

January/February 2012

Science & Technology

REVIEW



Science at the National Ignition Facility

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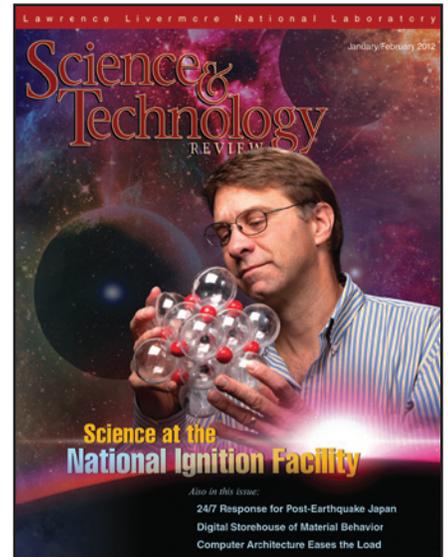
24/7 Response for Post-Earthquake Japan

Digital Storehouse of Material Behavior

Computer Architecture Eases the Load

About the Cover

The National Ignition Facility (NIF) offers unprecedented power, precision, and shot-to-shot reproducibility, allowing scientists to study material behavior under extremely high temperatures and pressures. NIF's capabilities are vital not only for stockpile stewardship and energy-related research but also for fundamental science research. The article beginning on p. 4 describes some of these initial pursuits. For example, Livermore physicist Jon Eggert (shown on the cover holding an atomic structure model) is collaborating on NIF experiments examining carbon under ultrahigh pressure to better understand the atomic structure of diamond. Such research takes a major step toward realizing the Laboratory's vision of developing NIF as an international user facility for scientific discovery in areas such as astrophysics, materials science, and nuclear physics.



Cover design: George A. Kitrinov

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New Moves Introduced for Monte Carlo Technique

A research collaboration involving Livermore biophysicist Jerome Nilmeier has developed a class of candidate moves based on nonequilibrium dynamics for Monte Carlo simulations—a breakthrough that allows the methodology to more efficiently simulate biological processes. Widely used to model systems, the Monte Carlo technique harnesses the power of computers to calculate the probable outcomes of equations with hundreds or thousands of variables.

Scientists working on the Manhattan Project first developed the sampling procedure to figure out how far neutrons might pass through various shielding materials. However, different types of systems have numerous variables that form a wide range of relationships. What works well for measuring how far a neutron will pass through different radiation shields may not function at all when applied to a biological system in which millions of molecules are moving rapidly in many directions but for very short distances.

To test the revised approach, the research team, which included scientists from Lawrence Berkeley and Argonne national laboratories and the University of California at Berkeley, used a chemical compound with two identical or similar subunits. Called a dimer, this compound served as a proxy for a reactive system where molecules are allowed to collide and form new molecules but can also dissociate into free atoms. “With the new technique, we can bias our simulation to sample the collision event more frequently and obtain better statistics,” says Nilmeier. Results from the team’s research appeared in the November 8, 2011, issue of *Proceedings of the National Academy of Sciences*.

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Separating Climate Signal and Noise

A study led by scientists at Livermore shows that temperature records must be at least 17 years long to discriminate between internal climate noise and the signal of human-caused changes in the atmosphere’s chemical composition. The research team also found that climate models can and do accurately simulate short, 10- to 12-year periods with minimal warming, even when the models are run with historical increases in greenhouse gases and sulfate aerosol particles. The team’s results appeared in the November 17, 2011, online edition of *Journal of Geophysical Research (Atmospheres)*.

When the scientists analyzed satellite measurements of the temperature in the lower troposphere (the region extending from Earth’s surface to about 8 kilometers into the atmosphere), they saw a clear signal of human-induced warming. Satellites use microwave radiometers to measure atmospheric temperature, and these recordings are independent from surface thermometer

measurements. The satellite data indicate that since 1979, when satellites first began to record temperatures, the lower troposphere has warmed by about 0.9°F. This increase is consistent with the warming of Earth’s surface estimated from thermometer records.

“Looking at a single, noisy 10-year period is cherry picking,” says Livermore climate scientist Benjamin Santer. Focusing on such a short period does not provide reliable information about differences across multiple decades, such as the presence or absence of human effects on climate. Santer adds that shorter periods generally have a small signal-to-noise ratio, making it difficult to identify a human-caused signal with high statistical confidence.

By analyzing multi-decadal records, scientists can eliminate the large year-to-year temperature variability caused by natural weather patterns such as El Niño and La Niña. According to Santer, this approach makes it easier to identify a slowly emerging signal arising from gradual, human-caused changes in atmospheric levels of greenhouse gases.

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Improved Focus for Proton-Beam Experiments

An international collaboration has discovered an approach for focusing protons with curved surfaces. Developed by scientists from Lawrence Livermore and Los Alamos national laboratories, the University of California (UC) at San Diego, Helmholtz-Zentrum Dresden-Rossendorf and Technische Universität Darmstadt of Germany, and General Atomics, the new method could be adapted to heat materials, create new types of matter, develop medical applications, and better understand planetary science.

Working with the Trident subpicosecond laser at Los Alamos, the team used a cone-shaped target to generate and focus a proton beam. The sheath electric field generated in this closed geometry effectively channels the proton beam through the cone tip, substantially improving beam focus. The results, which appeared in the December 4, 2011, online issue of *Nature Physics*, provide insights into the physics of proton focusing.

Lead author Teresa Bartal from UC San Diego says, “The ability to generate high-intensity, well-focused proton beams can open the door to new regimes in high-energy-density science.” For example, focusing a proton beam on a solid density or compressed material creates the extreme pressures required to examine the properties of warm dense matter, similar to that found in the interior of giant planets such as Jupiter. Laser-produced proton beams could also improve medical applications such as isotope production for positron emission tomography and proton oncology.

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Dawn of a New Era of Scientific Discovery

WITH the completion of the National Ignition Facility (NIF) in 2009, the international science community gained an important tool for pursuing fundamental scientific research. As the article beginning on p. 4 describes, NIF is maturing rapidly as an experimental facility and emerging as a premier capability for fundamental science. International research teams are preparing or already conducting science experiments on NIF, the world's largest and most energetic laser by far. These experiments are pushing the frontiers of science in a wide range of areas including astrophysics, nuclear physics, planetary physics, and the study of materials at extreme conditions.

NIF experiments have already demonstrated total laser energies up to 1.6 megajoules, 60 times greater than any operating laser. These experiments have been conducted with unmatched precision, repeatability, and reliability. NIF has also proven enormously flexible. For example, its 192 laser pulses can be customized according to the characteristics of the material being compressed to achieve the desired pressure, density, or temperature conditions for the experiment. More than 50 diagnostic instruments, many developed specifically for the giant facility, provide exceptional characterization of experiments.

The National Ignition Campaign (NIC) has played a major role in developing NIF as an experimental facility in support of stockpile stewardship, fundamental science, and other Laboratory missions. Part of the nation's Stockpile Stewardship Program, NIC is an international effort to demonstrate inertial confinement fusion ignition in a laboratory setting. With the accomplishment of ignition, we will possess an experimental capability to re-create the conditions that exist in stars and thermonuclear weapons, opening a new class of research—the study of burning plasmas. The fundamental science experiments in preparation or at the beginning stages are also showing promising results. What's more, there is a healthy interplay between the two research areas, with fundamental science providing new ideas and techniques for stockpile stewardship investigations.

NIF users include researchers from Department of Energy national laboratories, universities, and other U.S. and foreign research centers. Workshops held in the past several years have enabled the scientific community to learn more about fundamental science on NIF. For example, in May 2011, more than 100 scientific leaders from countries worldwide attended a workshop to discuss basic research directions for NIF during the next decade. A workshop report published in November identified

the scientific challenges and research directions for NIF-driven experiments in astrophysics, nuclear physics, materials science, planetary physics, and beam and plasma physics.

Another element in our ongoing effort to build a vigorous international user community is the NIF User Group, which will hold its next meeting at Lawrence Livermore in February. Some attendees have already participated in NIF experiments. Other researchers will be visiting for the first time to hear presentations regarding experiments on NIF and related facilities, including the Laboratory's Jupiter laser. Together, NIF and Jupiter provide the world's most sophisticated set of high-energy-density research tools located at one site.

One of the exciting avenues for fundamental research is astronomy, where NIF brings a new experimental dimension to existing observational efforts. With NIF, we can “explore” planets by duplicating the extreme interiors found in their interiors. In late 2011, researchers conducted the first university-based planetary science experiments on NIF, in which a diamond sample was compressed to a record pressure of 50 megabars (50 million times Earth's atmospheric pressure). By replicating the conditions that exist in the giant gas planets of our solar system and possibly the cores of recently discovered massive planets, the experiments will help scientists better understand how these planets might have formed billions of years ago. Experiments to look at the hydrodynamics of supernovas are also under way. Proposed experiments under consideration could even create a virtual time machine, permitting us to “travel” back to the big bang and “observe” some aspects of the birth of the universe.

Fundamental science research at NIF is in its early stages. Judging from the progress made and the success we've seen in this first generation of experiments, the next decade will indeed be an exciting time of scientific discovery at NIF.

■ Edward I. Moses is principal associate director for National Ignition Facility and Photon Science.

At the Fundamental



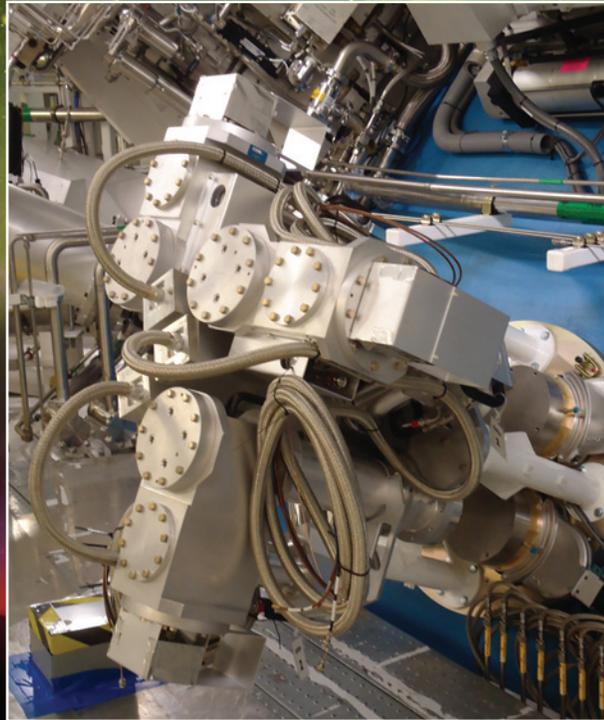
Livermore physicist Jon Eggert, shown with a powder x-ray diffraction image-plate holder, is collaborating on a fundamental science project to be conducted at the National Ignition Facility (NIF). This project is designed to study carbon under extreme pressures and thus better understand the atomic structure of diamond.

Frontiers of Science Research

The National Ignition Facility is maturing as an experimental facility and emerging as a premier resource for experiments in fundamental science.

THE National Ignition Facility (NIF), along with other new laser facilities in France, Japan, the United Kingdom, and elsewhere, is at the forefront of a significant worldwide thrust in scientific research: the study of matter under ultrahigh pressures and temperatures, conditions that have been inaccessible in laboratory experiments. Today, NIF is operating 24 hours a day. As the world's most energetic laser system, it is quickly becoming the premier facility in this exciting and rapidly evolving area of physical science. By focusing NIF's 192 laser beams onto a variety of targets, scientists for the first time can create extreme states of matter, replicating conditions that occurred during the big bang or a nuclear weapon detonation and those found at the interior of stars and planets. (See *S&TR*, June 2010, pp. 17–19; April/May 2010, pp. 4–11.)

Since NIF's completion in 2009, researchers have worked to make the giant laser's scientific promise a reality. Experiments conducted to date have achieved energies as high as 1.6 megajoules—approximately



More than 50 diagnostic systems are now online for NIF experiments. Shown here is the gamma reaction history diagnostic, which was developed for the National Ignition Campaign.

40 times greater than the level produced by other lasers—and a peak power of 420 terawatts. They have also demonstrated unprecedented shot-to-shot reproducibility as well as NIF's high-precision pulse-shaping capabilities.

The National Ignition Campaign (NIC) team and scientists working on the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program have commissioned more than 50 optical, x-ray, gamma, neutron, and charged-particle diagnostic systems and have developed techniques to fabricate the precision targets required for all NIF experiments. (See *S&TR*, July/August 2007, pp. 12–19.) The combination of laser, target, and diagnostic capabilities available at NIF are enabling experiments in new scientific regimes. In fiscal year

2011, 286 experiments were successfully executed in a wide range of programmatic and scientific areas with diverse demands on facility time and resources.

The most visible scientific effort at NIF is the demonstration of ignition via NIC and the subsequent exploration of the physics of burning plasmas. In addition, the broader scientific community is engaged in developing NIF as a tool for fundamental science. The importance of such research has been discussed in several reports, including *Basic Research Directions for NIF User Science*, a recent workshop report published jointly by NNSA and the Department of Energy Office of Science. In addition, scientists interested in pursuing fundamental science at NIF are organizing a user group, with Justin Wark, a professor from the University of Oxford, as interim

chair. The Laboratory will host the group's first meeting February 12–15, 2012. (See the box below.)

In recognition of NIF's scientific promise and user-community interest, Livermore executed a call for proposals for fundamental science research to be conducted at the facility. This competition, held in 2009 and 2010, received a strong response, with approximately 50 percent of the proposals from U.S. academic institutions, 25 percent from laboratories or institutions outside the NNSA complex, and 25 percent from international organizations. An external committee chaired by Robert Rosner, former director of Argonne National Laboratory and now a professor at the University of Chicago, reviewed the proposals.

Ten teams, some of which were approved prior to the proposal call, are now preparing fundamental science experiments on NIF to address a range of scientific questions, from observing new states of matter to

exploring the origin of ultrahigh-energy cosmic rays. Each team is paired with a Livermore scientist, who acts as facility liaison and collaborates on experiment design and execution. To make effective use of their allotted shot time, many teams first develop their experimental laser, diagnostic, and target setups at smaller facilities, such as the OMEGA and OMEGA EP lasers at the University of Rochester's Laboratory for Laser Energetics and the Jupiter Laser Facility at Livermore. They then perform fully integrated experiments on NIF.

Material Behavior at a Planet's Core

One fundamental science project on NIF is studying how planets outside our solar system form and evolve. Over the past 16 years, nearly 700 extrasolar planets have been identified, some smaller than Earth and others a dozen times more massive than Jupiter. Observational data provides only a rough estimate of an object's size and mass, so scientists must

supplement exploration with modeling. This approach, however, has its own limitations because models are based on our own solar system, and many planetary systems do not closely resemble ours. Accessing densities and temperatures similar to those deep within planets through laboratory experiments would allow scientists to refine their calculations and models so they can better understand the structure and formation of bodies both distant and close to home.

A major factor in unraveling the interior structure of planets is accurately predicting material behavior, or determining the relevant equations of state, under extreme pressure. Equations of state are used to generate computational models that simulate material behavior, revealing for example the temperatures and pressures at which diamond melts. NIF experiments designed to replicate the conditions believed to exist in the cores of "super-Earth" extrasolar planets (those 3 to

Campus Environment Fosters an International User Community

Lawrence Livermore has made progress toward installing the infrastructure required to support the fundamental science and other NIF user communities. A campus for high-energy-density science research allows collaborators from various disciplines and different institutions to more easily work on NIF experiments. The campus also provides a venue where users from the national security, basic science, and energy communities can discuss ongoing projects and research dilemmas—interactions that facilitate a "cross-pollination" of ideas and ultimately benefit all researchers involved in NIF experiments.

The campus includes office space for visitors and a dedicated user office to facilitate work by scientists from outside the Laboratory. A visitor office provides the staffing needed to make all arrangements for short- and long-term visits by external users. The campus will also complement the resources at the Livermore Valley Open Campus. (See *S&TR*, March 2011, pp. 22–24.)

The Laboratory's vision is to operate NIF as an international user facility and to provide a research environment that allows users to obtain maximum scientific benefit from this important national resource. Chris Keane, director of the NIF User Office, says, "Our goal is for NIF to be known as a center for scientific excellence—a facility that will make significant contributions to national security, scientific discovery, and energy independence."

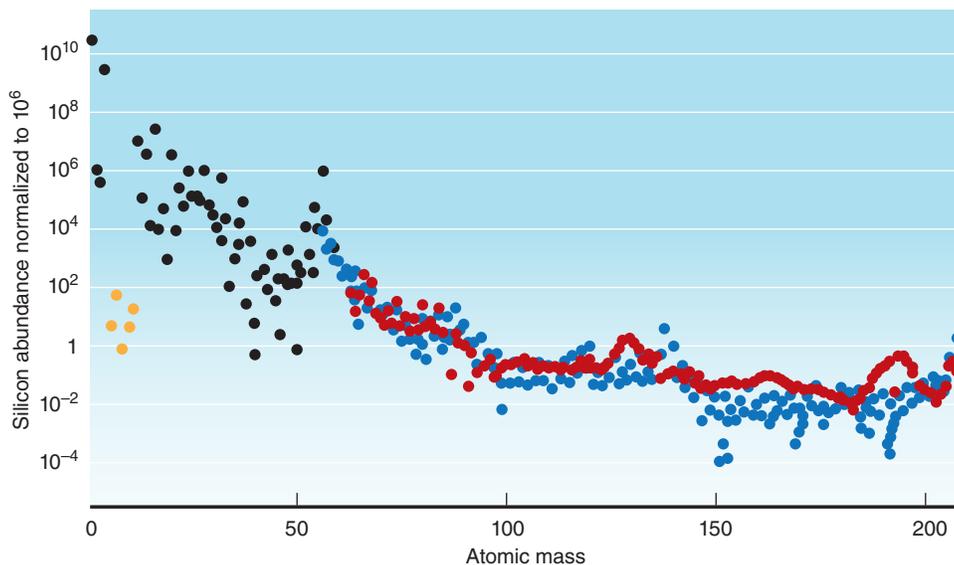


20 times more massive than Earth) will provide clues to planet formation and structure as well as to the exotic behavior of materials at high densities.

The standard technique for studying material conditions relevant to planetary interiors is through compression in a diamond anvil cell, which is limited to peak pressures near 300 gigapascals (GPa). Pressures in planetary cores, however, are higher, ranging from 350 GPa for Earth to 3,000 GPa for extrasolar planets and 7,000 GPa for Jupiter, for example. Lasers are proving to be an excellent platform for these higher pressures.

A team of scientists led by Raymond Jeanloz from the University of California at Berkeley and Tom Duffy from Princeton University has gradually compressed a diamond sample to a record pressure of 5,000 GPa (50 million times Earth's atmospheric pressure). This experiment at NIF reached more than six times the previous highest measurement, a record set by the same team using the OMEGA laser.

The researchers have also developed a time-dependent, ramp-wave compression



This plot shows abundance of elements formed during the big bang and carbon–nitrogen–oxygen burning in stars (black dots), by cosmic rays (gold dots), and by complex processes in stars that result in elements heavier than iron and nickel. NIF can be used to study the slow (s) process (blue dots), which burns the helium shell to form asymptotic giant-branch stars, and the rapid (r) process (red dots), which creates Type II supernovae and merging neutron stars. (Data adapted from E. Anders and N. Grevesse and from F. Kappeler, H. Beer, and K. Wisshak.)

technique to keep the compressed material relatively cool—less than 10,000 kelvins compared with 30 million kelvins in NIC ignition targets. With ramp compression, materials also remain in solid form at higher pressures than they would in standard, nearly instantaneous shock physics experiments. (See *S&TR*, June 2009, pp. 22–23; July/August 2007, pp. 20–21.) “The reduced level of heating offered by ramp-wave compression makes these experiments relevant to the study of planetary interiors,” says Livermore physicist Ray Smith, the project liaison.

Data are gathered with the Velocity Interferometer System for Any Reflector (VISAR), which is also used extensively in NIC experiments. VISAR records velocity versus time at various points in the target during the ramp compression. Measuring how a material such as carbon responds to stress compression will help researchers determine its equations of state and the different structures it may take as it evolves under extreme pressure.

Carbon in its many forms, including diamond, is of great interest to planetary researchers. Icy, giant planets such as Uranus and Neptune contain large quantities of methane, which decomposes at high pressures and temperatures and thus may form interior diamond-rich layers. Previous shock experiments and an earlier series of ramp compression experiments on OMEGA have furthered the understanding of diamond phases and material strength. Before the NIF experiments, however, researchers had not explored the behavior of diamond in solid state from 1,000 to 10,000 GPa.

Smith notes that NIF's laser pulse-shaping capability was also critical to the team's success. Researchers had to customize the pulse shape precisely to match the material being compressed. Otherwise, the laser pulse might have generated a shock and melted the sample. These NIF experiments are the first to demonstrate that scientists can access the relevant pressure regime for extrasolar planet interiors.



In upcoming experiments, Smith's team hopes to push even further into the high-pressure regime with diamond—up to 10,000 GPa. The researchers will then apply ramp compression to examine other materials relevant to planetary interiors, such as iron. They are eager to study iron's compressibility and crystal structure because supermassive planets are expected to have an iron core. The ramp compression techniques are also being used in NIF stockpile stewardship experiments on tantalum, which are already producing initial evidence of a new high-pressure phase.

A related fundamental science experiment will explore carbon using ramp compression and an x-ray diffraction diagnostic that is under development. The goal of this effort is to observe the atomic structure of diamond (and later, other materials) as it is compressed. The traditional view among physicists has been that materials have a simple structure at high pressure. New observations, however, indicate increased structural and behavioral complexity for many materials.

Theoretical calculations predict that at ultrahigh pressure, carbon will undergo several phase transitions. One of these phases, BC8, is thought to have similar

atom bonding as that found in diamond. The university team, led by Wark and Jon Eggert at Livermore, plans to look for evidence of a phase transition to BC8.

Accelerating Element Formation

Nucleosynthesis, or element formation, occurs at extreme stellar temperatures and pressures, making it difficult to simulate in the laboratory. (See *S&TR*, July/August 2007, pp. 22–23.) Elements heavier than iron are formed either slowly, during the life of a star, or rapidly, during a star's last few seconds. NIF can more realistically replicate the hot, dense stellar plasma where both processes occur in nature than is possible in other laboratory experiments. Livermore physicist Lee Bernstein leads a project to study the slow nucleosynthesis process, or s-process, deep within asymptotic giant branch stars.

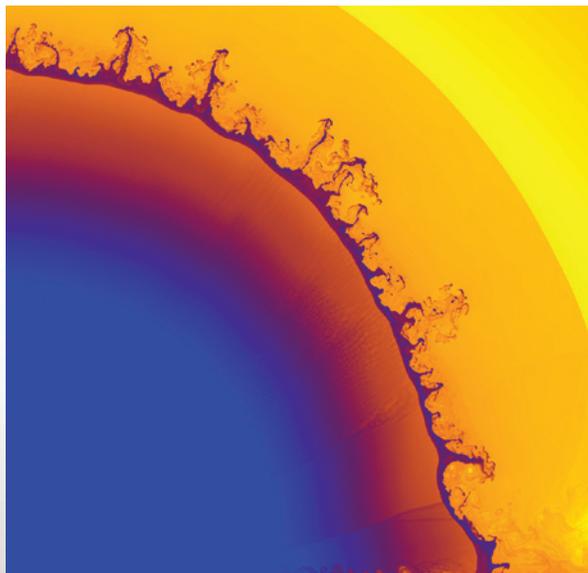
Two important reactions occur during the s-process. In neutron capture, the mass of the nucleus increases by one unit, while the charge stays constant. In beta decay, the charge of the nucleus increases or decreases, and the mass remains unchanged. For neutron capture to occur, free neutrons must be available, but an unstable nucleus undergoes beta decay automatically and then waits for the next neutron capture.

Sometimes, capture rates are comparable to the rate of beta decay by a particular isotope, forming a “branch point” in the s-process. A portion of that isotope will undergo neutron capture, while another portion transforms through beta decay. The likelihood for a particular isotope to take a given path depends on how easily a neutron can hit the nucleus, which in turn depends on physical conditions such as temperature and neutron density inside the star.

Accelerator experiments have measured the rates for neutron capture and beta decay, called cross sections, for most stable nuclei. However, measuring cross sections of unstable, short-lived nuclei has been impossible, in part because such studies would require unsafe quantities of radioactive materials. Models that extrapolate cross sections from stable nuclei and apply them to unstable nuclei are limited in accuracy. Another complication is that nuclei in a stellar plasma often exist in excited states that modify capture probability.

“If we could determine these capture probabilities, then the s-process could tell us amazing things,” says Bernstein. “We could use the information to help determine the heat, compression, and density of star interiors.” Knowing the neutron capture processes and probabilities would also improve star and planetary formation models and could explain big bang nucleosynthesis puzzles, such as the unexpected abundance of certain isotopes in the universe. Accessing the hot, dense stellar environment is important for stockpile stewardship as well.

NIF holds some advantages over accelerators—and nature. Laser experiments require a much smaller quantity of radioactive material than accelerators would, allowing the experiments to be safely performed. Radioactive (or short-lived) elements can also be directly created at NIF, but not in accelerators. When bombarding a tiny fuel pellet with laser energy, scientists can produce stellar conditions with much higher neutron quantities. In



One series of NIF experiments is studying hydrodynamic instabilities in supernovae. This simulation, created by team member Tomasz Plewa from Florida State University, shows Rayleigh–Taylor instability growth during a supernova in a red supergiant star.

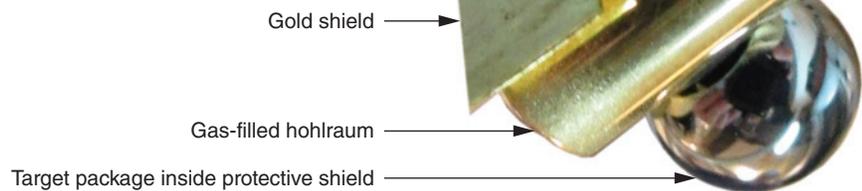
addition, the laser energy compresses the target, reducing its area by a factor of 1,000, boosting the density of nuclei, and increasing the probability of a neutron hitting a nucleus. Because of the additional neutrons and the extremely dense target material, an astonishing 2,800 years of stellar neutron capture occurs in every NIF shot. Even for short-lived nuclei, multiple reactions are possible in a single shot, potentially advancing scientific understanding of nucleosynthesis far more rapidly than accelerator-based experiments.

Livermore physicist Dick Fortner, who works on the nucleosynthesis project, says, “The first key physics question is can we generate and measure low-energy neutrons to simulate the conditions the astrophysics community is interested in?” Fast-moving, high-energy neutrons generated by a typical NIC experiment hit the wall of the target chamber, lose energy, and generate a background signal that interferes with astrophysically relevant, low-energy neutron measurements. In fact, most neutrons hit the wall a fraction of a second after the experiment. The team needed a device that could rapidly detect and measure low-energy neutrons before the more energetic neutrons have a chance to muddy the signal.

The gamma reaction history (GRH) diagnostic proved to be ideal for this purpose. This tool was developed for NIC experiments by a team led by Wolfgang Stoeffl at Livermore and Hans Herrmann at Los Alamos. When the relevant low-energy neutrons exit the gold target enclosure (or hohlraum), neutrons are captured on the gold, just as they would be in a star. This process generates a surge of gamma rays detectable by the GRH diagnostic, which consists of four detectors operating at independently tuned energy thresholds.

Analysis of GRH data from a 2011 shot provided the first evidence of a low-energy neutron signal in the laboratory. More low-energy neutrons were produced than predicted, by a factor of two or three. To date, says Bernstein, the team has used NIC shots for detection, calibration,

In supernova experiments on NIF, a target package is attached to the side of the hohlraum inside a thin, aluminum-coated plastic shell. The shell protects the package from the unconverted light in the target chamber.



and preliminary data gathering. Future experiments to be fielded on NIF will focus exclusively on nuclear physics research, using target fuels that maximize low-energy neutron production.

The team eventually aims to measure branch-point cross sections for nuclei in both ground and excited states and study nuclear processes within a plasma on NIF. Although the work is still in the early stages, the neutron-generation results suggest that NIF will be a powerful tool for exploring nuclear physics. Meanwhile, the analysis of GRH low-energy neutron data is helping NIC scientists better understand and interpret the ignition-relevant data the diagnostic produces.

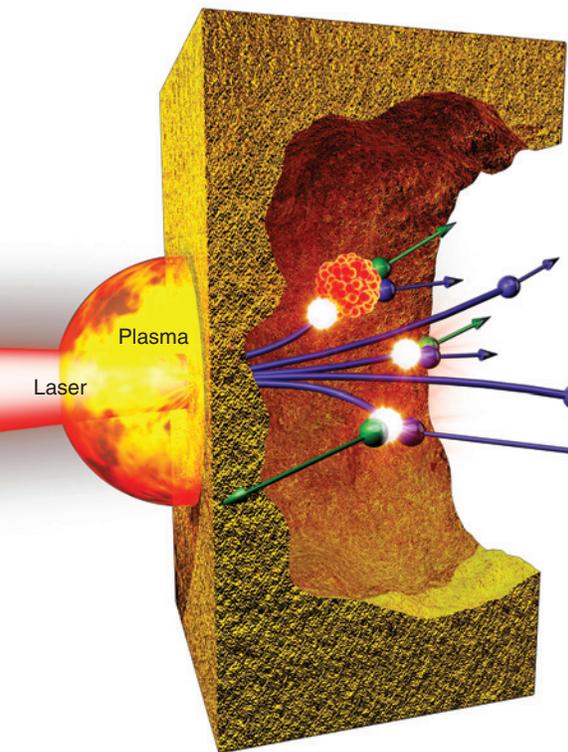
Simulating Supernovae

Another fundamental science project at NIF is investigating the evolution of turbulence in supernova explosions. In a core-collapse supernova, a star with 10 times or more mass than our Sun uses up the nuclear fuel at its core element by element, starting with hydrogen and working up the periodic table. As each fuel is consumed, the star develops an onionlike structure, with layers differing in density and material.

Once the fusion process can no longer compete with the pull of gravity, the star’s core collapses in a few seconds, triggering a powerful explosion that sends a shock wave back through the star. Propelled by the shock wave, fingers of matter from heavier layers penetrate the overlying lighter shells, resulting in Rayleigh–Taylor hydrodynamic instabilities.

A research team led by Carolyn Kuranz from the University of Michigan has begun a series of NIF experiments to understand how an unstable interface is affected when heated by a shock in a supernova explosion.

To simulate this process in scaled experiments, the researchers will use the laser beams to create the extreme radiation, temperature, and pressure conditions of a supernova-type environment. They will then observe the changes in a rippled target package via x-ray radiography. The targets are designed to enhance the radiographic contrast between the rippled iodine-doped polystyrene component, which mimics the dense supernova core, and the foam component, which mimics the interstellar medium. Measuring the ripple growth will provide information on supernova evolution, in particular, how it is affected by the extremely radiative conditions.



In positron generation experiments, the short-pulse Titan laser fires a tightly focused “photon bullet” at a tiny gold disk. The laser tears electrons from their atoms and accelerates them through the gold target. As high-energy electrons interact with the gold nuclei, they are transformed into a lower energy electron (green) and its mirror, a positron (purple). (Rendering by Kwei-Yu Chu.)

work, notes, “We always have surprises in developing NIF-class experiments.”

Adding thicker gold shielding to the hohlraum would ensure that the background signal did not overwhelm the emissions being studied. However, debris ejected from the shield during the experiment could skew results. This concern prompted the team to request that simulations be performed to predict debris behavior.

The three-dimensional calculations run on Laboratory supercomputers were perhaps the most complex of their kind performed to date and are now being applied to other experiments. According to Kuranz, access to the Laboratory’s computing capabilities—which include both codes and computing power not available at universities—has been essential to this project, whether calculating the necessary hohlraum temperature for the experiments or determining the behavior of experimental debris.

The next step for the team will be to perform integrated experiments to record instability growth in the rippled NIF targets at several radiation temperatures. Simulations indicate that x-ray radiation may stabilize the instabilities. If results

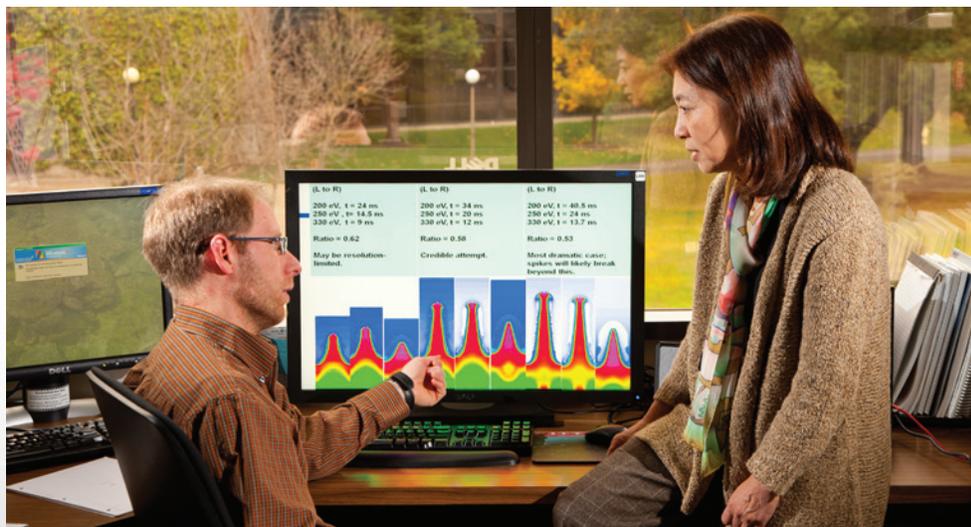
from NIF experiments verify this effect, they will offer important insight into supernova hydrodynamics. Supernovae occur only once every few hundred years in our galaxy. Supplementing astronomical observation with scaled laboratory experiments provides the best opportunity of understanding these brief and violent events, elements of which also shed light on ignition experiments and nuclear weapon detonations.

Another NIF astrophysics project aims to produce the first relativistic electron–positron pair plasmas in a laboratory, enabling experiments on a state of matter found only in gamma-ray bursts, black holes, active galaxies, and the universe shortly after the big bang. Scientists first theorized nearly 40 years ago that ultraintense lasers could generate antimatter. In the 1990s, small numbers of positrons were produced using the Laboratory’s Nova petawatt laser. Experiments in 2008 on the short-pulse Titan laser at the Jupiter Laser Facility were the first to generate a substantial source of antimatter, or positrons, using a laser.

Within tens of picoseconds, each shot on Titan creates about 10 billion positrons. This rate is several orders of magnitude greater

Preliminary investigations to validate the experimental design are already yielding important results. A by-product of this work was a high-energy hohlraum imager that is now used for most NIF experiments.

Measurements taken with DANTE and other diagnostics have demonstrated a radiation temperature on NIF equivalent to 330 electronvolts (roughly 3.8 million kelvins), one of the highest ever recorded in a gas-filled hohlraum. This temperature surpasses the 300 electronvolts required to replicate supernova conditions. The team was surprised to find that the shot produced much higher levels of x-ray background than expected. Hye-Sook Park, a veteran NIF experimentalist and the liaison scientist for the supernova



Aaron Miles (left) and Hye-Sook Park discuss the simulation results of diagnostic predictions for NIF experiments designed to replicate the conditions of a supernova.



Future NIF experiments are being designed to produce electron–positron jets to study what may lie at the heart of the universe’s brightest objects: split-second gamma-ray bursts generated by black holes. In this image of Centaurus A taken by the Chandra X-Ray Observatory, opposing jets of high-energy particles extend from a supermassive black hole. (Courtesy of National Aeronautics and Space Administration, Chandra X-Ray Observatory, Harvard-Smithsonian Center for Astrophysics, and R. Kraft et al.)

than positron production from radioactive decay processes and is comparable to that in large-scale linear accelerators, the only other positron sources available to scientists. Physicist Hui Chen leads the team of researchers who performed the groundbreaking Titan experiments and will soon be bringing this research to NIF.

The team’s experiments are producing jets with several times more electrons than positrons. To better imitate nature, the researchers are working to produce a higher density, charge-neutral jet with equal numbers of electrons and positrons. This charge-neutral jet is expected to be produced in NIF experiments using the Advanced Radiographic Capability. (See *S&TR*, December 2011, pp. 12–15.)

“If we can produce an antimatter plasma at a relativistic regime, it will help us understand many fundamental plasma physics processes,” says Chen. Though the experiments are in the early stages, powerful lasers are proving to be the first available tools to access the antimatter plasma phenomena observed in nature. Ultimately, colliding two such charge-neutral jets may provide a tool to simulate gamma-ray bursts and other exotic astrophysical phenomena.

Research to Capture the Imagination

NIF’s array of experimental capabilities is revealing the laser’s potential as a frontier science platform. “Experience shows that open user facilities—operating as they do with a healthy mix of collaboration and competition—lead to the best ideas and high-quality science,” says Wark. The promise of an open user facility with extraordinary capabilities has drawn strong interest from the international scientific community. As more results are published in papers and presented in conferences, demand is only expected to grow.

Fundamental science research offers many practical benefits for the Laboratory. Bill Goldstein, associate director for Physical and Life Sciences, is a strong supporter of this type of research. “Advancing fundamental scientific understanding is critical to the Lab’s national security mission,” he says. “Such work frequently leads to solutions for the hardest applied problems the Lab faces.” Much of the fundamental science research will benefit NIF and other Livermore mission areas.

In addition, these experiments will help the Laboratory attract and retain top scientists because the nature of such

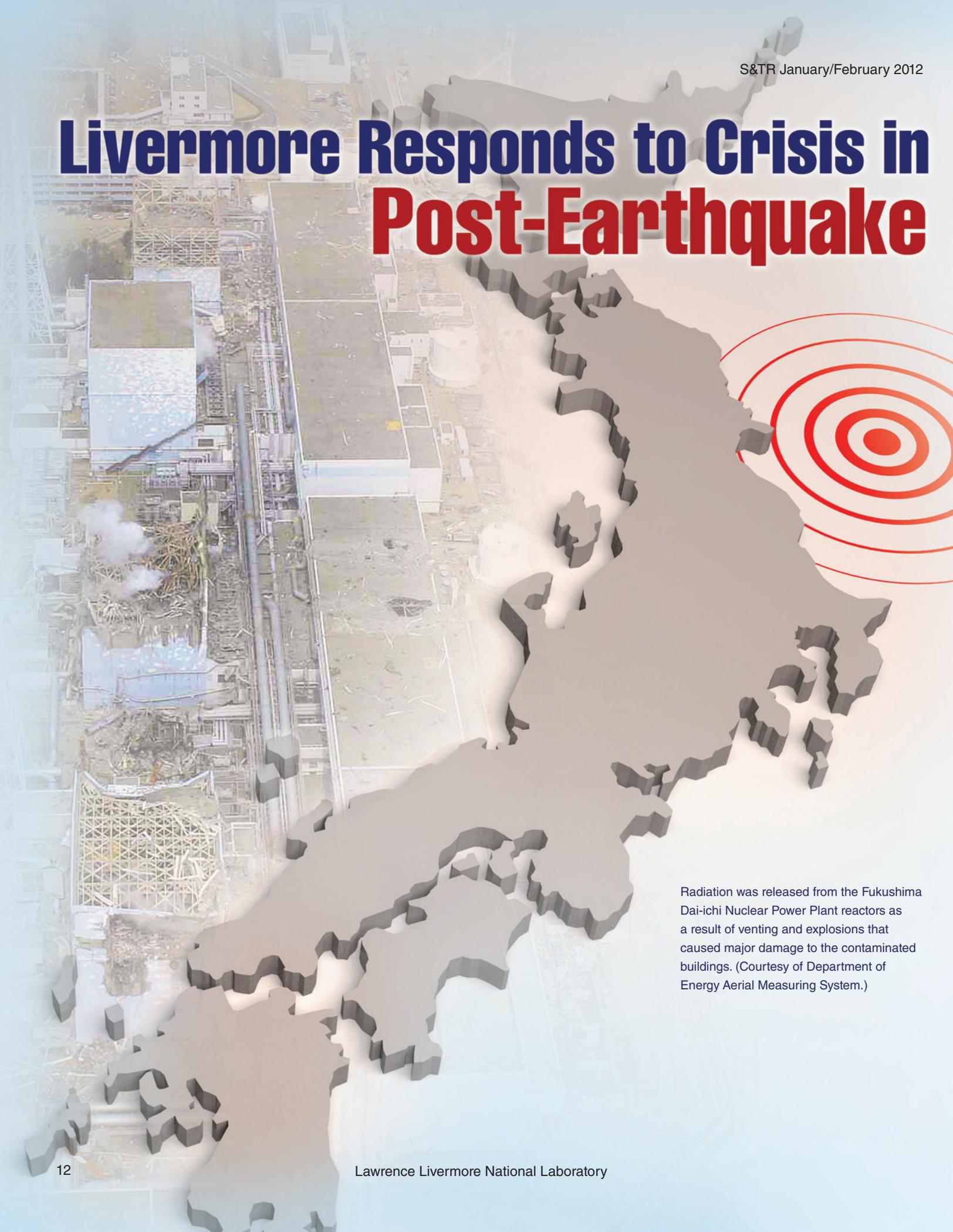
work captures the imagination. Says Wark, “The most exciting aspect of fundamental science experiments on NIF is that they will allow scientists to ‘visit’ parts of the universe we have never before been able to access.” Planetary scientists and astronomers have had to collect light and particles to study distant objects. But now, for a brief moment in time, they can create a tiny sun, or the center of a giant planet, in the laboratory. Those few billionths of a second are long enough to gather detailed information about an object’s properties and start unraveling the mysteries about the birth, life, and death of stars and planets.

—Rose Hansen

Key Words: antimatter, beta decay, high energy density, hohlraum, hydrodynamic instability, materials science, National Ignition Campaign (NIC), National Ignition Facility (NIF), neutron capture, nucleosynthesis, phase transition, positron, ramp-wave compression, Rayleigh–Taylor effect, s-process, stellar plasma, stockpile stewardship, supernova, x-ray diffraction.

For further information contact Chris Keane (925) 422-2179 (keane1@llnl.gov).

Livermore Responds to Crisis in Post-Earthquake

The image features a background aerial photograph of a large industrial complex, likely a nuclear power plant, showing significant structural damage and debris. Overlaid on the right side of the image is a 3D map of the United States, with a red target symbol consisting of concentric circles centered over the East Coast. The overall color palette is muted, with greys, blues, and browns from the photograph, and a light blue background for the text and map elements.

Radiation was released from the Fukushima Dai-ichi Nuclear Power Plant reactors as a result of venting and explosions that caused major damage to the contaminated buildings. (Courtesy of Department of Energy Aerial Measuring System.)

Japan

For several months in 2011, Livermore scientists contributed to the nation's response to the nuclear accident at the Fukushima Dai-ichi Nuclear Power Plant complex in Japan.

ON March 11, 2011, an earthquake of historic proportions unleashed its 9.0-magnitude destructive power on the northeast coast of Japan, triggering a devastating tsunami that turned cities to rubble and claimed thousands of lives. Soon the news got even worse: Japan found itself on the brink of a major nuclear crisis after a 14-meter (45-foot) wave struck the Fukushima Dai-ichi Nuclear Power Plant complex. The plant itself survived, but electrical power to cool the reactors was lost and backup generators were damaged. The resulting heat buildup in reactor cores and in spent fuel pools then led to the release of radioactive materials.

As the world held its collective breath, the scientific community swung into action to assess the extent of the crisis

and help guide protective actions. Among the responders was a team of Livermore experts who have developed sophisticated computer systems that model the spread of nuclear materials in the atmosphere. Their goal was to provide government officials in the U.S. and Japan with answers to some of the most urgent questions on everyone's mind: how much radiation was being released, where it would travel, and what protective actions might be warranted.

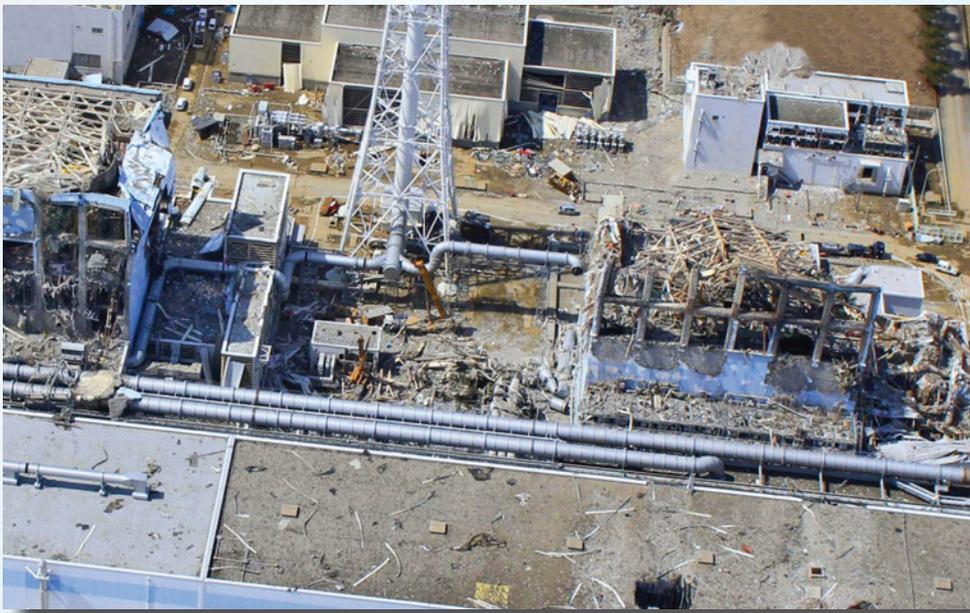
Livermore's National Atmospheric Release Advisory Center (NARAC) was activated on March 11 to provide top governmental authorities and emergency response teams both in the U.S. and Japan with daily meteorological forecasts and atmospheric dispersion predictions. The center's analyses provided scientifically based guidance that was used in making

decisions affecting U.S. citizens in Japan, including the potential need for evacuation, sheltering, or iodine administration.

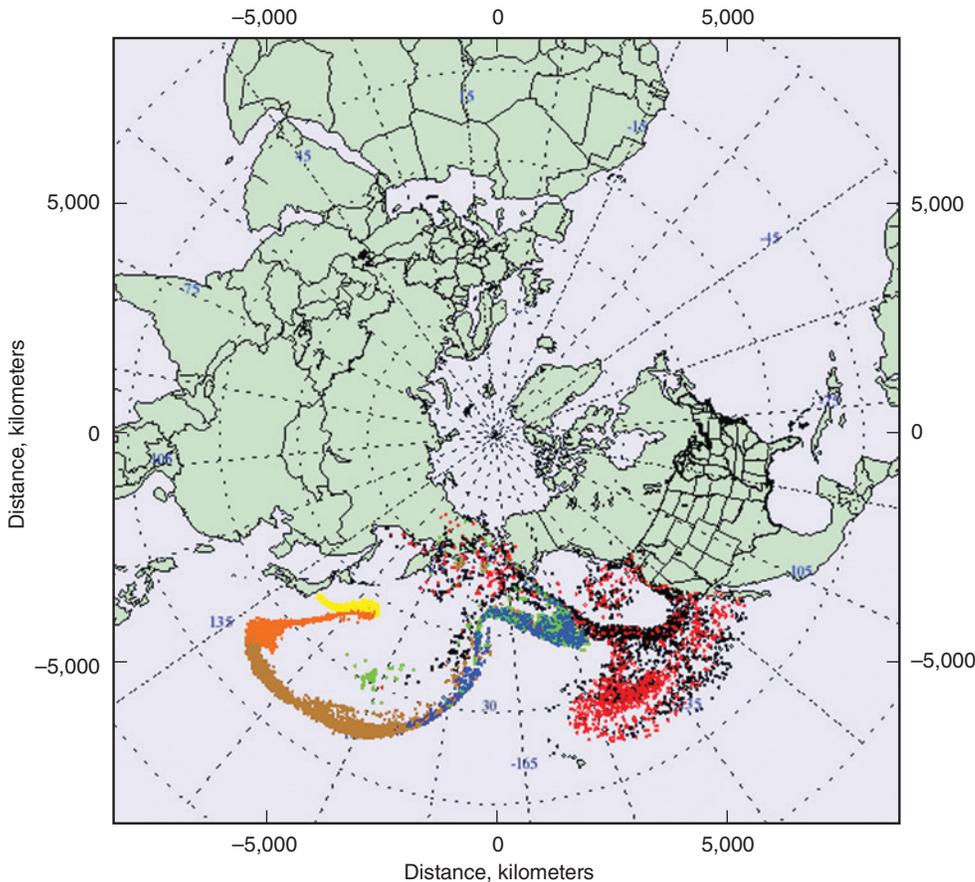
Based in part on NARAC projections and Nuclear Regulatory Commission (NRC) guidance, on March 16, the U.S. Department of State advised American citizens living within 80 kilometers of the damaged nuclear power plant to evacuate or take shelter indoors. Factors such as weather and wind direction were cited by the embassy as key reasons for this recommendation. "None of the recommendations were based solely on model results," says Gayle Sugiyama, program leader for NARAC. "But modeling analyses were certainly important in providing guidance, especially in the early phases of the crisis."

NARAC was tasked with making projections of plume arrival times in U.S. territories with corresponding radiation doses. NARAC models correctly estimated an initial four- to five-day transit time before radioactivity would reach the West Coast and predicted that the radioactivity was unlikely to reach the U.S. at hazardous levels after the trans-Pacific journey. Measurements subsequently confirmed these projections.

NARAC operated as part of the Department of Energy's (DOE's) Consequence Management Home Team (CMHT), a network of national laboratory scientists who complement each other in their respective areas of expertise. The CMHT was drawn from scientists working at the Remote Sensing Laboratory in Las Vegas, Nevada, and in



The National Atmospheric Release Advisory Center's (NARAC's) team of multidisciplinary scientists, engineers, technicians, and administrators worked around the clock for weeks during the height of the 2011 Japan nuclear reactor crisis. Principal Deputy Administrator Neile Miller (center in yellow) of the Department of Energy's (DOE's) National Nuclear Security Administration visited Livermore on March 29, 2011, to thank the team members for their efforts.



This NARAC model of plume transport from Japan to U.S. territories shows the complexity of the trans-Pacific dispersion. Colored particles represent airborne radioactivity, with different colors indicating different days of potential releases from Japan.

Washington, DC, as well as personnel from Lawrence Livermore, Sandia, Los Alamos, and Savannah River national laboratories.

Areas of staff expertise included radiological monitoring, sample collection and analysis, atmospheric dispersion, and dose assessment. CMHT scientists provided DOE with information to support the U.S. government in advising its citizens on protective actions, the Department of Defense in conducting humanitarian assistance and disaster relief operations, and the Japan government in developing its own guidelines for population relocation. NARAC served as the CMHT plume modeling center, analyzing data supplied by other members to use in its models and predictions.

Decades of Atmospheric Modeling

Founded in 1979 as part of the response to the Three Mile Island nuclear power plant accident, NARAC has been on the cutting edge of the science of atmospheric dispersion modeling ever since. Its multidisciplinary staff of physicists, atmospheric scientists, computer scientists and technicians, engineers, and health physicists has access to high-performance computers

and sophisticated modeling software. The center's stored databases of geographical and meteorological information are combined during real-life events with disaster-zone data to create three-dimensional maps of hazardous plumes.

The center serves the nation by responding to U.S. and global disasters, from fires and toxic spills to nuclear accidents. Its thousands of users include federal, state, and local agencies and emergency operations centers both in the U.S. and around the world. As the modeling center for radiological and nuclear events for DOE's National Nuclear Security Administration (NNSA), NARAC has responded to dozens of nuclear emergencies over the years, including the 1986 Chernobyl nuclear reactor disaster and the 1999 nuclear fuel accident in Tokaimura, Japan. As such, it was especially well positioned to lend its expertise to this latest crisis in Japan.

"What's unique about our center is how we integrate all the pieces: knowledge of nuclear material and atmospheric transport, understanding of radiological monitoring data and radiological dose, access to the multidisciplinary talent at the Laboratory, and collaborations with other DOE organizations," says John Nasstrom, NARAC's deputy leader. "We can put all these pieces together and then translate science into information that decision makers can act on."

One of NARAC's major tasks during the Japan response was to work with NRC, DOE, and the White House to construct a wide range of hypothetical scenarios, or "what-if" predictions, for the atmospheric dispersion and deposition of radioactive releases. NARAC scientists used scenarios provided by NRC to develop products such as maps of potential evacuation and sheltering areas. Says Brenda Pobanz, an atmospheric scientist with NARAC for the past 20 years, "Based on a given source term (the amount of radioactive material released) and the location of people in the

area, we projected whether dose levels warranting sheltering or evacuation would or would not be reached."

A Challenge Second to None

For all of NARAC's experience, nothing approached the complexity and urgency of responding to the nuclear accident in Japan—by far the most challenging event in the center's history. In the response to Chernobyl, NARAC experts provided longer range and fewer assessments. This time, they were part of the daily action throughout the crisis, constantly revising their models in response to data streaming in at all hours of the day and night.

The center needed to deal with ever-changing meteorological conditions, Japan's complex topography, and the overwhelming amount of data. Winds were shifting continually, alternating

between blowing offshore and onshore. To compound a bad situation, rain washed radioactivity out of the air in some areas, resulting in complex patterns of ground contamination.

NARAC computational resources and personnel were frequently strained to respond to the stream of requests. "So many reactors were experiencing problems over so many days that the requests for simulations were immense," says Nasstrom. "And each simulation had complicated atmospheric release characteristics, requiring simulation of weather and radioactive material transport over multiple days."

The scientific challenge, however, was only part of the equation. Throughout the crisis, NARAC supplied information to DOE, which in turn passed the information on to other U.S. agencies, the Department of State, and the White



DOE activated NARAC on March 11, 2011, to provide daily meteorological forecasts and atmospheric dispersion predictions to government officials in the U.S. and Japan. The center provided over 300 plume analyses, such as this one, in collaboration with DOE's Consequence Management Home Team, the Nuclear Regulatory Commission, and other agencies. (Background map courtesy of Google.)

House. A Web site hosted by NARAC also shared model projections and monitoring data with DOE and other government organizations.

“We dealt with a constant stream of requests from Washington,” says Sugiyama, who was in regular contact with government authorities. “Understandably, everyone wanted more information, more quickly. But NARAC staff supplemented by other scientists from the rest of the Laboratory rose to the challenge in an extraordinary way. We have practiced being able to do something like this for years, and that practice paid off.”

Making Sense of a Tsunami of Data

During the early days of the crisis, data were scarce. The tsunami brought down power lines, and many stations were off-line. But within days, the floodgates of 21st century communications opened up. NARAC carried out calculations based on

information from a multitude of sources—weather and monitoring stations in Japan, the DOE teams deployed to Japan, other national laboratories, NRC, and a plethora of Web sites and e-mail streams, many of which had to be translated and checked for accuracy.

Once in Japan, DOE’s Aerial Measuring System and ground-monitoring teams began to send large volumes of valuable data to CMHT, as did Japanese organizations. Soon, NARAC was flooded with an abundance of riches. “Having to process, quality assure, and analyze all the data so they could be used in support of modeling efforts was a major challenge,” says Sugiyama.

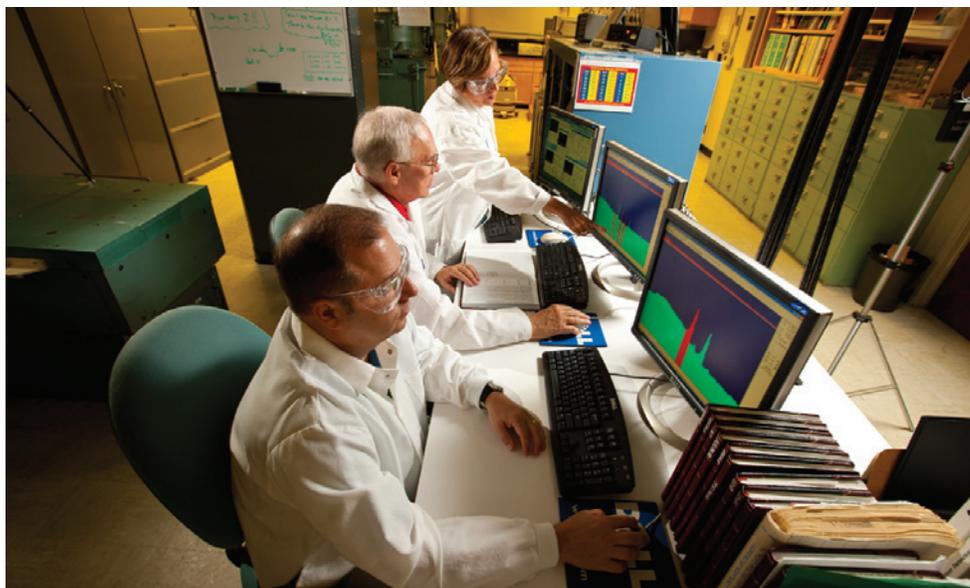
Counting on Nuclear Experience

While NARAC used real-time weather data to develop computerized forecasts and models, another team at Livermore supported DOE with radiological analysis

of air and soil samples sent directly from Japan by the DOE team deployed there. The Livermore Japan Response Lab Analysis Support Project and the DOE Triage Program leveraged the Laboratory’s expertise with radionuclide analysis and gamma spectrometry to answer two key questions: Had actual nuclear fuel been released into the environment, and is the amount of radiation released posing a real danger to U.S. and Japanese citizens? To determine the physical state of the reactor fuel, scientists looked for the presence of actinide signatures in the samples. High-resolution gamma-ray spectroscopy was used for dose assessment. The sample analysis also provided NARAC scientists with measurement data they could use to refine their predictions.

The Lab Analysis Support Project collaborated with other institutions as part of DOE’s CMHT. Livermore’s Carolyn Wong coordinated the distribution of Japanese samples to multiple laboratories for analysis. As the primary analysis laboratory, Livermore performed the bulk of these tasks, including sample screening, gamma spectrometry, depth profiling, and actinide analysis. Savannah River conducted strontium analysis, gamma spectrometry on soils, and actinide analysis. Los Alamos also performed a few strontium and actinide analyses. In addition, Livermore team members who normally serve as part of the DOE Triage Program supported analysis of hundreds of gamma spectral measurements taken in Japan and provided technical peer review of analytical products, such as correlating and corroborating results from CMHT members.

From the end of March through the end of June, hundreds of field samples from Japan arrived at Livermore, testing to the extreme the capabilities of personnel and facilities that had never responded to a crisis of this magnitude. “The system had



Gamma spectroscopists P. Todd Woody (foreground), Bob Haslett (center), and Cindy Conrado (standing) of the Laboratory’s Nuclear Counting Facility analyzed Japan air and soil samples for radionuclides measured with high-purity germanium gamma detectors.



Livermore chemists Rachel Lindvall (left) and Amy Gaffney (right) analyzed Japan air particulate samples for uranium and plutonium isotopic composition with Nu Plasma HR™, a multicollector, inductively coupled plasma mass spectrometer.

not been exercised for such a sustained period of time in many years,” says project lead Steve Kreek, who heads the Nuclear Detection and Countermeasures Research Program in Global Security. “We had not experienced anything even remotely similar since the end of nuclear weapons testing in 1992.”

Samples collected by DOE personnel in Japan, many from the Remote Sensing Laboratory in Las Vegas and other laboratories, included paper and charcoal air filters that trap airborne particulates, surface soils and swipes used to assess ground deposition of radionuclides, and soil cores collected for depth profiling to assess how quickly radioactive isotopes migrate into the ground.

On arrival at Livermore, the samples were delivered to the Radiological Measurements Laboratory, where they were barcoded for sample tracking and screened for gross alpha and beta activity

to assess radioactivity levels and to monitor for contamination. Next, all of the air filters and charcoal cartridges and some of the soil samples were sent to Livermore’s Nuclear Counting Facility for gamma spectroscopy. A few were also analyzed at the mass spectrometry laboratories in Livermore’s Chemical Sciences Division to determine if actinides (uranium, plutonium, americium, and curium) were present.

“Five to seven days later, we had peer-reviewed analytical products we could confidently present to DOE for dose assessment,” Kreek says. “We could not have done this work had we not been a weapons laboratory with a long history of performing such analyses. We needed a large nuclear counting facility and large analytical laboratories.”

At the Nuclear Counting Facility, the samples were placed in gamma counters for measuring and then analyzed

with GAMANAL, a software program developed by the Laboratory during the nuclear testing program for gamma spectra analysis. “We extended the program’s use to environmental and emergency response samples,” says Bryan Bandong, head of the Nuclear Counting Facility.

Gamma spectroscopy was used to identify the presence of various radionuclides, including cesium and iodine isotopes, and for dose assessment. Chemical separation and purification followed by mass spectrometry and alpha spectroscopy determined whether actinides such as uranium and plutonium were present. For gamma spectrometry, Bandong says, “Most radioisotopes have signature gamma rays by which we can identify them. Depending on the intensity of the peak, we can tell how much of the radioisotope is present in the sample.”

The rate at which samples came in combined with the tight turnaround requirements imposed by the ongoing crisis forced the facility to put all its ongoing research and development operations on hold. According to Bandong, DOE needed analytical results in as few as two days, and more than 90 percent of the time, his team delivered on time. Meeting the requirements was both the greatest challenge and the greatest accomplishment for the Nuclear Counting Facility staff. “Working long days and weekends for several weeks definitely got us tired, but we felt good knowing we could support the government at a time of crisis,” he says.

Measuring Success

By the time NARAC ended its active operations in late May and the lab analysis team at Livermore sent its last data set to DOE on August 19, Livermore had invested more than 7,600 person-hours of time in support of the Japan response effort. NARAC produced more than 300 analyses and predictions, the lab analysis team



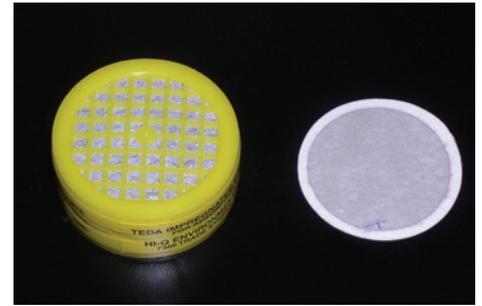
Soil samples collected by the DOE field team from locations throughout Japan were sent to DOE national laboratories, including Livermore, for radionuclide analysis.

performed more than 1,500 analyses, and the DOE triage team processed hundreds of field gamma spectra. NARAC's Web site had received 3 million hits.

"Our computer systems, containing millions of lines of codes, functioned 24 hours a day, seven days a week for three months, well beyond any anticipated requirement," Sugiyama



Particulate filter (left) and carbon cartridge (right) samples were barcoded for analysis tracking and mounted on holders for gamma counting.



Air samples were collected by a 5-centimeter-diameter particulate glass fiber filter (right) and passed through a 5-centimeter-diameter carbon cartridge (left) filled with triethylenediamine.

says. "As we look back, we realize it was a remarkable accomplishment."

People seemed to be as indestructible as the machines, with the NARAC core team working for 22 days straight during the height of the crisis, manning the center 24 hours a day in rotating shifts, nights and weekends. The lab analysis and triage teams did much the same during the height of samples arriving at Livermore. "It was difficult to keep up the pace in the early phase," says Kreek, "and changing requirements complicated our ability to respond and optimize our throughput."

A total of 78 people contributed to the combined efforts. For their outstanding contributions in support of the Japan emergency, the Laboratory honored the teams with Gold Awards, Livermore's highest honor, on July 8, 2011.

The true measure of NARAC's efforts came down to the quality of the modeling products it put out, as judged against actual measurements. "Given the many complexities involved in modeling this release, we were surprised that all of our calculations, using different sets of data, produced similar estimates of release quantities," Sugiyama says. "But much work still remains to be done to accurately reconstruct the Fukushima releases."

Ultimately, what Livermore scientists accomplished during the Japan response effort lies at the heart of the Laboratory's fundamental mission: to harness the power of high-level science, Laboratory expertise, and computing and apply them to real problems affecting the nation and the world. Livermore can bring together specialists from many fields, integrate their efforts, and sustain their expertise over the decades.

Says Nasstrom, "Science has advanced so much over the years. We can do many things now that we could not have done 10 or 20 years ago. Seeing the payoff from that investment in science is especially rewarding."

—Monica Friedlander

Key Words: actinide analysis, alpha spectroscopy, atmospheric dispersion model, Consequence Management Home Team (CMHT), gamma spectroscopy, National Atmospheric Release Advisory Center (NARAC), nuclear accident, Nuclear Counting Facility, Radiological Measurements Laboratory.

For further information on NARAC, contact Gayle Sugiyama (925) 422-7266 (sugiyama1@llnl.gov); on the Lab Analysis Support Project, contact Steven Kreek (925) 423-2594 (kreek1@llnl.gov).

A Comprehensive Resource for Modeling, Simulation, and Experiments

ACCURATELY predicting how materials will perform under a variety of conditions is essential to countless research programs in national security, lasers, and energy. For the past two decades, Livermore scientists have combined experiments and simulations to predict the performance of materials and help researchers understand how and why materials change over time and ultimately fail. This predictive capability is particularly important for stockpile stewardship, the National Nuclear Security Administration's (NNSA's) program to ensure the safety and reliability of the nation's nuclear stockpile.

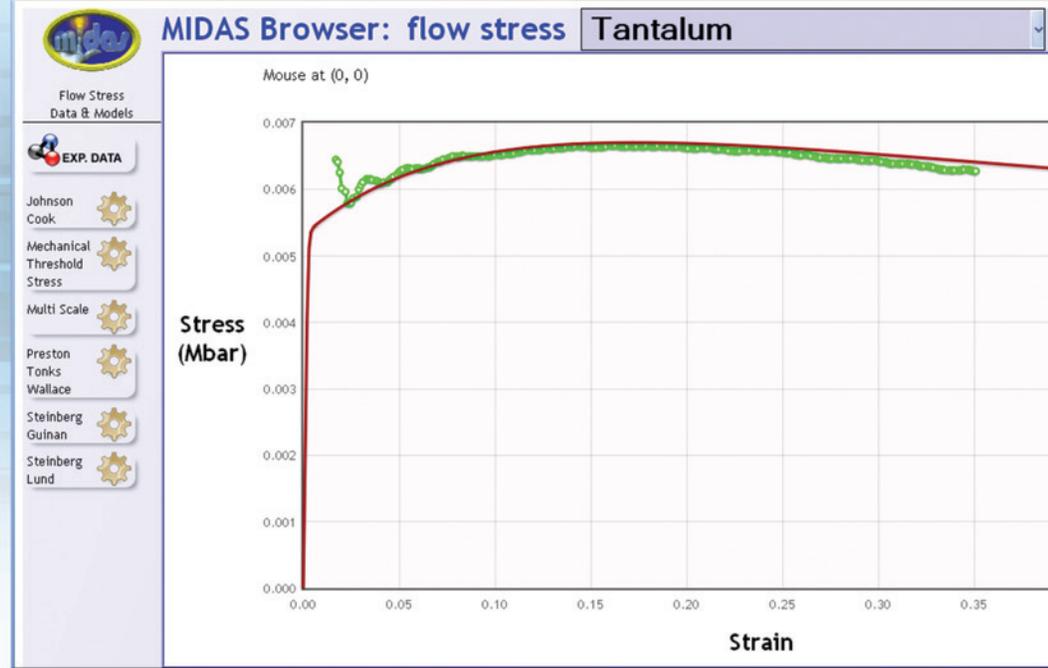
Recent experiments at Livermore's High Explosives Applications Facility (HEAF) and National Ignition Facility (NIF) and at Sandia National Laboratories' Z-pinch machine are providing new experimental data about material properties at a record pace. At the same time, other scientists are perfecting new computer models that more faithfully reflect how materials perform under different conditions, especially extreme pressures and temperatures.

Until recently, researchers had to search in different locations for the most relevant data on past experiments to help plan and guide new experiments and simulations. Likewise, Livermore code developers did not have one single resource to support their efforts to build new computer models and refine older ones. In response, a team of physicists, materials scientists, engineers, and computer scientists has developed MIDAS (Material Implementation, Database, and Analysis Source). This Web-based program is strictly access controlled and designed to be a comprehensive central repository for material properties, experimental data, and computer models. MIDAS is used in experiments and simulations involving materials of interest to stockpile stewardship and other national security programs.

The MIDAS development effort is headed by physicist Meijie Tang, together with Peter Norquist, Nathan Barton, Kevin Durrenberger, Jeff Florando, Armand Attia, and Janine Taylor. The effort is sponsored by the Advanced Simulation and Computing

(a)

(a) A MIDAS user investigates the strength of tantalum by comparing how closely a standard stress–strain model called Preston–Tonks–Wallace (red line) matches, or fits with, experimental data (green line). (b) Another MIDAS screen shows the relevant parameters used in running the Preston–Tonks–Wallace model. (c) The Experimental Data Panel from the MIDAS browser window lists the selected data from an experiment on tantalum, which was conducted at 293 kelvins and a strain rate of 0.003 per microsecond. Clicking on the Info button would display documentation on the experiment.



Campaign’s Physics Engineering Models thrust, led by Brad Wallin. Advanced Simulation and Computing is a key component of NNSA’s mission to extend the lifetime of nuclear weapons in the nation’s aging stockpile. NNSA’s ability to model the extraordinary complexity of nuclear weapons systems is essential to maintaining confidence in the stockpile.

Tang says that Livermore researchers are always seeking to enhance their understanding of how materials age in the extreme environments found within nuclear warheads. They also need to assess the likely effects of these changes under conditions relevant to weapons performance. For both purposes, researchers need robust models that permit true-to-life simulations.

Material Properties Key to Simulations

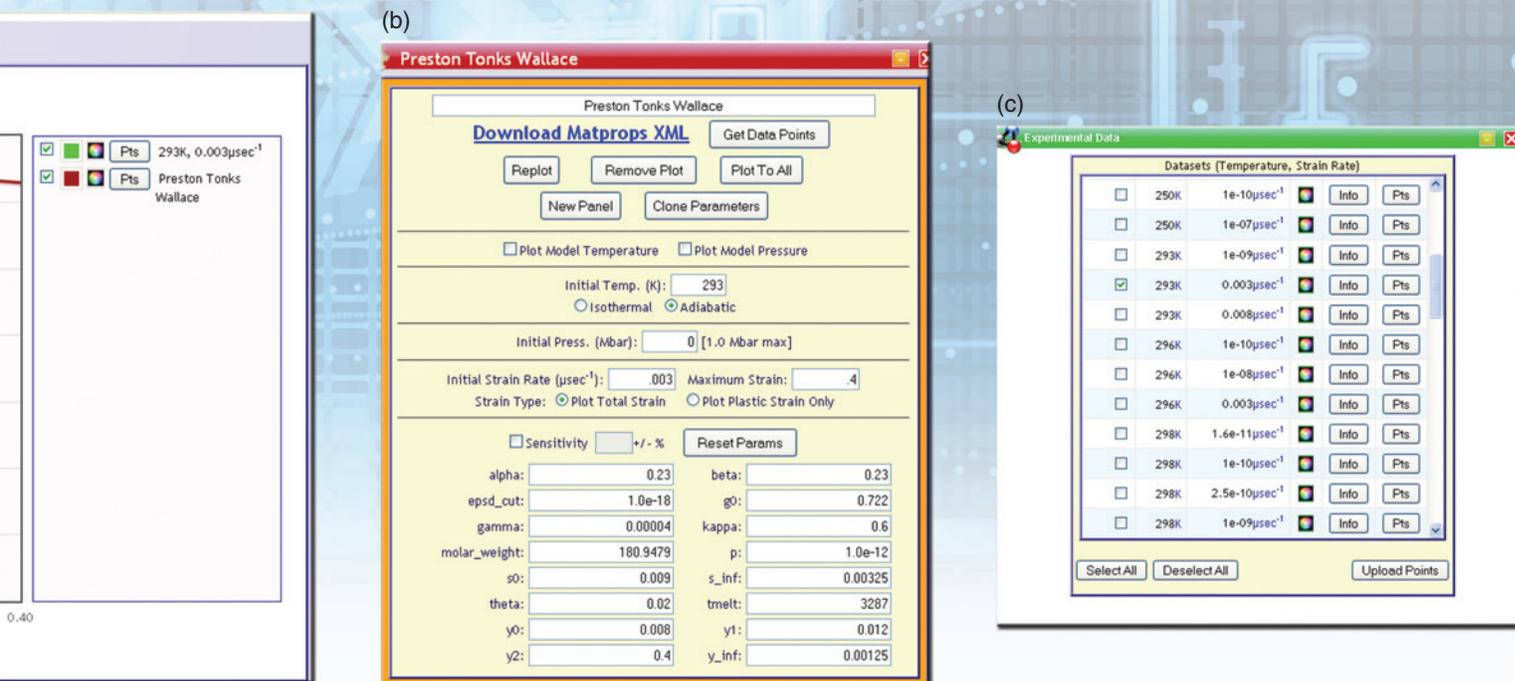
“Many simulations are performed at the Laboratory, and all depend on using the most accurate material properties generated by experiments or theories,” says Tang. She notes, however, that accurate properties can be difficult to obtain. A common repository of experimental results for dozens of materials relevant to stockpile stewardship does not yet exist.

Even when the most relevant data are located, thorough documentation, such as the exact experimental conditions and the purity of materials used in the experiments, may be missing. Researchers also may not have access to the latest models or

revisions to the most popular models. In addition, when a newer model is developed, scientists may not have the needed source code to implement the model into their application codes. Plus, few tools help researchers determine the best parameters to use for a given physical regime when they run a simulation or prepare to conduct an experiment.

In the past, Livermore scientists traditionally relied on a “bluebook,” developed by the late Livermore scientist Dan Steinberg. The bluebook contains standard strength data and equation-of-state models and parameters for many materials. However, researchers continually need to include new materials, new experimental data, advanced models and the relevant source codes, and new model “fits” showing to what degree a particular model matches experimental results—all of which the bluebook does not easily accommodate.

In place of a printed bluebook, MIDAS provides a simple Web-based program that houses, organizes, and deploys experimental data, models, and their parameters for a growing list of materials. It also provides a flexible interface to the hydrocode applications. When fully developed, MIDAS will provide a comprehensive resource application and framework for many material properties. For now, the team has focused on the all-important material strength data and the related models. Currently, 42 material data sets are available, with up to six models for each



material. Tang's goal is for MIDAS to accommodate a much larger amount of data, more types of material properties, and more models and parameters for materials of interest under different temperature and pressure regimes.

MIDAS allows registered users to view and interact with experimental data, references, and corresponding material strength models. The program accesses components already in existence at Livermore, including databases of materials properties, experimental results, and material model source codes. In the current phase of development, much of the MIDAS effort has focused on the computer framework required to provide easy interfaces between these components.

A registered user signing onto MIDAS could, for example, choose to view all experimental data that reference the hard metal tantalum and select a strength model for the material. The browser then plots the experimental data and the modeled results on a graph known as a stress-strain plot. (See the box on p. 22.) The user can easily determine to what degree data from past experiments fit various strength models. The user can then modify the model parameters to see how those changes affect the corresponding stress-strain behavior. Another feature downloads the model parameters examined at the browser so a user can add the data to their application codes. If a user is unsure what parameters are needed, MIDAS provides "blessed" or default parameters.

Only Pedigreed Data Permitted

Most experimental data on the Web site is "pedigreed"; that is, scientists can attest to the veracity of the data and the purity of materials used for the experiment. Says materials scientist Florando, "A researcher reviewing a previous experiment on tantalum needs to know the amount of impurities as well as microstructural features, such as the size of the tantalum grains." Such detailed knowledge is critical because these features dictate the overall mechanical behavior. In addition, examining the compiled experimental data can reveal where the MIDAS team needs to add experimental data. The team is currently engaging the broad scientific community to obtain additional experimental data.

MIDAS also serves as a central location for documentation of the various models and their source codes. Users can easily compare differences between model versions. MIDAS links the model version with its developer because a user may need to know the model development history and background. Users can also test the sensitivity of model fits to various parameters in the models. Additional plot types, such as strength versus temperature, provide more insight into rate- and temperature-dependent material behavior.

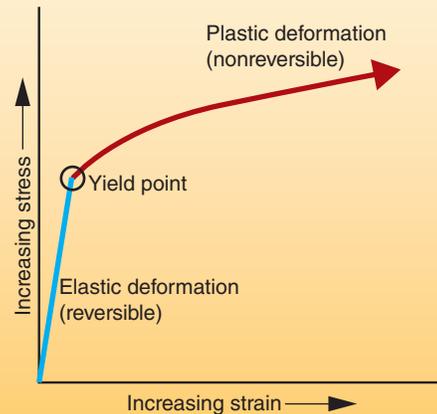
MIDAS users will be encouraged to upload new experimental data and model fits. However, all uploaded data will be checked and reviewed to ensure completeness and quality before these resources become part of the central database.

The Stress and Strain on Materials

A typical model represents a small piece of “physics” for a given material under a set of physical forces. For example, one of the simplest models that Livermore scientists use is for obtaining a stress–strain curve, a graph that shows the relationship between the stress (intensity of the applied force) and the strain (relative deformation) of a particular material.

The nature of the stress–strain curve varies from material to material. Livermore materials scientist Jeff Florando explains, “If one takes a small metal spring and starts to pull it a little bit and lets go, the spring goes back to its original shape, which is called elastic deformation and represents the initial linear portion of the stress–strain curve.” If one continues to pull, the spring begins to permanently or plastically deform and does not return exactly to its original shape. The point at which the material transitions from elastic to plastic deformation is called the yield point. On the example stress–strain plot (at right), it is the point where the line starts to curve. If a person continued to pull on the spring, it would eventually break.

Bending samples of gold and aluminum produces different results because the metals have different properties. Models account for these material differences. The more accurate the model, the better the modeled results will match, or fit to, experimental data. And the closer this fit, the more confidence scientists will have in using the information in simulation codes.



A stress–strain plot shows the relationship between the intensity of the applied force (stress) and the resulting relative deformation (strain) of a particular material. The point at which the line starts to curve is called the yield point. It indicates a material's transition from elastic (reversible) to plastic (nonreversible) deformation.

The model source library will soon be able to interface with Livermore application codes written in programming languages such as C, C++, and FORTRAN. Application codes simulate an entire system such as a weapon system or a NIF experiment. The codes involve multiscale modeling, which solves physical problems that have important features at multiple spatial or temporal scales (or both). Florando explains, “We want our source codes to seamlessly feed the pertinent parameters from the material properties database into an application code.”

The number of Livermore researchers now using MIDAS continues to grow. The development team plans to make the Web-based program available to other DOE national laboratories as well as the Department of Defense Joint Munitions Program and the U.S. Army Research Program.

Although the current focus is on materials strength, the MIDAS team wants to integrate other properties such as fracture, failure,

and high-explosives properties. The team is also developing the capability to examine temperature change and material strength during deformation. The plan is to add to the list of materials and eventually include important compounds. “The overall goal,” says Tang, “is to make people’s jobs easier, and in so doing, advance stockpile stewardship as well as scientific understanding of what makes materials age and ultimately fail.”

—Arnie Heller

Key Words: Advanced Simulation and Computing, MIDAS (Material Implementation, Database, and Analysis Source), stockpile stewardship, stress–strain curve.

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Finding Data Needles in Gigabit Haystacks

IN the ever-connected world of faster and faster computers with more and more memory, researchers in many fields suffer from an avalanche of data. It is an embarrassment of riches that is nearly impossible to grasp and manipulate, particularly when the goal is to find the one anomalous bit in a million (or billion, or trillion). As a result, scientists at Lawrence Livermore and elsewhere are exploring innovative ways to store, index, retrieve, assimilate, and synthesize mountains of raw data into useful information.

One way that computer scientists are tackling this challenge is by developing and optimizing algorithms and architectures that interact closely with large volumes of data. These data-intensive computing approaches combine techniques from computer science, statistics, and applied mathematics to speed up data manipulation in fields as diverse as astrophysics, bioinformatics, and social networks.

Not the Usual Data-Crunching

Computer scientist Maya Gokhale leads a team in the Laboratory's Center for Applied Scientific Computing that is creating computer architectures to address this "data overload" problem. "Not only is the amount of data being generated growing exponentially," explains Gokhale, "but when the raw data are analyzed, more data—called metadata—are generated as well. It's truly an issue of 'drowning in data.'"

The solutions evolving to address these problems are vastly different from those developed to manage the data generated by large number-crunching physics simulations. Many physics problems, such as modeling a solid piece of metal as a shock wave moves through it, can be characterized as three-dimensional (3D) mesh problems. Computationally, these problems are modeled as "cells" in a 3D space. In this way, each cell's behavior is influenced only by its nearest neighboring cells, where shared "edges" exist.

Physics computations run efficiently on huge supercomputers, such as Livermore's BlueGene/P, because those machines have many compute nodes, each of which can map to a spatially contiguous collection of cells. These systems have a favorable ratio of computation to communication; that is, each node can perform a lot of computing before it needs to communicate with other nodes. Thus, relatively little memory is required on each node. In general,

the data of interest for solving these problems have been generated and are being used within the computer system.

However, not all problems map well to the physics-oriented computer architecture. For some, the data to be analyzed are stored externally, on hard disks and other storage devices. These data might be millions of star images gathered from telescopes all over the world, detailed tables of genomic data, or data on social networks. (See the figure on p. 24.)

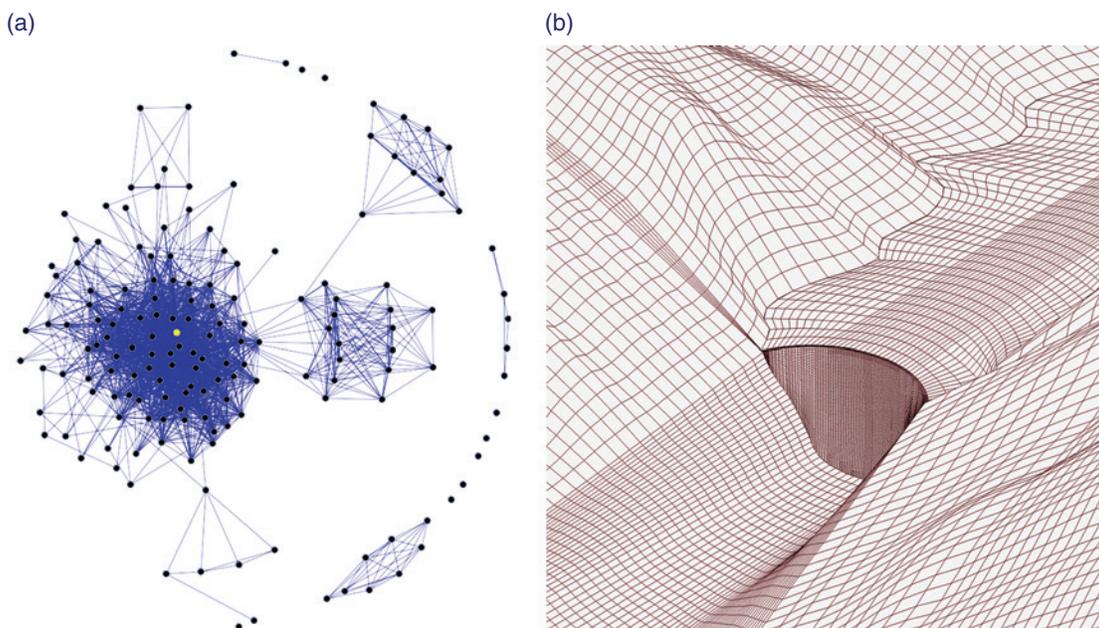
With social networks, for example, each person would be characterized as a "cell" or node, and the connection between one person and another would be an edge. The number of edges between nodes can vary immensely: A person might have a connection to only one other person on the network or connections to tens, hundreds, even thousands of people. "Methods have been developed to access such data for analysis," says Gokhale, "but when speed is of the essence, we want faster, more convenient ways to access and analyze data. One solution is to have an architecture in which the database exists 'closer' to where the work is done."

Bringing Data Closer

To meet the data-intensive computing requirements, Gokhale and her team are working on an innovative hardware technology project that is funded by the Laboratory Directed Research and Development Program. The technology, called "persistent" memory, incorporates large, parallel arrays of solid-state storage devices within the compute node. Persistent memory is embodied as flash memory, for example, in a USB memory stick.

Options for storing data range from permanent to transient memory. Permanent memory can be stored on devices such as hard disk drives and flash drives (or memory sticks) outside the computer. Transient memory, such as dynamic random access memory (DRAM) and central-processing-unit (CPU) cache, exists

(a) A social network graph displays the complex interconnections (purple lines) between different people, each represented by a node (black dots). Most people have many connections that often overlap, but some have only one or even zero. (b) Physics data-crunching solutions use three-dimensional meshes with cells and edges, such as this simulation of the Morrow Point Dam region in southwest Colorado. The two types of computational problems require different approaches for data storage.



within a computer. DRAM consists of capacitors that each store a bit of data within integrated circuits in the computer. CPU cache holds copies of data from the computer's main memory that are frequently used by the processor.

Permanent and transient memories each have their pluses and minuses. Pull the plug from the wall, and permanent memory data remain, but transient memory data vanish. On the other hand, access to data on permanent memory is slow: a factor of 100,000 slower than data stored on DRAM. Persistent memory embraces the best of both permanent and transient memory. Data stored in persistent memory are both permanent and close to the compute node, allowing for fast access and manipulation.

"Plentiful, inexpensive persistent memory in the form of flash storage array technology makes it possible to create very large databases that can be accessed later for searches," says Gokhale. "However, we still need to address the research challenges in organizing and accessing such databases in flash memory arrays, which have, at best, 1,000 times the access latency of main memory." Latency, or delay, is defined as the time required for a data packet to travel from one point to another, or in this case, from memory to a compute node. Gokhale and colleagues have made inroads on the latency problem by developing a highly multithreaded parallel algorithm for flash storage arrays that allows flash memory to outperform a serial algorithm in plentiful main memory by a factor of four.

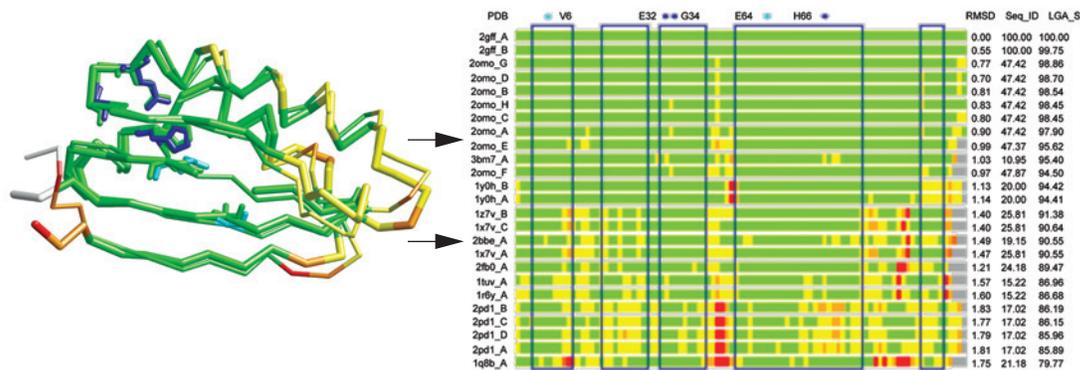
From Galaxies to Global Security to Genomes

One area that will benefit from the team's novel approach is astrophysics, including the Large Synoptic Survey Telescope

(LSST), a project for which the Laboratory is a contributing member. When completed in 2013, the telescope will have the world's largest digital camera to survey the entire visible sky. Researchers will use the resulting images to study dark matter through its light-bending gravitational effect in an effort to chart the expansion history of the universe and probe the nature of dark energy.

LSST will generate 30 terabytes of data every night, yielding a total database of 100 petabytes. "They will do triage on the data right away," says Gokhale. "A software pipeline will look for starlike objects, compare them to a template, and store likely candidates for immediate consideration. The raw data will be saved and stored. One challenge is how to later retrieve and examine the raw data for a very specific item; that is, identify an anomaly in that enormous database. Our persistent-memory architecture will speed up such tasks."

Global security is another arena that will benefit from the team's inventive solution for data-intensive computing. Scott Kohn of the Information Operations and Analytics Program is enthusiastic about the possible application to cybersecurity efforts. A primary concern in cybersecurity is getting a big picture view, or situational awareness, of how machines are communicating with each other in a network. These communications are modeled as a graph, but the graph is so large that to store and analyze it typically requires the memory resources of a small supercomputer. "Maya's work is exciting," says Kohn. "It may allow us to analyze these massive communication graphs on a relatively inexpensive workstation instead of spending tens of millions of dollars on a custom supercomputer."



Work in data-intensive computing solutions such as persistent-memory technology will benefit a multitude of research areas from astrophysics to bioinformatics. For bioinformatics problems such as the one shown, access to very large, low-latency memory on a single node can provide orders of magnitude improvements compared with calculations that use distributed memory on a computing cluster optimized for physics codes.

The team's work can also be applied to bioinformatics. Tom Slezak, associate program leader for Informatics, explains that bioinformatics has a class of problems in which large amounts of DNA sequence data are analyzed, creating an efficient data-indexing structure called a hash table. Researchers need to easily and quickly exploit the data in the large sequence hash table. Slezak says, "Although there appears to be an easy way to break up the table and distribute the data across many compute nodes, communication latency makes this approach too slow to be practical." Latency comes into play when a given node requests part of a hash table that is stored on another compute node. The seek-request-and-fetch operation is then at least 2 to 3 orders of magnitude slower than it would be if the entire hash table were in local memory for any compute node accessing it—a difference that translates into a job running in 1 day versus 100 or 1,000 days.

With persistent memory, the huge hash tables can be stored completely and accessed with a very low latency compared to going across the "grid" to another computer node. "Persistent memory will enable us to attempt bioinformatics computations that simply are not feasible with other architectures," says Slezak.

Among the bioinformatics problems that will benefit from this approach are those related to rapid and thorough analysis of complex (metagenomic) sequence data. These problems involve billions of DNA "short reads" (currently between 36 and 110+ bases in length). "Although portions of this problem can be mapped to multiple compute nodes, the need to access the enormous data structure argues for a single multicore system," says Slezak. Large persistent memory will likely outperform any other architecture currently feasible."

Persistent Memory Graphs a Winner

The viability of this novel computer architecture was proven in the June 2011 international Graph 500 competition. Two entries from Gokhale and Roger Pearce, a Lawrence Scholar working under her direction, ranked at 7 and 17. Graph 500 gets its name from graph-type problems—algorithms that are a core part of

many analytics workloads in applications, such as those for cybersecurity, medical informatics, and social networks. Rankings indicate which computer and algorithm combination solved the largest instance of the problem and had the fastest time to solution for a particular problem size. A machine on the top of this list can quickly and efficiently analyze huge quantities of data to find the proverbial needle in the haystack.

The Graph 500 benchmark calculations were run on Livermore's Kraken, a large memory server with 32 cores, 512 gigabytes of DRAM, and 2 terabytes of direct-attached flash memory. The approach, which used a highly multithreaded, shared-memory algorithm, was unique among the competitors in achieving high performance on a single compute node with very large memory. "The graph problem is part of our research that seeks to enlarge the memory available to a compute node by augmenting DRAM with high-performance, direct-attached flash arrays," says Gokhale. "This configuration enables higher utilization of the cores by giving each core more aggregate memory, a combination of DRAM and flash. It also reduces the energy required by the node, trading power-hungry DRAM for flash."

The team has since developed a multinode version of the algorithm and tested it in distributed memory runs on the Hyperion Data Intensive Testbed at Livermore and the Trestles machine at the San Diego Supercomputing Center. As for what's next, says Gokhale, "We are working on additional flash-based, multithreaded graph-analysis algorithms including Google's page-rank search algorithm and connected components identification, which finds clusters of nodes in a graph that indicate close relationships."

—Ann Parker

Key Words: bioinformatics, computer algorithm, computer architecture, database, data-intensive computing, flash memory, Large Synoptic Survey Telescope (LSST), persistent memory.

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Awards

Two scientists who previously worked as postdoctoral researchers at Livermore are among the 94 recipients of the **Presidential Early Career Award for Scientists and Engineers** named by **President Barack Obama**. This award is the highest honor bestowed by the U.S. government on science and engineering professionals in the early stages of their careers.

Fotini Katopodes Chow, now an assistant professor of Civil and Environmental Engineering at the University of California at Berkeley, was honored for research conducted between 2004 and 2005. The Laboratory nomination cited her for “original contributions to atmospheric flow simulation in areas with complex terrain, and leadership in bridging the gap between meteorology researchers and weather forecasters.”

Logan Liu is now a professor in the Electrical and Computing Engineering Department at the University of Illinois Urbana-Champaign. He was nominated for innovative research in understanding the interactions between photons, plasmons, and electrons. His research has contributed to the development of miniaturized spectroscopic and sensing systems with applications in homeland security, renewable energy, and health care.

Steve MacLaren, a physicist with Livermore’s Weapons and Complex Integration Principal Directorate, received the **Employee of the Quarter Award** from the **National Nuclear Security Administration’s Defense Programs**. Award recipients are recognized for going beyond the call of duty in supporting the Defense Programs’ mission. MacLaren was recognized for his work as the lead designer for several high-energy-density experiments on the National Ignition Facility at Livermore and the Z machine at Sandia National Laboratories, New Mexico. These experiments delivered validation data for three-dimensional simulations that allowed Laboratory researchers to develop and implement key physics-based models for the Stockpile Stewardship Program.

The **Blue Gene/Q Prototype II** supercomputer, now located at IBM’s T. J. Watson Research Center in New York and soon to be installed at Livermore as the Sequoia system, won **first place** on the annual **Graph 500** list. Blue Gene/Q traversed more than 254 billion graph edges per second, a rate that is more than 2.5 times greater than the next machine on the list. The ranking corroborates the new machine’s data-intensive computing abilities, which were developed in support of the nation’s Advanced Simulation and Computing Program.

Livermore submitted multiple entries to this year’s Graph 500 competition, including several by **Maya Gokhale** and **Roger Pearce** that used solid-state drive storage arrays to hold the graphs. (See the article beginning on p. 23.) Leviathan, a system

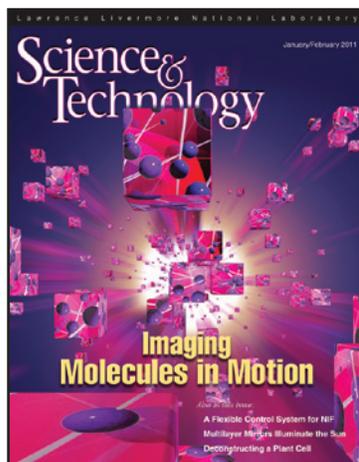
with a single 40-core node, 1 terabyte of memory, and 12 terabytes of flash storage, processed a graph of 1 trillion edges, larger than the Laboratory’s top-ranked entry.

Graph 500 ranks the world’s most powerful computer systems for data-intensive computing. The list gets its name from graph-type problems, or algorithms, that are a core part of many analytics workloads, including applications for cybersecurity, medical informatics, and data enrichment.

The **Department of Energy** named Laboratory geochemist **Tom Guilderson** the 2011 winner of its prestigious **Ernest Orlando Lawrence Award**. Guilderson is the senior research scientist in the natural carbon research group at the Laboratory’s Center for Accelerator Mass Spectrometry and a lecturer and researcher in the Department of Ocean Sciences and Institute of Marine Sciences at University of California at Santa Cruz. He is honored for groundbreaking radiocarbon measurements of corals, advancements in understanding the paleohistory of ocean currents and ocean processes that reveal past climate variability, and the explanation of how physical and biogeochemical oceanic processes affect the global carbon cycle.

The E. O. Lawrence Award honors midcareer scientists and engineers for exceptional contributions in research and development supporting the Department of Energy’s National Nuclear Security Administration and its mission to advance the national, economic, and energy security of the United States. Named for the physicist who cofounded Lawrence Livermore, it comes with a citation signed by the Secretary of Energy, a gold medal bearing the likeness of Ernest Orlando Lawrence, and \$20,000. Guilderson is the 28th current or former Laboratory employee to receive the award.

Laboratory researchers **Roger Aines, Tom Buscheck, Mark Havstad, Wayne Miller, Christopher Spadaccini, and Todd Weisgraber** received the **Secretary of Energy’s Achievement Award** for their contributions to flow-rate calculations for the Macondo Well in response to the Deepwater Horizon oil rig disaster. The six scientists were part of the Flow Rate Technical Group and Nodal Analysis Team, led by the National Energy Technology Laboratory. This collaborative effort included research teams from Lawrence Livermore, Los Alamos, Lawrence Berkeley, Oak Ridge, and Pacific Northwest national laboratories and the National Institute of Standards and Technology, each of which used different methods to estimate the well’s flow rate. The Livermore calculations were based on the properties of the oil, well-bore geometry, and damage caused by the explosion. The collective work of the teams also accounted for the sequence of attempts to cap the well.

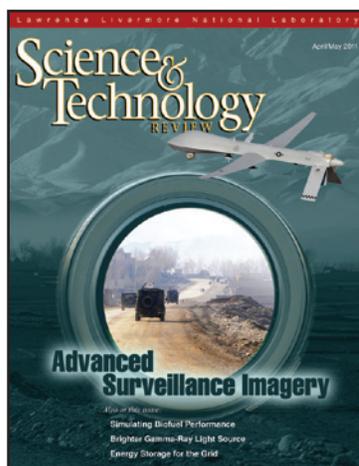
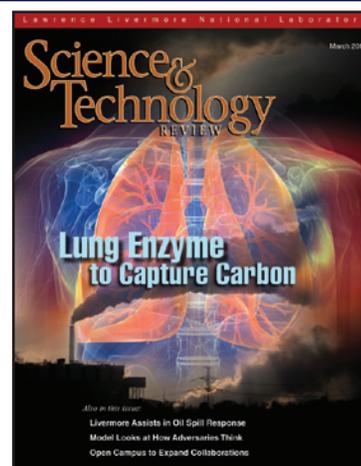


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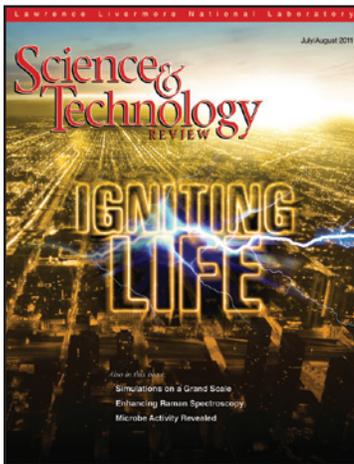
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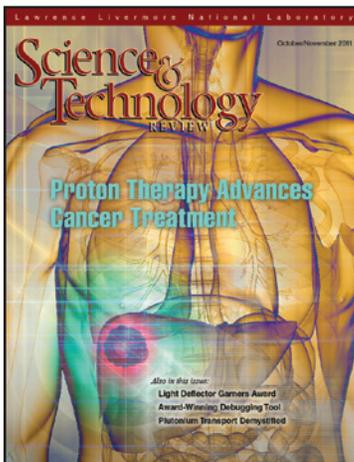
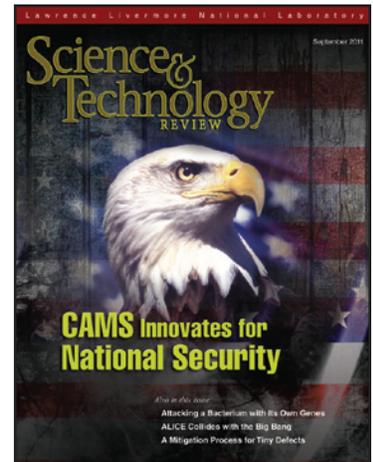


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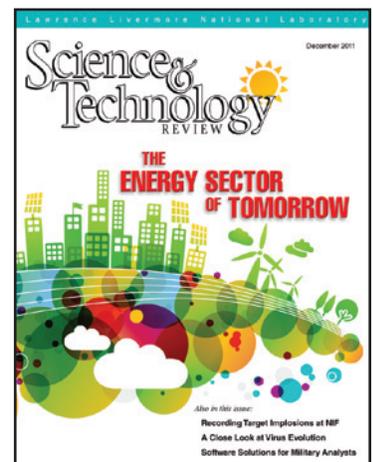


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At the Frontiers of Fundamental Science Research

The National Ignition Facility (NIF)—the world’s most energetic laser—was completed in 2009 and is rapidly emerging as the premier facility for studying matter under extreme temperatures and pressures. NIF’s unprecedented power, precision, and reproducibility, coupled with its sophisticated target fabrication and diagnostic capabilities put in place via the National Ignition Campaign (NIC) and other ongoing experimental campaigns, is enabling leading edge experiments in fundamental science. The Laboratory provides domestic and international researchers an opportunity to perform fundamental science experiments on NIF through a competitive selection process similar to that used at other major Department of Energy user facilities. This activity is a major step toward the Laboratory’s vision of developing NIF as an international user facility for scientific discovery. NIC, fundamental science, and other NIF experiments are already demonstrating the laser’s potential for advancing research in areas such as astrophysics, materials science, and nuclear physics. A NIF User Group will meet for the first time in 2012, and Lawrence Livermore is putting the infrastructure in place to support the broader NIF user community.

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Livermore Responds to Crisis in Post-Earthquake Japan

On March 11, 2011, a 9.0-magnitude earthquake erupted on the northeast coast of Japan, triggering a devastating tsunami that turned cities to rubble and claimed thousands of lives. When a 14-meter (45-foot) wave struck the Fukushima Dai-ichi Nuclear Power Plant complex, Japan found itself on the brink of a major nuclear crisis. Electrical power was lost, and backup generators were damaged. The resulting heat buildup in reactor cores and spent fuel pools led to the release of radioactive materials. Worldwide, scientists swung into action, assessing the damage and developing guidelines for protective actions. Among the responders were Livermore experts who helped model the spread of nuclear materials in the atmosphere and performed radionuclide analyses of air and soil samples sent from Japan. Throughout this challenging, multidisciplinary effort, the Livermore teams demonstrated their passion for the Laboratory’s fundamental mission: to harness the power of high-level scientific expertise and computational resources and apply them to real problems affecting the nation and the world.

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Life Extension for an Aging Weapon



Stockpile stewards have begun a multiyear effort to extend the service life of the W78 warhead.

Also in March

- *Material microstructures go three-dimensional with improved additive manufacturing techniques developed at Livermore.*
- *Laboratory researchers are exploring strategies that use electrogenic bacteria in microbial fuel-cell technologies to produce clean, renewable energy and to purify water.*
- *A new nanowire sensor that operates without batteries could improve field applications in such areas as homeland security and medicine.*

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