University are applying a hybrid particle-in-cell plus fluid code, known as LSP, to simultaneously model positron generation and hot-electron excitation in three dimensions. LSP provides large-scale plasma simulations that model laser–plasma interactions. The model generates and tracks charged particles and photons through solid dense plasmas and calculates the interaction between particles and the electromagnetic fields they create. "This work will allow us to perform, for the first time, an integrated simulation that includes all the physical effects believed to occur in laser-generated pair production, and to specifically see the connection between the escaping positrons and the hot electrons that created them," says Wilks. Although LSP is not typically used for positron research, the team has developed a plug-in Monte Carlo code that works in conjunction with LSP to effectively model positron origination and propagation.

Electron energy and distribution cannot be measured through experiments alone because the electron excitation process occurs in front of the solid surface and the large electric potential inhibits electrons from escaping the solid. However, because the positron energy is directly correlated with the electron and photon energies that created it, this data can provide insight into the actual electron distributions inside the solid. Using their Grand Challenge allocation, Wilks and his colleagues have access to the computational resources necessary for simulating every aspect of these interactions. The data they obtain about the excitation and propagation of hot electrons and positrons can be used to design experiments for a variety of HED physics applications. "This knowledge could have tremendous implications for several applications involving ultraintense lasers," says Wilks. "Tabletop acceleration of ions may be useful in cancer therapy and homeland defense, and the successful demonstration of fast ignition may lead to the practical application of nuclear fusion for power generation."

Seeking the Unknown

Livermore's Grand Challenge program is an excellent mechanism by which scientists can achieve scientific breakthroughs. "When we allot time on our supercomputers, we want researchers to use these machines to expand their scientific scope and go beyond what is currently known in their fields," says Streitz. Over the last five years, Grand Challenge allocations have provided Livermore scientists with access to some of the most advanced tools for conducting research, allowing them to take scientific exploration to whole new dimensions and to visualize science in truly "grand" ways.

—*Caryn Meissner*

Key Words: Grand Challenge Program, high-energy-density (HED) physics, high-performance computing (HPC), Institute for Scientific Computing Research, Multiprogrammatic and Institutional Computing (M&IC), supercomputing.

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Going Smaller, Raising Sensitivity

Researchers (clockwise from bottom) Tiziana Bond, Mihail Bora, Allan Chang, and Elaine Behymer fabricate rectangular arrays of vertical resonant cavities for use in surface-enhanced Raman spectroscopy (SERS).

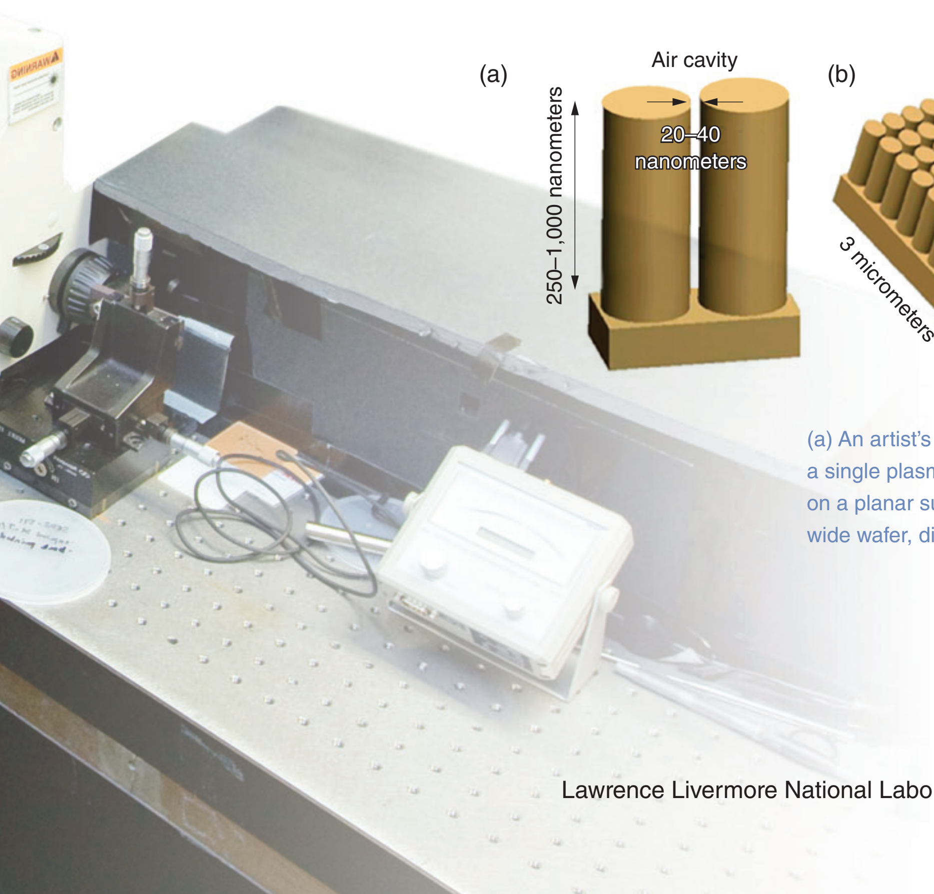
RAMAN spectroscopy has been used for decades to analyze the composition of complex liquids, gases, and solids. In this method, laser light excites molecular vibrations, which shift the energy of the laser light in a way that uniquely depends on the molecular structure. The method's popularity derives from both its high specificity and its noninvasiveness. Forensic investigators, when stymied by the diversity of sample mixtures they must analyze, often turn to Raman spectroscopy because it can produce excellent analytic data. In the 1970s, scientists accidently discovered that a roughened silver surface smeared with metal nanoparticles would dramatically increase the light signal and improve the sensitivity. With this new modification, "surface-enhanced" Raman spectroscopy (SERS) allowed researchers to pick out one molecule among a million others, making it an excellent tool for nondestructively identifying substances for forensic analysis and other purposes. A problem lingered, however. Each roughened surface was slightly different—neither entirely uniform nor experimentally repeatable. For some testing procedures, these imperfections were not a problem. But for the detection of extremely low concentrations in a sample, a better technique was deemed essential.

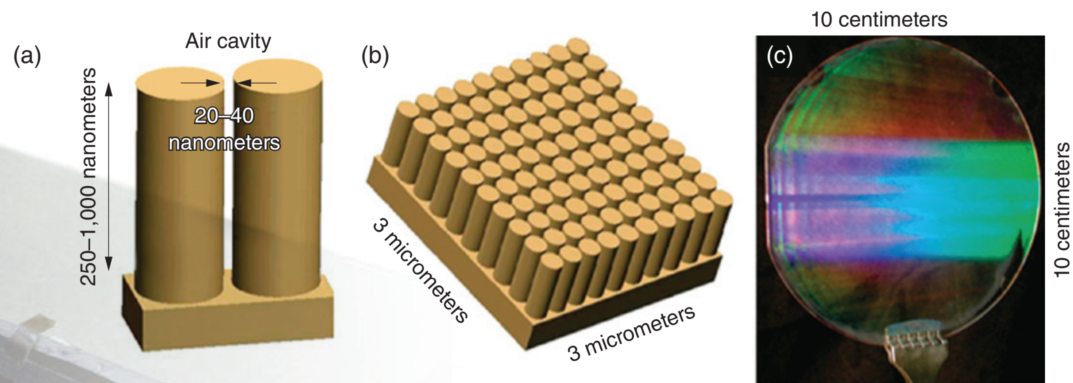
A team of scientists from Livermore and the University of Illinois at Urbana-Champaign has found a solution that enables researchers to detect solids, liquids, and gases with sensitivities thousands of times higher than previously possible. The team has replaced the irregular metal nanoparticle surface with carefully engineered nanoscale pillars. "We have exploited the Livermore speciality of laser interference lithography, which was developed for patterning over whole semiconductor wafers," says team leader Tiziana Bond of the Engineering Directorate's Center for Micro- and Nanotechnologies. The highly uniform SERS wafers are able to produce intense electric fields when laser-illuminated, which strengthens the Raman effect. For the first time, 10- to 15-centimeter-wide wafers can be identically fabricated. "Batch processing is essential for this tool to be truly useful," says Bond.

The Pillars of Raman

Although a roughened surface enhances interaction of the sample molecules with the metal surface, a substrate with uniform topographic features yields a more consistent Raman signal. The team's tapered and cylindrical nanopillars are just 100 to 150 nanometers in diameter and 250 to 1,000 nanometers tall. (For comparison, a human hair is about 50 micrometers across or approximately 1,000 times wider than one nanopillar.) Both pillar shapes perform as nanometer-size antennae, or so-called hot spots. The tapered pillars have generally offered better sensitivity than their straight-sided siblings.

The sensitivity of the cylindrical pillar has recently been raised by exploiting another step in the SERS wafer fabrication process to produce extremely small cavities between the tightly packed pillars. In these plasmonic resonant cavities, crowded electromagnetic waves concentrate energy into nanoscale dimensions thousands of times smaller than the wavelength of light. Incoming laser light interacts with the sample and coating on the nanopillar array, and the pillars act as highly confining waveguides at the interface with the sample, sending electronic oscillations upward and downward into the cavities. As is characteristic of Raman spectroscopy, the standing waves between pillars interact with the sample and, as a result, generate a shifted wavelength pattern. "By confining the light to such tight spaces, we can create intense electronic fields that increase the spectroscopic signal," says Bond. For the Defense Advanced Research Projects Agency, the team has successfully detected the explosive simulants bis(4-pyridyl)ethylene and benzenethiol



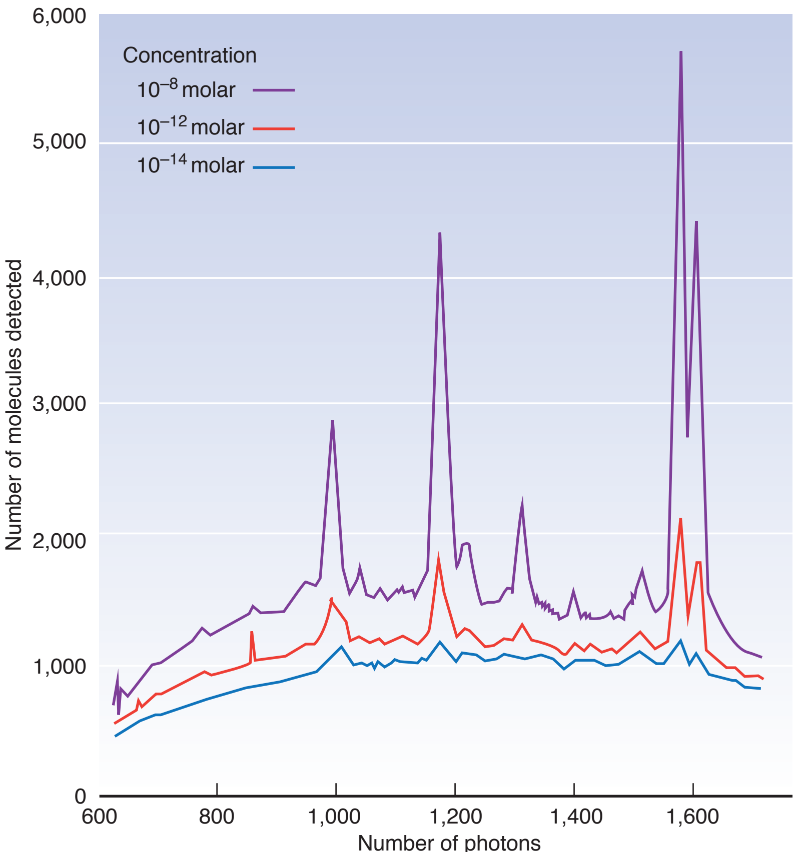


(a) An artist's rendering shows two gold nanopillar waveguides separated by a single plasmonic resonant cavity and (b) an array of pillars and cavities built on a planar substrate. (c) In an experiment using a fabricated 10-centimeter-wide wafer, diffraction patterns are observed at a high-viewing angle.

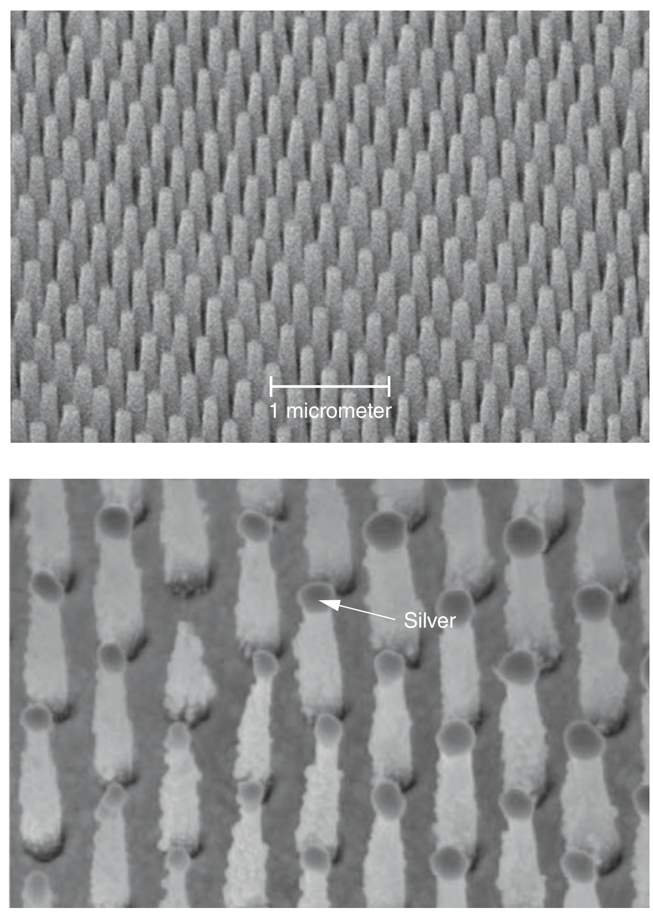
with femtomolar sensitivity, essentially picking out one molecule among a quadrillion others.

To achieve a deeper understanding of the observed improvement in SERS and its fundamental physical and chemical effects, the Livermore researchers collaborated with Gang Liu's NanoBionics Laboratory at the University of Illinois. The Illinois team used density functional theory, a quantum mechanical modeling method that aids in the investigation of the electronic structure of atoms, molecules, and solid materials, specifically their electron density. Using density functional theory and other studies, the team demonstrated computationally the mechanism that is potentially responsible for the remarkable enhancement: a strong local electrostatic field caused by what is known as the Schottky barrier at the junction of the metal wafer and the sample molecule. The study provided an explanation for the typical low repeatability of previous SERS experiments as well as the improved Raman peak shifts in raw spectra. These studies demonstrated that the strong electrostatic field at the metal–molecule junction along specific orientations could result in an enhancement in SERS of hundreds and even many thousands of times.

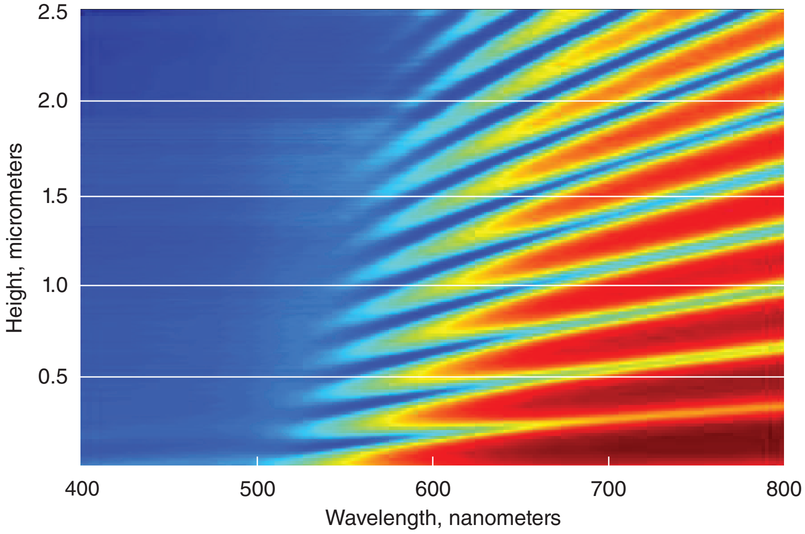
Ongoing efforts to optimize the system include experimenting with various metallic coatings on the pillars and with a range of pillar geometries. The goal is to maximize the absorbance and subsequent light emission as well as the adsorption of the sample molecules on the coatings, which together can enhance spectroscopic analysis and therefore sensitivity. Livermore



This graph shows Raman vibrational resonances of bis(4-pyridyl)ethylene molecules at various concentrations when they are excited by 660-nanometer laser light on a nanopillar substrate. The bottom (blue) curve represents the lowest concentration for effective detection.



(top) A SERS substrate is built with tapered pillars. (bottom) The substrate then receives an 80-nanometer silver coating.



Electromagnetic simulations measure the reflected power of gold coating as a function of wavelength and pillar height. Enhancing absorbance is a primary goal and it is derived as a function of reflectivity. The taller pillars, with more blue, indicate more resonances and greater absorbance.

photonics experts build the wafers of silica pillars, and electrical engineer Allan Chang evaporates a metallic coating onto them. “So far, we have worked with gold, silver, aluminum, and most recently an alloy of silver and palladium coatings,” says Chang. After coating the nanopillar arrays, he examines test objects spectroscopically to determine the coating’s effectiveness. Physicist Mihail Bora uses electromagnetic modeling to test the benefits of different pillar geometries. “We have found that with the taller pillars, the number and depth of resonances increases, and the absorbance rate is higher,” says Bora.

A Future of Enhancement

With funding from the Laboratory Directed Research and Development Program, the researchers have been testing SERS for use in the detection of gases in nuclear weapons. To advance this capability, a member of the Lawrence Scholar Program from the University of California at Santa Cruz recently began work on incorporating advanced SERS into microscale fiber-optic sensors. “Initially,” says Bond, “a sensor will have a tiny SERS device on its tip. In the future, we want to develop a technique to coat the optical probe.”

The new SERS technology is expected to eventually be enormously useful for monitoring aging weapons materials and assessing the health of closed systems. The Laboratory is responsible for ensuring the safety and reliability of the Livermore-designed nuclear weapons in the nation’s stockpile. Sensors are embedded in the weapons to constantly and nondestructively monitor changes over time.

Jim McCarrick, who leads embedded sensor development in the Engineering Directorate, is excited about SERS nanosensors because of their extraordinary sensitivity. “We already have a gas detection capability, but the SERS technology increases the sensitivity available by many thousands of times,” says McCarrick.

A further step toward higher enhancements is to increase the number of hot spots. More closely packed nanopillar arrays are being set in miniature bowls, or dimples, using block copolymers, which are combinations of chemical “blocks” that can be coupled in various ways to create exotic structures of all kinds. Recent research suggests that they may be useful for creating semiconductor and carbon nanotube arrays. This new platform could be used not only for SERS but also for advanced lithography. A student from the Swiss Federal Institute of Technology in Zurich is at Livermore for a year working on developing these higher density arrays.

In addition to applying SERS to defense efforts and forensics, a future goal is to detect very small amounts of biological material in a sample. Says Bond, “All of these applications are critical for the Laboratory’s national security mission.”

—Katie Walter

Key Words: Center for Micro- and Nanotechnologies, enhanced surveillance program, nanoscale engineering, surface-enhanced Raman spectroscopy (SERS), ultraviolet laser interference lithography.

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New Insight into the Unseen World

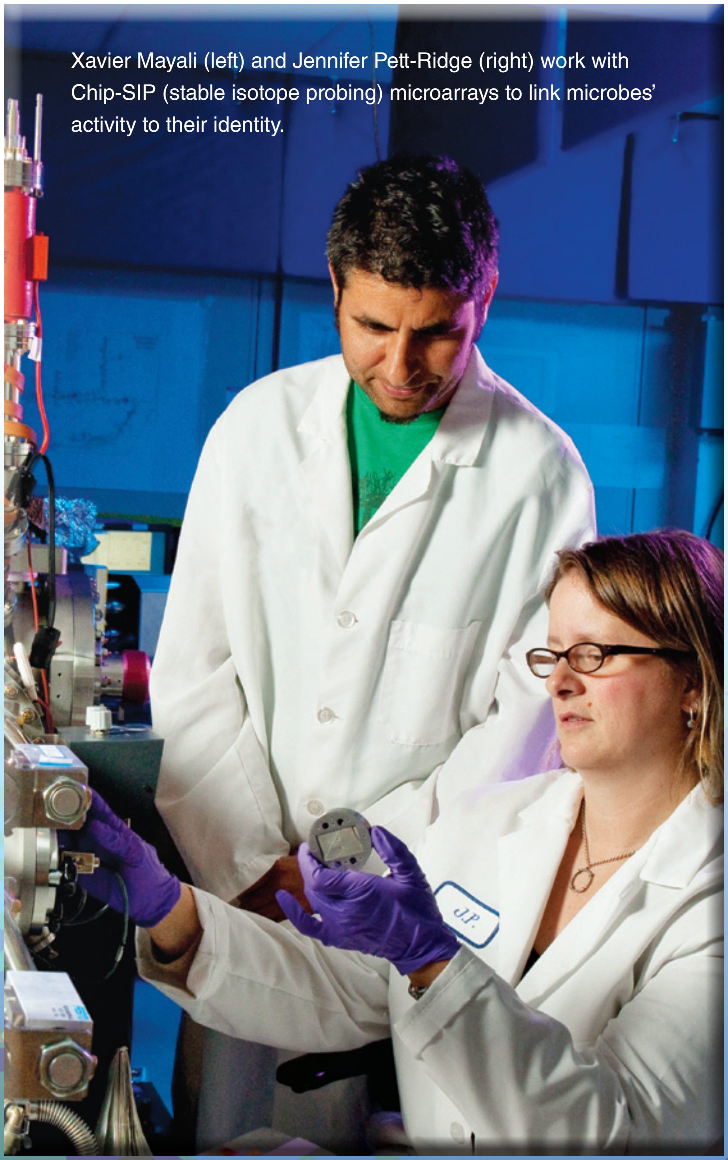
MICROORGANISMS—bacteria, fungi, microscopic algae such as plankton, and other tiny life forms—live all around us but are invisible to the naked eye. The oceans worldwide are teeming with microbial life. Microbes can be found virtually everywhere: in soil and hot springs, on and beneath the ocean floor, high in the atmosphere, and deep inside rocks within Earth's crust. Even our skin is fruitful territory for bacteria of all shapes and sizes.

Despite their small size, microbes play many important roles on Earth, including breaking down organic materials. They are also expert chemists and excel at finding solutions to their environmental problems so they can survive and prosper. At Livermore, environmental microbiologist Jennifer Pett-Ridge, marine microbiologist Xavier Mayali, and Peter Weber, Paul Hoeprich, and Shalini Mabery of the Physical and Life Sciences Directorate have taken a significant step forward in answering one of the "Holy Grail" questions in microbiology: what jobs do the hundreds of thousands of microorganisms perform in a given environment? "If that can be determined, we might be able to predict which organisms can best help with bioremediation of polluted sites," Pett-Ridge says. "Microbes also play a critical role in the production of biofuels, and they help turn atmospheric carbon dioxide into usable carbon at a rate of about 50 gigatons a year. The more we know about them, the better we understand their essential roles in our environmental challenges."

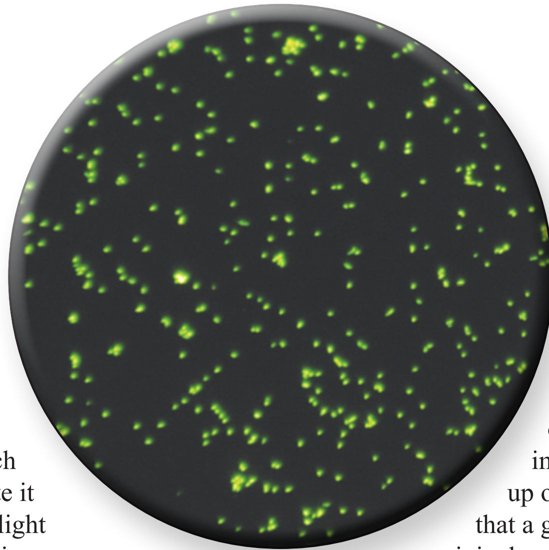
Who Does What, and How Much?

With early funding support from the Laboratory Directed Research and Development Program, the Livermore team has developed Chip-SIP, a high-throughput, high-sensitivity technique for linking the activities of microbes to their identity. The Chip-SIP method combines several technologies unique to Livermore and takes its name from the combined use of a microarray slide (the "chip") and an analytical method commonly used by microbial ecologists called stable isotope probing (SIP). Pett-Ridge says, "In the microbiology community, many researchers hypothesize that if organisms are closely related in taxonomy, they probably do the same job in the environment. However, in experiments using the Chip-SIP technique, we have shown that identity and function are not always related."

Chip-SIP is based on the same premise as traditional SIP, a suite of techniques used to link the identity and functional role of microorganisms in environmental samples. Researchers expose microbial communities to food sources labeled with rare isotopes, such as carbon-13 and nitrogen-15, which are not naturally



Xavier Mayali (left) and Jennifer Pett-Ridge (right) work with Chip-SIP (stable isotope probing) microarrays to link microbes' activity to their identity.



A drop of seawater treated with a fluorescent stain that binds to DNA shows microbes as green spots. A single liter of seawater, once thought to contain about 100,000 microorganisms, can actually hold more than 1 billion.

abundant. Active organisms in the system “eat” this food and incorporate the isotopic tracer into their cells, specifically into their DNA and ribosomal ribonucleic acid (rRNA).

Mayali says, “Traditional SIP looks at activity, measured by food source consumption, and asks questions about who’s doing what. However, processing rRNA samples using the SIP approach can take weeks.” Researchers have to collect all the DNA and rRNA from a sample, which contains a variety of organisms, and separate it based on density into isotopically heavy or light bands of nucleic acids that contain information on the organisms’ genetic identity. The assumption is that the denser samples are enriched with carbon-13 or nitrogen-15. “But because SIP is not quantitative, it’s hard to know how much of the food each microbe is taking up. With Chip-SIP, we’ve essentially reversed the process, by first separating nucleic acids by organism and then determining how enriched in the rare isotope it is,” Mayali says.

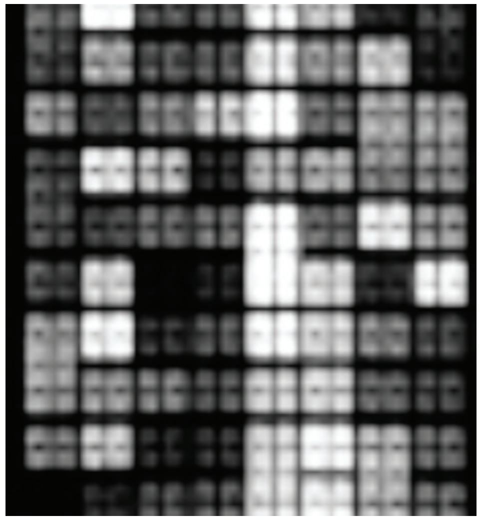
In the Livermore Microarray Center (LMAC), the team uses devices called microarrays to help sort the extracted nucleic acids and identify the dominant active organisms in a sample. LMAC provides onsite access to state-of-the-art microarray equipment for analyzing DNA and proteins. The microarrays are made of glass, nylon, or silicon slides with special Livermore-developed coatings on which tiny amounts of DNA from known organisms are printed in a regular pattern of spots.

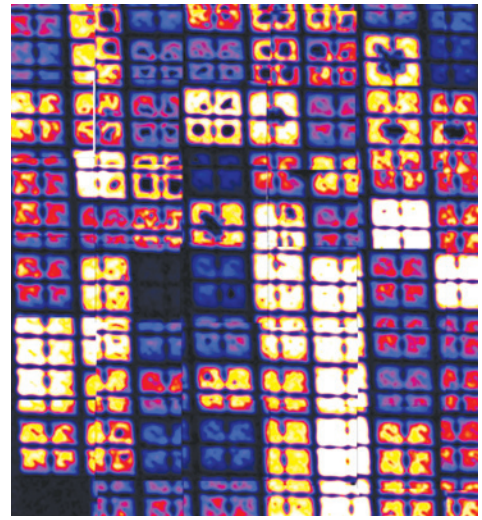
Match Game

The specific region of DNA that provides the most information about identity and evolutionary relatedness is the 16S rRNA gene. This gene is present in all bacteria, and related forms occur in other cell types. LMAC microarray slides can be spotted with up to 300,000 unique probe spots of 16S rRNA, representing tens of thousands of different sequences. Pett-Ridge says, “We design these probes to complement gene sequences of one or more organisms, called taxa, that we’re interested in studying.” When fluorescently labeled strands from the extracted nucleic acids of a sample bind, or hybridize, to matching counterparts immobilized on the slide, the match shows up on a fluorescence scan and indicates that a given taxa was present and active in the original sample.

Chip-SIP then combines these data with a scan of the same microarray by a nanometer-scale secondary-ion mass spectrometer (NanoSIMS), an ultrahigh-resolution imaging ion microprobe. The NanoSIMS beam scans across the surface of the microarray and creates an image that looks like a checkerboard, with each bright square depicting a probe spot. (See the figure on p. 26.) Chip-SIP researchers look for places where the ratio of carbon-13 to carbon-12 is higher than the normal terrestrial value, indicating that a microorganism took up the carbon-13 in its food. A darker square indicates the normal ratio, called natural abundance. The brighter a square is, the higher above normal the ratio is, and the more active the microorganism has been in feeding on the isotopically labeled food. Chip-SIP thus provides quantitative isotopic data not available through traditional methods.

The team validated the Chip-SIP method for the first time with aquatic samples from the San Francisco Bay. The seawater was incubated with carbon-13, enriched with mixed amino acids, fatty acids, ammonium, glucose, and nucleic acids. In a fraction of the time it would have taken with older methods, the researchers tested about 100 combinations of organisms and food sources from a complex microbial community. “Because we could identify organisms by their 16S sequence and determine which ones had consumed the labeled food sources, we could relate their taxonomic relationships to what role they play in the





(left) A microarray fluorescence image shows RNA hybridization to DNA probe spots. Bright spots indicate the highest signal. (right) A nanometer-scale secondary-ion mass spectrometer montage of carbon-13 enrichment shows the same area of the array providing quantitative isotopic data.

environment," Mayali says. A series of such experiments yielded a substrate-use diagram, or a food web, providing even more insight.

Traditional SIP is not only a more time-consuming analytical technique than Chip-SIP, it is also not as sensitive, requiring an isotopic enrichment of 20 to 40 percent to produce a strong enough signal for detection. "If we add a huge amount of food, we are actually fertilizing and changing the community," Pett-Ridge says. Chip-SIP can detect an enrichment of just 1 percent. Another advantage of Chip-SIP is that it can simultaneously analyze both carbon and nitrogen, which are intimately linked in the environment.

Bacterial Buddy System?

Microorganisms have been historically difficult to study because 99 percent of them are not easily cultivated in a laboratory environment. According to Pett-Ridge, this difficulty is partially because scientists do not completely understand what makes microorganisms tick, and therefore they do not have a way to duplicate their surroundings perfectly. "Millions of different taxa exist, yet we haven't identified the majority of them," she says. "We also don't know what makes some of them thrive in the field, or which 'buddies' they need to grow in a laboratory environment."

The Department of Energy's Genomic Science Program is funding the development and use of Chip-SIP in two very different environments. By examining the hindgut of beetles that eat wood, the team will seek to understand which microbial enzymes efficiently degrade cellulose and produce acetate and hydrogen gas, important information for biofuels research. In another study, the team hopes to learn more about the enzymes and energy web of microbial mats, films of layered bacterial communities that develop in intertidal, hypersaline regions and produce copious quantities of hydrogen, a potentially important biofuel. If the mats have figured out a better way to quickly produce hydrogen, the organisms or their enzymes might be used to bioengineer more tractable microbes, such as *Escherichia coli*, to produce large quantities in a semi-industrial manner.

Pett-Ridge says, "We can also foresee Chip-SIP being useful in a number of other settings, such as in the medical field, where it could help identify the organisms that perform particular tasks in the human gut. There's still a great deal to learn about microbes' role in health and disease."

—Kris Fury

Key Words: biofuel, bioremediation, Chip-SIP, Livermore Microarray Center (LMAC), microarray, microorganism, nanometer-scale secondary-ion mass spectrometer (NanoSIMS), nucleic acids, stable isotope probing (SIP), taxa, taxonomy.

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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

Slip Casting Nanoparticle Powders for Making Transparent Ceramics

Joshua D. Kuntz, Thomas F. Soules, Richard L. Landingham, Joel P. Hollingsworth
U.S. Patent 7,922,965 B2
April 12, 2011
A method for making a transparent ceramic includes mixing processed or unprocessed nanoceramic powders with deionized water to produce a slurry, sonifing the slurry to completely wet the powder and suspend it in the water, and then separating very fine particles from the slurry. Finally, the slurry is molded and cured to produce the transparent ceramic.

Dispersion-Free Radial Transmission Lines

George J. Caporaso, Scott D. Nelson
U.S. Patent 7,924,121 B2
April 12, 2011
This dispersion-free radial transmission line (DFRTL) for linear accelerators has two plane conductors, each with a central hole. An electromagnetically permeable material (EPM) is positioned between the two conductors and surrounds a channel connecting the two holes. At least one of the material parameters of relative magnetic permeability (dielectric permittivity) and axial width of the EPM is varied as a function of radius, so that the characteristic impedance of DFRTL is held substantially constant and pulse transmission is substantially dispersion-free. Preferably, the EPM is divided into concentric radial sections, with the varied material parameters held constant in each respective section but stepwise varied between sections as a step function of the radius. The radial widths of the concentric sections are selected so that pulse traversal time across each section is the same, and the varied material parameters of the concentric sections are selected to minimize traversal error.

Method of Preparation of Bonded Polyimide Fuel Cell Package

Jeffrey D. Morse, Alan Jankowski, Robert T. Graff, Kerry Bettencourt
U.S. Patent 7,931,993 B2
April 26, 2011
In this process for fabricating microfluidic fuel-cell systems with embedded components, micrometer-scale features are formed by bonding layers of DuPont Kapton™ polyimide laminate.

Awards

Three Lawrence Livermore scientists were awarded $7.5 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.

Yongqin Jiao, a scientist in the Laboratory's Biosciences and Biotechnology Division, received the award for her research in how microbes play a major role in the stability and transportation of uranium in natural aquatic systems. **Peter Lindstrom**, a computer scientist in the Data Analysis Group at the Laboratory's Center for Applied Scientific Computing, was selected for his research in alleviating the data-movement bottleneck in extreme-scale computing to accelerate numerical simulation and data analysis. **Sofia Quaglioni**, a scientist in the Laboratory's Computational Nuclear Physics Group, was chosen for her work in providing the research community with the theoretical and computational tools that will enable an accurate prediction for the fusion reactions that power stars and Earth-based fusion facilities.

The **Laboratory** was recognized as one of the **Top 25 engineering and technology companies** in 2010 by the ***Black Equal Opportunity Employment Journal***, America's leading African American business and career magazine. The publication serves as a resource to African Americans seeking employment and business opportunities within corporate America and strives to connect, educate, and promote equal opportunity. The journal annually reviews and evaluates the nation's employers in such areas as diversity plans and policies, minority recruitment, hiring, retention, and advancement opportunities.

Livermore climate scientist **Ben Santer** was elected a **member** of the **National Academy of Sciences** (NAS) for his research in human-induced climate change. Santer, an expert in the climate change research community, has worked in the Laboratory's Program for Climate Model Diagnosis and Intercomparison for nearly 20 years and is a frequent contributor to congressional hearings on the science of climate change. The NAS is an honor society of distinguished scholars engaged in scientific and engineering research, dedicated to the furtherance of science and technology and to their use for the general welfare. "We are defined by our humanity—not by awards received or the number of letters before or after our name," says Santer. "It has been a great privilege to work with and learn from my colleagues and friends at Livermore and other research institutions around the world."

The **Laboratory's Computations Directorate's Building 451** received a **silver-level rating** under the **Leadership in Energy and Environmental Design** (LEED) Green Building Rating System developed by the **U.S. Green Building Council**. LEED is an internationally recognized certification system providing third-party verification that a building or community was designed and built using strategies aimed at improving performance in areas such as energy savings, water efficiency, and carbon dioxide emissions reduction. The building, which houses some of Livermore's largest high-performance computing clusters, is the fourth building on site to be LEED-certified and the second to achieve a silver rating.

The Laboratory in the News (*continued from p. 2*)

Looking into Properties of Warm Dense Copper

Lawrence Livermore researchers, in conjunction with Lawrence Berkeley National Laboratory colleagues, have combined experiment and theory to characterize a fast-changing system in the growing field of warm dense matter physics. This emerging field of science bridges the gap between condensed matter and plasma physics. Warm dense matter exists in Earth's core, in giant planet interiors, and at the edge of the inertial confinement fusion capsule that will be used for experiments at the National Ignition Facility.

In order to measure the ever-changing conditions in this regime, the experimental team, led by Lawrence Berkeley's Phil Heimann and Lawrence Livermore's Yuan Ping, used a picosecond x-ray pulse and a streak camera to capture the time history of electron temperature in warm dense copper at Lawrence Berkeley's Advanced Light Source. "The Advanced Light Source provided a bright probe and a fast camera, bright and fast enough to capture a clear snapshot," says Ping.

In combination with a theoretical effort carried out by Lawrence Livermore's Tadashi Ogitsu and Alfredo Correa Tedesco and former postdoctoral researcher David Prendergast (now a staff scientist at Lawrence Berkeley), the team discovered that the rate of heat exchange between electrons and ions strongly depends on electron temperature. Because many material properties depend on the electron–ion coupling, this finding will change how scientists understand the behavior of copper in the warm dense regime. The team's research appeared in the April 22, 2011, issue of *Physical Review Letters* and was supported with funding from the Department of Energy's Basic Energy Sciences Program at Lawrence Berkeley and the Laboratory Directed Research and Development Program at Lawrence Livermore.

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Viral Disease May Spread through Shedding Skin Cells

Laboratory scientist Michael Dillon has proposed that virus-infected skin cells could be a source of infectious foot and mouth disease virus (FMDV) aerosols. His proposal is based on the facts that the foot and mouth disease virus is found in skin and that airborne skin cells are known to transmit other diseases. FMDV is highly contagious and capable of causing widespread epidemics in livestock.

"The airborne pathway may play a role in some outbreaks by causing disease 'sparks,' that is, disease spread to regions remote from a primary infection site," says Dillon. "If the disease isn't detected quickly, these sparks can lead to major outbreaks." Dillon cites the widespread dissemination of FMDV during the catastrophic 2001 United Kingdom outbreak, which is thought to have been caused by the inadvertent transport of animals with unrecognized FMDV infection from one farm to areas previously free of FMDV.

Mammals actively shed skin cells into the environment. Skin cells comprise a significant fraction (1 to 10 percent) of measured indoor and outdoor aerosols and indoor dust. These cells—and the bacteria, yeast, fungi, and viruses known to be present on the surface of or inside skin cells—can become airborne by being shed directly into the air or when dust is disturbed.

Dillion's proposal could lead to new methods for surveillance of foot and mouth disease, the development of more effective control measures, and improved studies of the persistence of the disease in the environment. The research, which appeared in the June 22, 2011, issue of the *Proceedings of the Royal Society B,* also may be applicable to the spread of other infectious diseases.

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New Form of Diamond Is Lighter Than Ever

A Livermore team has created a nanocrystalline diamond aerogel from a carbon-based aerogel precursor using a laser-heated diamond anvil cell. Aerogels are a class of materials that exhibit the lowest density, thermal conductivity, refractive index, and sound velocity of any bulk solid. Aerogels are among the most versatile materials available for technical applications because of their many exceptional properties.

In creating diamond aerogels, lead researcher Peter Pauzauskie, a former Lawrence fellow now at the University of Washington, infused the pores of a standard, carbon-based aerogel with neon, preventing the entire aerogel from collapsing on itself. Then, the team subjected the aerogel sample to pressures above 20 gigapascals and temperatures in excess of 1,500 kelvins, forcing the carbon atoms within to shift their arrangement and create crystalline diamonds.

The new form of diamond has a very low density—only about 40 times denser than air. The diamond aerogel could have applications in antireflection coatings, a type of optical coating applied to the surface of lenses and other optical devices to reduce reflection. Less light is lost, improving the efficiency of the system. The coating can be applied to telescopes, binoculars, eyeglasses, or any other device that may require reflection reduction. The diamond aerogel also has potential applications in enhanced or modified biocompatibility, chemical doping, thermal conduction, and electric field emission.

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Abstracts

Igniting Our Energy Future

A Livermore-led effort, called Laser Inertial Fusion Energy, or LIFE, addresses the need for safe, secure, and sustainable energy. The development effort includes contributions by dozens of Livermore physicists, engineers, and materials scientists, along with input from other laboratories, universities, and industrial partners. LIFE builds on the accomplishments of the National Ignition Facility (NIF) and the U.S. government's five decades of investment in inertial fusion. Inertial fusion uses powerful lasers to compress and heat the hydrogen isotopes deuterium and tritium to the point of fusion, liberating more energy than was put into the reaction. Demonstration of ignition on NIF will establish that the physics underpinning laser-driven fusion energy are fundamentally sound and ready to be exploited. The next step toward commercial LIFE plants would be a five- to seven-year technology demonstration program, followed by building a prototype power plant. Projections indicate that commercial LIFE plants could deliver 25 percent of U.S. electrical generation by 2050. Estimates of LIFE's capital and operational costs are strongly competitive with other baseload power plants.

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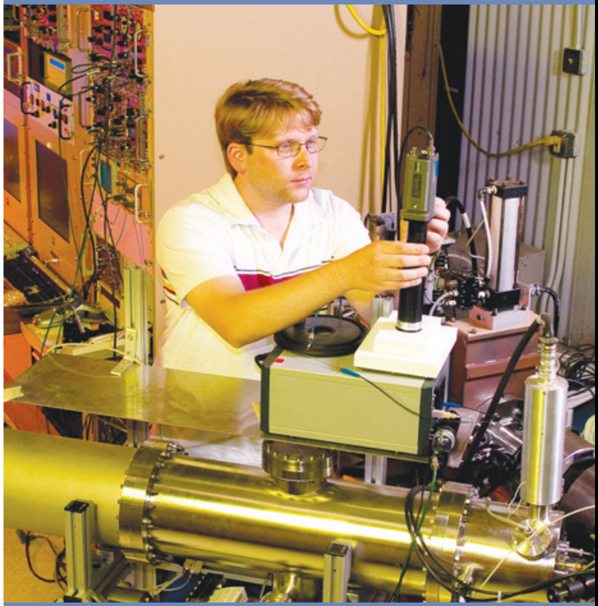
A "Grand" Way to Visualize Science

The Laboratory's high-performance computing (HPC) machines consistently make headlines as some of the fastest, highest capability computers in the world, enabling simulations of physical processes that cannot be investigated by experiment alone. The Grand Challenge Awards Program aims to further scientific innovation while advancing supercomputing capabilities. Grand Challenge projects look to push the frontiers of computational science and achieve scientific breakthroughs that would not be possible without HPC resources. More than 400 million computing hours are allocated to teams from across the Laboratory for work on unclassified, mission-relevant projects that meet Grand Challenge objectives. Each year, 10 to 12 projects are given allocations of time on the HPC machines. This article highlights five Tier 1 projects—those with the highest allocations—that were awarded in November 2010 to teams studying a wide range of high-energy-density physics topics. Simulations are run on the unclassified BlueGene/L and Sierra machines, both of which perform over 200 trillion floating-point operations per second.

Contact: Fred Streitz (925) 423-3236 (streitz1@llnl.gov).

Coming Next Issue

Focusing on National Security



Researchers at the Center for Accelerator Mass Spectrometry find new ways to advance Laboratory science.

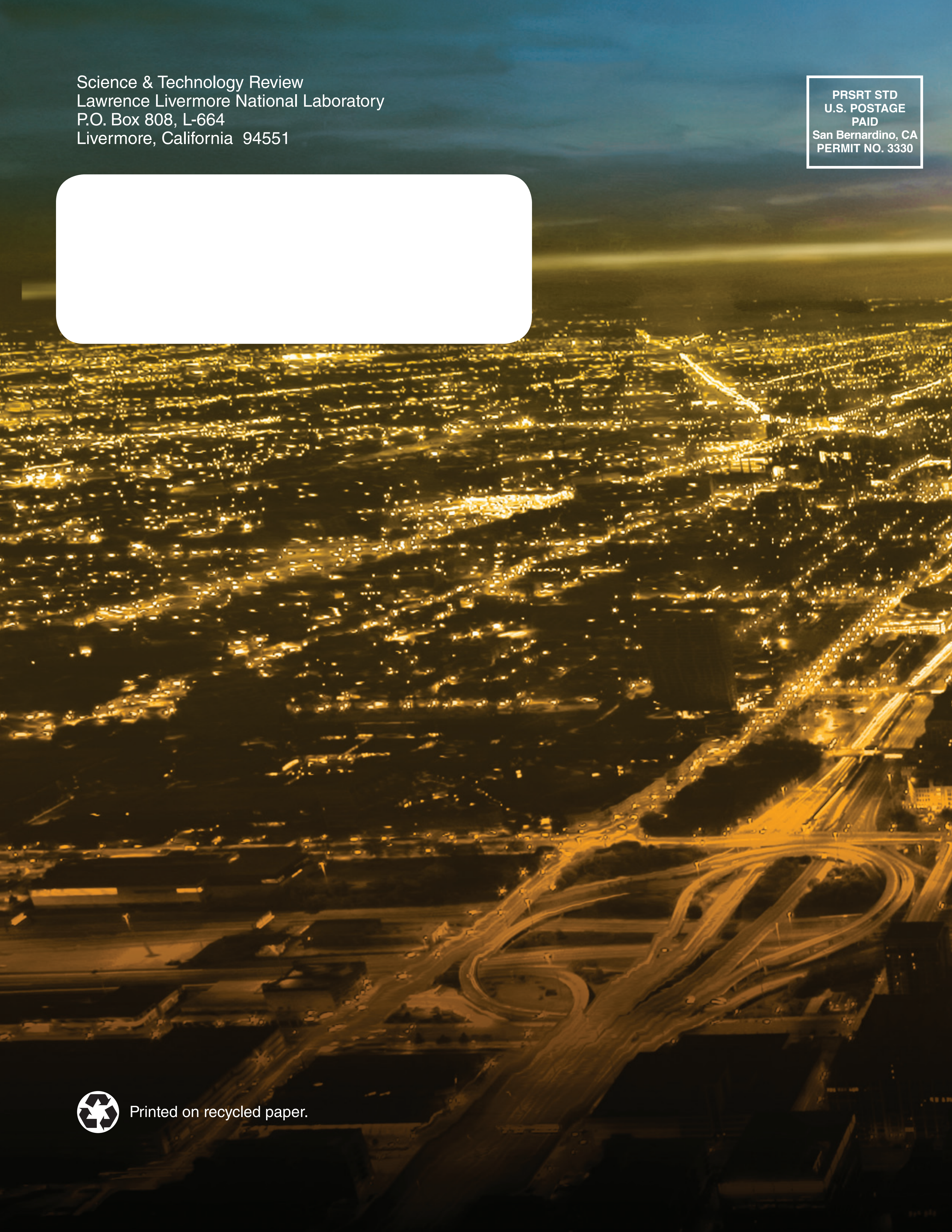
Also in September

- *Experiments at the Large Hadron Collider, the world's largest particle accelerator, are helping Laboratory scientists learn about the universe in the first moments after the big bang.*

- *Livermore biotechnology researchers fight antibiotic resistance by turning a bacterium's own genes against it.*

- *A new process improves the damage resistance of fused silica optics for the National Ignition Facility.*

U.S. Government Printing Office: 2011/770-075-50006



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