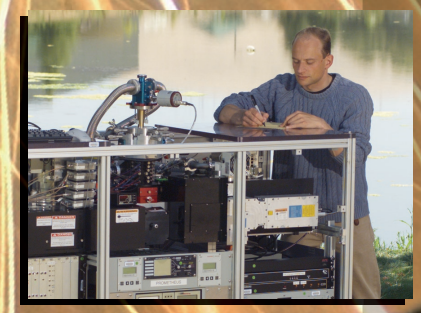
Science & Technology REVIEW

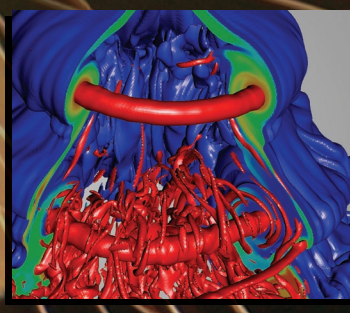
October 2005

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Award-Winning Science and Technology

2005 R&D 100 Awards





Also in this issue:

- Simulating the Phases of Water
- Aerogel Targets for Laser Experiments

About the Cover

Livermore researchers garnered four R&D 100 awards in *R&D Magazine*'s annual competition of the year's top 100 inventions. This issue of *Science & Technology Review* highlights the four award-winning technologies. On the cover, a NanoFoil® is pulsed with energy in a soldering operation. Shown below it are (from left) ARAM, the adaptable radiation area monitor; BAMS, the bioaerosol mass spectrometry system; and results from a simulation rendered in graphics format by VisIt, the open-source visualization software. Since 1978, Laboratory researchers have won 106 R&D 100 awards. (NanoFoil photograph reprinted courtesy of Reactive NanoTechnologies.)

Cover design: Kitty Madison

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str.

National Nuclear Security Administration

Prepared by LLNL under Contract No. W-7405-Eng-48

Science & Technology REVIEW

October 2005

Lawrence Livermore National Laboratory

Contents

S&TR Staff

Scientific Editor
Maurice B. Aufderheide III

Managing Editor
Ray Marazzi

Publication Editor
Carolin Middleton

Writers
Arnie Heller, Ann Parker, Gabriele Rennie, and Katie Walter

Art Director and Designer
Kitty Madison

Illustrator
John Maduell

Compositor
Louisa Cardoza

Proofreader
Pamela MacGregor

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Policy, Planning, and Special Studies.

S&TR is available on the Web at www.llnl.gov/str.

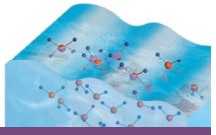
Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

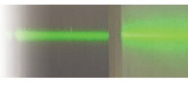
UCRL-TR-52000-05-10
Distribution Category UC-99
October 2005

2005 R&D 100 Award Highlights

Features



Research Highlights



Departments

Carbon storage measured in the Amazon River basin

Radiocarbon measurements of the Amazon River basin indicate that the watershed is returning carbon to the atmosphere much faster than scientists believed. This project, led by Emilio Mayorga of the University of Washington and Anthony Aufdenkampe of the Stroud Water Research Center, found that carbon outgassing from the waters in the 6.2-million-square-kilometer basin had been stored in the surrounding landscape for about 5 years. Tom Brown from Livermore's Center for Accelerator Mass Spectrometry (CAMS) and researchers from Rice University and University of São Paulo, Brazil, collaborated on this study.

Each year, the trees, plants, and soil of the Amazon rainforest absorb millions of tons of carbon dioxide during photosynthesis. As components of these organic materials decompose, rains and groundwater carry the produced carbon compounds into waterways. Microorganisms, insects, and fish in the waterways ingest that carbon and then generate carbon dioxide, which quickly returns to the atmosphere.

Previous measurements indicated that carbon in the downstream sections of the Amazon basin was 40 to more than 1,000 years old. Those findings led researchers to believe that tropical forest regions might store carbon for decades or even centuries. These regions thus might serve as a potential site for the long-term storage of atmospheric carbon dioxide, the human-produced greenhouse gas. However, in the recent radiocarbon survey, researchers found that the cycle time is much shorter. That is, most of the landscape carbon entering the basin waters was from very recent sources and was rapidly returned to the atmosphere rather than being carried downstream and sequestered in longer term deposits.

Livermore's University Relations Program and CAMS funded the carbon-14 measurements. The team's results appeared in the July 28, 2005, issue of *Nature*.

Contact: Tom Brown (925) 423-8507 (tabrown@llnl.gov).

Truck armor kits deployed to Iraq

Gun truck armor kits developed by Laboratory researchers are now providing convoy protection for U.S. troops on the roads of Iraq. Livermore researchers created a modular, easy-to-assemble armor protection kit that, with the addition of several machine guns, allows the military to convert 5-ton supply trucks into gun trucks to protect convoys. About 30 trucks have been outfitted with the armor protection kits and are being used in convoys on Iraqi roads. Kits for another 80 trucks have been requisitioned.

The main threats to convoys are hidden bombs or improvised explosive devices, sometimes followed by ambushes. Thus, the kit designers' primary goal was to protect truck occupants from the initial blast. The gun truck kits have proven popular and helpful to U.S. soldiers in Iraq. In fact, one transportation battalion honored the Livermore team with a commendation for exceptional service.

Each gun truck kit consists of readily available, low-cost armor steel and ballistic fiberglass panels, designed to provide a wall of protection around the back of the truck and for the truck cab. The side walls are topped by transparent armor to protect machine-gun operators. In addition to having a simple design and ample ballistic redundant protection, the kits can be assembled by a team within 5 hours and are easy to repair.

Livermore's Manufacturing and Materials Engineering Division completed the first prototype gun truck in March 2004. After ballistics and safety testing at the U.S. Army's Aberdeen Proving Ground in Maryland, the prototype was shipped to a transportation battalion at Camp Anaconda in Balad, north of Baghdad. Since then, the Laboratory has transferred the technology to U.S. companies for production. AB Fabrication and Machining of New Holland, Pennsylvania, is the project's main contractor. Other participating firms include Waco Composites of Waco, Texas; Conklin Equipment Company of Fallbrook, California; and Protective Armored Systems of Lenoxdale, Massachusetts.

Contact: Steve DeTeresa (925) 784-6513 (deteresa1@llnl.gov).

Radiocarbon dating used to study the brain

A research collaboration between CAMS and the Karolinska Institute in Sweden applied carbon dating to DNA to confirm that cells in the brain live longer than other cells. Carbon dating is typically used in archeology and paleontology to date the age of artifacts. However, in this application, which was described in the July 15, 2005, issue of *Cell,* the scientists used the pulse of radiocarbon to pinpoint, within 2 years, the birth dates of individual cells.

Radiocarbon, or carbon-14, is naturally produced by the interaction of cosmic rays and air and is present at low levels in the atmosphere and food. Its concentration has remained relatively constant during the past 4,000 years. But atmospheric testing of nuclear weapons from 1950 to 1963 produced a global increase in atmospheric radiocarbon.

In the Livermore–Karolinska collaboration, the team used carbon dating to determine whether the body creates neurons after birth. Because DNA does not exchange carbon after cell division, it provides a time capsule for pinpointing cells' date of birth.

Using research cadavers, the scientists dated neurons in people born before 1950 and after 1963—the year aboveground nuclear testing ended. The neurons in people born before 1950 showed no spike in radioactive carbon from the atmospheric testing. Those born after 1963 had levels consistent with the level of atmospheric radiocarbon at the time of their birth. The team concluded that neurogenesis does not occur in the cortex after birth—people do not produce new neurons during their lives.

The research collaboration received funding from the National Institutes of Health and the multinational Human Frontier Science Program. Further research will delve into other brain regions to determine the origin of neurodegenerative diseases.

Contact: Bruce Buchholz (925) 422-1739 (bbuchholz@llnl.gov).

Commentary by Cherry A. Murray

Important Missions, Great Science, and Innovative Technology

LAWRENCE Livermore National Laboratory's commitment to applying the best of science and technology to meet important national needs is clearly evident in the articles in this issue of *Science & Technology Review* (*S&TR*). The stories highlight a strong focus on mission; a multidisciplinary approach to research and development; effective partnerships with industry and universities; and signature strengths of the Laboratory in high-energy-density physics, computations, materials science, and biodefense sciences.

One indicator of the creativity of Laboratory researchers is their success in *R&D Magazine*'s annual competition for the top 100 technological advances that contribute to meeting an important national or societal need. In 2005, the Laboratory and its partners earned four R&D 100 awards, and beginning on p. 4, *S&TR* highlights these award-winning technologies. Livermore has now captured 106 of these "Oscars of invention" since 1978.

Our focus on mission is particularly striking in two of the award winners, both of which strengthen homeland security. The first, the bioaerosol mass spectrometry (BAMS) system, can analyze individual aerosol particles to almost instantly identify the presence and concentration of harmful biological particles. BAMS is designed for operation in office buildings that could be targets for a terrorist attack using an agent such as anthrax. Alternatively, it can be used at ports of entry such as airports or train stations to monitor for potential epidemic diseases.

A second R&D 100 Award was earned by a team of Livermore researchers who developed the adaptable radiation area monitor (ARAM). ARAM is a highly sensitive system designed to detect small amounts of nuclear material. The system can be used as a fixed detector to monitor slow-moving packages, luggage, or pedestrians; as a roadside detector to monitor high-speed traffic; or as a portable detector. Livermore shares this award with Innovative Survivability Technologies of Goleta, California, which licensed the technology and rapidly put this easy-to-operate system into production.

Our national security mission is further highlighted in the article on aerogels, lighter-than-air materials that have been the subject of considerable pioneering research at Livermore. Beginning on p. 20, we examine efforts to dope aerogels with materials that efficiently produce high-energy x rays when pulsed with a laser. The x rays would be used to diagnose future high-energy-density experiments for stockpile stewardship and other applications at the National Ignition Facility.

Expertise in materials science and nanotechnology is preeminent in our third R&D 100 Award–winning technology, a nanoengineered heat source, dubbed NanoFoil®. This unique nanotechnology was featured last year in *The National Nanotechnology Initiative Strategic Plan.* NanoFoil heats only the interface being joined and permits large and small components to be metallically bonded with no thermal damage. Developed with Reactive NanoTechnologies of Hunt Valley, Maryland, and Johns Hopkins University, the technology potentially has wide application—from airplanes to computers.

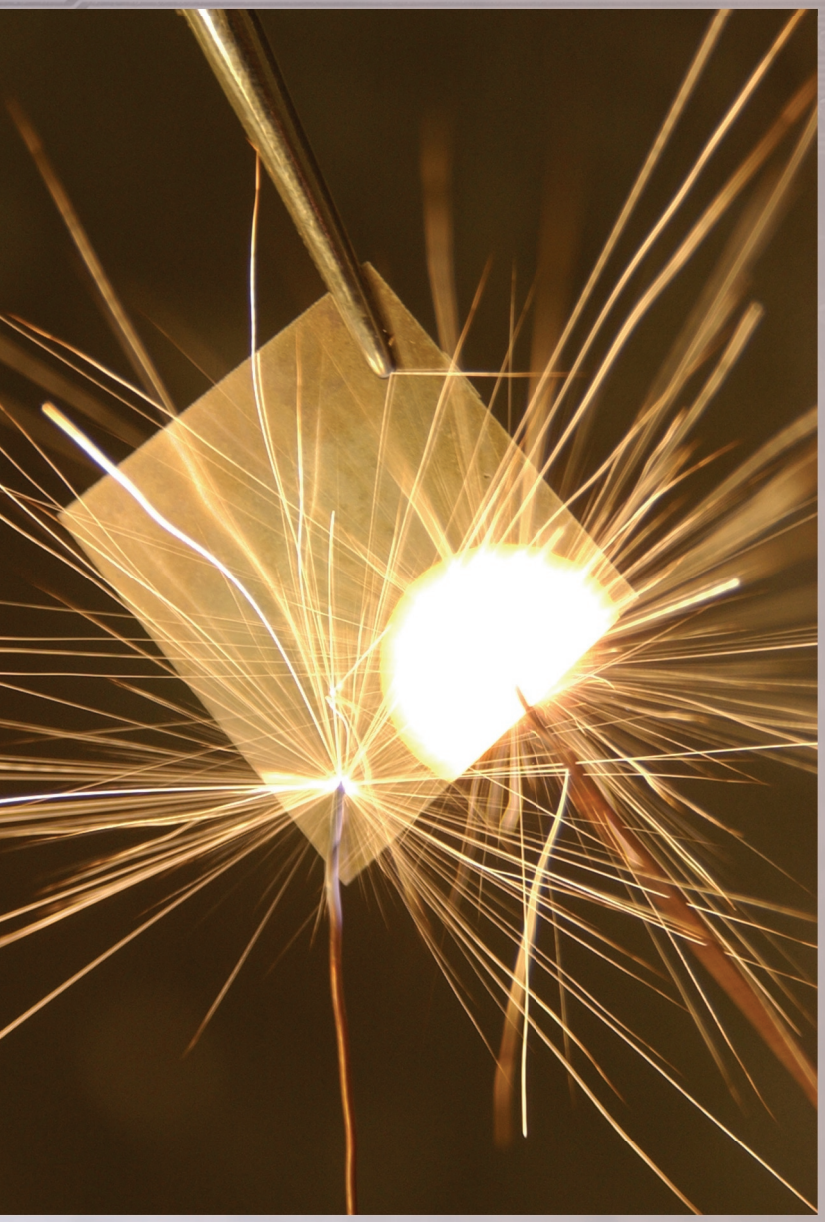
Computations is the area of our fourth R&D 100 Award. With several of the world's largest and fastest computers on site, Livermore is facing the issue of how to extract knowledge from trillions of bytes of data. VisIt is a visualization tool geared toward just that—parallel processing the large amounts of data produced from simulations and rendering them in graphic form. Problems that run for days or weeks on the Laboratory's supercomputers can be visualized and displayed within seconds using VisIt. This free, interactive tool has been downloaded more than 25,000 times by users throughout the world.

An important application of supercomputers is in studying material properties. For example, part of Livermore's national security mission requires that we understand how materials behave at the extreme conditions present in an exploding nuclear weapon. The feature article beginning on p. 12 describes supercomputer simulations of a common but surprisingly complex substance: water. Laboratory scientists are examining the structure of water at the liquid–vapor interface, and they are modeling the dynamic properties of water under the conditions that might exist inside giant planets.

Important missions, great science, and innovative technology—all come together to make Lawrence Livermore an exciting place to pursue multidisciplinary research and development in the national interest.

■ Cherry A. Murray is deputy director of Science and Technology.

NanoFoil® Solders with Less Heat



When a NanoFoil® is soldered, the reaction propagates outward at about 5 meters per second. In the reaction region (white area), the temperature has jumped to 1,500°C, while the remainder of the foil is still at room temperature. (Image courtesy of Reactive NanoTechnologies.)

HEAT is becoming one of the most critical issues in computer and semiconductor design," says Intel Corporation's Chief Technology Officer, Pat Gelsinger. As microprocessors in computers operate faster, they produce more heat. However, the difficulty of conducting this increased heat out of a chip is limiting both chip performance and reliability. The most effective way to get heat into the heat sink would be to attach the chip package with a conductive metallic bond such as a solder. But soldering the components in a hot furnace can damage or destroy the chip. Epoxies do not damage the chip, but they tend to degrade over time, and their bond is weaker and conducts substantially less heat than a metallic soldered joint.

Enter NanoFoil®, a revolutionary product that creates a strong, thermally conductive bond between a heat sink and a chip, with no damage to the chip. NanoFoil delivers just enough heat to melt the solder but not enough to damage a chip. When one end of the foil is pulsed with energy, NanoFoil's thousands of nanolayers of nickel and aluminum begin to chemically react and release heat into the surrounding solder material. This reaction front self-propagates across the foil, causing the temperature of the reacted area to leap to more than 1,500°C while the remainder of the foil is still at room temperature. This process energizes the formation of what is termed a NanoBond™. The NanoBond process works in air, in a vacuum, or in argon gas, and it is completed in a second or less.

NanoFoil grew out of technology used to fabricate multilayer x-ray and extreme-ultraviolet optics at Lawrence Livermore. Materials scientist Troy Barbee, Jr., began much of the early work on reactive foils as part of a broad multilayer, nanolaminate project initially funded by Livermore's Laboratory Directed Research and Development Program. Postdoctoral researcher Timothy Weihs and Barbee worked on reactive nanolaminate materials as part of a Cooperative Research and Development Agreement in the mid-1990s. In 1995, Weihs joined the faculty at Johns Hopkins University where he teamed with Omar Knio (then a professor at Johns Hopkins) and others to further develop reactive foils for use as localized heat sources for soldering and brazing. In 2001, Weihs and Knio founded Reactive NanoTechnologies (RNT) in Hunt Valley, Maryland, to commercialize NanoFoil.

Manufactured and sold exclusively by RNT, NanoFoil can be used to bond metals, ceramics, semiconductors, and polymers. It can also bond dramatically dissimilar kinds of materials without causing the materials to crack. NanoFoil is a new class of material and is one of the most mature nanotechnologies available today.

Because of NanoFoil's unique properties, the technology is getting considerable high-profile exposure. It was featured on the cover of the *Strategic Plan for the National Nanotechnology Initiative* published in December 2004 by the Executive Office of the President. More recently, RNT, Lawrence Livermore, and Johns Hopkins University won an R&D 100 Award for NanoFoil.

Benefits Abound

The NanoFoil technology can replace reflow soldering, a common process for mounting components on printed circuit boards that requires multiple, time-consuming runs through a furnace. NanoFoil also eliminates the need for potentially toxic, lead-based solders.

Compared with other joining methods, NanoFoil is a major cost saver. It can replace expensive capital equipment such as the furnaces and torches used in conventional soldering or brazing operations. Similarly, newer bonding methods such as laser and resistive welding, developed to get around the limitations of traditional soldering and brazing, have significant capital costs up front.

NanoFoil can be manufactured in a range of sizes, allowing both large and small components to be bonded, and it can be customized for specific uses. The properties of the chemical reaction, such as velocity and temperature, can be controlled by varying the thickness of individual nanolayers or the average chemistry or total thickness of the foil. The velocity of the reaction increases significantly as the thickness of each aluminum–nickel bilayer decreases. In thinner layers, the atoms intermix more easily, and the reactions propagate faster. Each bilayer typically is about 50 nanometers thick with approximately 25 atoms across its thickness. RNT engineers can adjust the thickness to within a few nanometers to obtain the NanoFoil properties needed for a particular job.

From Chips to Missiles

RNT has identified many potential uses for NanoFoil besides attaching computer chips to heat sinks. It offers a replacement for epoxies and solder in manufacturing circuit boards, saving money and time and eliminating the need for lead-based solders. RNT developed the NanoBond process for mounting radio-frequency connectors on printed circuit boards in conjunction with Agilent Technologies of Palo Alto, California.

As the first technology to create strong, large-area metallic joints between ceramic and metal, NanoFoil may be used in the near future to attach ceramic armor tiles to U.S. Army tanks and trucks. Epoxies are used now, although their bonds are weak and typically fail with a single ballistic hit. Worse yet, when a single tile is hit, the shock wave causes neighboring armor tiles to pop off. BAE Systems, an international defense and aerospace contractor, has an exclusive development agreement with RNT for the use of NanoFoil to mount armor on military vehicles.

NanoFoil can also be used to mount magnetron sputtering targets; to hermetically seal photocells, capacitors, sensors, and other devices; and to ignite solid propellants. Other possible applications are as infrared decoys to defeat heat-seeking missiles and in intercepting missiles to provide structural integrity and to release energy on impact.

Joining and bonding materials are important to almost every commercial and defense market. The NanoBond process is fast, strong, inexpensive, and environmentally friendly—and it promises significant benefits to U.S. manufacturing.

—Katie Walter

Key Words: computer industry, NanoBond™ process, NanoFoil®, nanotechnology, R&D 100 Award.

For further information contact Troy Barbee (925) 423-7796 (barbee2@llnl.gov).

Troy Barbee, a materials scientist at Livermore, worked on the NanoFoil team.

Detecting Radiation on the Move

TERRORISTS beware. If you're considering bringing material for a "dirty bomb" into the U.S., a new Livermore technology can almost literally stop you in your tracks. Try hauling radiological material over the border in a fast-moving truck, and the adaptable radiation area monitor (ARAM) will be able to detect it. ARAM detectors, which have already been installed at many border crossings, are designed specifically for fast, accurate detection without interrupting the flow of traffic and commerce.

The adaptable radiation area monitor (ARAM) can detect small amounts of radioactive material hidden in a vehicle moving at highway speeds.

The ARAM technology won a 2005 R&D 100 Award, which Livermore scientists, led by physicist Dan Archer, share with Innovative Survivability Technologies (IST) of Goleta, California. IST licensed the technology in January 2004.

"The ARAM system can serve as a stand-alone radiation monitor, or it can be networked into a system of monitors to cover a large area," says Archer. In addition, the system can be used as a fixed detector to monitor slow-moving packages, luggage, or pedestrians and as a portable detector. ARAM is optimized to detect even small quantities of radioactive materials moving at highway speeds. This capability makes ARAM a crucial element in the effort to protect the nation from radiological weapons of mass destruction.

Improving Time Resolution

ARAM is an automatic, highly sensitive system that uses a thallium-doped sodium iodide crystal to detect even small amounts of radiation in different scenarios. The crystal may be shielded on as many as four sides to "point" the detector in a particular direction, or it may not be shielded at all. The crystal detects full spectral data by dividing the spectrum into 1,024 energy bins, or channels. It counts single photons, unlike most other detectors, which collect gross counts or divide the spectrum into only 10 channels. ARAM's method, known as list mode, produces large quantities of raw, time-stamped data that can be analyzed in any number of ways. List mode increases overall sensitivity and the signal-to-noise ratio for spectral data analysis, thereby increasing the probability of a proper identification. This feature is particularly important for detecting radioactive materials hidden inside moving vehicles.

"ARAM is unique because it combines shielding, a large crystal, and the very brief time during which the radiation source needs to be in front of the detector," says Archer. "ARAM can achieve the highest signal-to-noise ratio to date among comparable detector systems."

The software for the ARAM system provides near-real-time results. With Ethernet connectivity standard on all units, ARAM can be interfaced to a variety of radiation detector technologies. Third-party detector systems can be connected for data archiving and processing. Digital cameras may be attached to further document events, and multiple annunciation mechanisms are available, including e-mail, local paging, liquid crystal displays, and Ethernet-attached annunciators. Radiation levels and spectra are archived by the software and made available via the Web (and secure Web transmission) for remote telemetry and viewing.

By acquiring data in list mode, ARAM can produce output with much finer time resolution than similar programs. Fine time resolution offers numerous advantages: Small sources of radiation moving at highway speeds can be detected and identified, and the

direction of the radiation source's motion may be determined. Fine time resolution also protects the source spectrum from contamination by background radiation collected immediately before or after an event. Eliminating this spectral contamination results in better data for radionuclide identification.

When a spectral anomaly is detected, "trigger" algorithms operate on the acquired data and produce detailed, easily read event reports. These advanced algorithms include enhancements to improve performance in difficult scenarios, such as roadside monitoring, and to substantially reduce false alarms—for example, when the shielding effect from a large truck causes a change in the level of background radiation.

Members of the ARAM development team: (left to right) David Pletcher, Mike Mercer, Brock Beauchamp, David Trombino, Vincent Riot, Tom Schaffer, Joe Mauger, Daniel Archer, Karl Nelson, and Guy Urbina.

No Choke Point to Slow Traffic

Monitoring for radiological material involves three steps: detection, localization, and identification. Each step could require a different piece of equipment, depending on a system's design. For example, in some systems, a large portal monitor might perform the initial detection phase of all vehicles. Suspect shipments would then be inspected using smaller handheld detectors to localize and identify the material. The ARAM design combines detection and identification into a single step.

Comparing ARAM to other commercially available radiation monitors is difficult. Many systems have been designed to detect small quantities of smuggled nuclear materials leaving nuclear plants. Detectors also monitor scrap metal entering steel mills to avoid contaminating the mills, because hiding nuclear material in scrap steel is a common disposal method. Several of these detectors indicate the presence of radiation but provide little identification capability. The nuclear fingerprint that ARAM's system supplies reduces the need for secondary screening. Thus, ARAM minimizes the number of labor-intensive inspections on suspect shipments and keeps commerce moving. In addition, many radiation monitors require people and material to pass through a narrow detection area, which becomes a choke point that slows traffic. In contrast, ARAM can operate in a pass-by mode so traffic continues to move freely.

ARAM's adaptability has been thoroughly tested. ARAM was used as a fixed device to monitor packages for Federal Express in its air-cargo facility at the Denver International Airport. Another version of ARAM was integrated into a vehicle, in which the operator could perform his or her normal job and be able to monitor for radioactive materials. In this configuration, ARAM can operate like a portal monitor that can be moved from site to site, or it can be used in a mobile mode, testing for radiation anomalies while the vehicle is in motion. Yet another version of ARAM was part of a demonstration in which 14 independent systems were networked to detect and identify multiple radiation sources of varying strengths.

California is the first state to install radiation detection units such as ARAM at border crossings, and other states have expressed interest in the technology. According to IST, a major port authority has proposed integrating more than a dozen ARAM units into a system to monitor people at marinas and a ferry terminal. With ARAM around, people and vehicles carrying illicit radiological material can run, but they can't hide.

—Katie Walter

Key Words: adaptable radiation area monitor (ARAM), homeland security, radiation detection, R&D 100 Award.

For further information contact Daniel Archer (925) 423-6018 (darcher@llnl.gov).

Identifying Airborne Pathogens in Time to Respond

AMONG the possible terrorist activities that might threaten national security is the release of an airborne pathogen such as anthrax. Because the potential damage to human health could be severe, experts consider 1 minute to be an operationally useful time limit for identifying the pathogen and taking action. Many commercial systems can identify airborne pathogenic microbes, but they take days or, at best, hours to produce results. The Department of Homeland Security (DHS) and other U.S. government agencies are interested in finding a faster approach.

To answer this national need, a Livermore team, led by scientist Eric Gard, has developed the bioaerosol mass spectrometry (BAMS) system—the only instrument that can detect and identify spores at low concentrations in less than 1 minute. BAMS can successfully distinguish between two related but different spore species. It can also sort out a single spore from thousands of other particles—biological and nonbiological—with no false positives. (See *S&TR*, September 2003, pp. 21–23.)

The bioaerosol mass spectrometry (BAMS) system—about the size of three lecterns—can identify bioagents, such as anthrax, and it has the potential to differentiate between normal and cancerous cells.

The BAMS team won a 2005 R&D 100 Award for developing the system. Livermore's Laboratory Directed Research and Development (LDRD) Program funded the biomedical aspects of the BAMS project, and the Department of Defense's Technical Support Working Group and Defense Advanced Research Project Agency funded the biodefense efforts.

Developing a detection system that can analyze small samples so quickly has been challenging. Livermore engineer Vincent Riot, who worked on the BAMS project, explains, "A typical spore weighs approximately one-trillionth of a gram and is dispersed in the atmosphere, which contains naturally occurring particles that could be present at concentrations thousands of times higher. Previous systems also had difficulty separating benign organisms from those that are pathogenic but very similar, which has resulted in false alarms."

Sorting between Harmful and Benign

BAMS operates by drawing air through a nozzle and removing nearly all the particles too small to be biological threat agents. The remaining particles—each about 0.5 to 10 micrometers in diameter—are focused into a tight beam. A particle accelerates to a velocity determined by its size and shape, which provides information on a particle's type. The system then probes each particle to determine if it contains biological material. For this operation, a pulsed-laser beam excites the particles. Biological materials, if present, emit fluorescent light, which can be recorded by the detector, but nonbiological particles, such as dirt in the atmosphere, do not emit light. This step reduces the number of particles for further analysis by 90 percent.

In the system's final step, a mass spectrometer identifies the particles. Most mass spectrometers operate by measuring either positive or negative ions. BAMS uses a dual-polarity mass spectrometer, which can process a particle's positive and negative ions at the same time. The positive and negative ions formed are further separated by polarity and mass-to-charge ratio. Real-time pattern-recognition software developed at the Laboratory then

analyzes and categorizes the resulting spectra. Every organism produces a unique signature, which BAMS compares with spectra in a database of organisms. The system can analyze thousands of particles per second, so it can distinguish a very small concentration of biological aerosol from a much larger concentration of background aerosol.

To test the system, the Livermore team used *Bacillus subtilis var. niger*, a surrogate of anthrax (*B. anthracis*), and *B. thuringiensis*, an organic pesticide that differs from *B. anthracis* in two short sections of its DNA. BAMS successfully distinguished between the two. The instrument also identified other bacterial cells and spores, biological toxins, and viruses. "BAMS is the only system that can identify harmful biological agents in enough time to evacuate an area," says Riot, "and it can do so with almost no false positives, which is essential in reducing the panic that alarms can cause."

In a recent study, the team placed BAMS in the international terminal at San Francisco International Airport to help DHS determine the cause for false positives registered by other equipment. The instrument has also been used in preliminary studies at Livermore's Site 300, where BAMS successfully distinguished particles in the atmosphere and surrounding soil from those generated by a detonation of conventional high explosives.

The system's ability to analyze particles or cells could benefit other fields in addition to biological threat detection. Potential applications include medical diagnostics, explosives detection, meteorological studies, and nonproliferation programs. For example, the BAMS team hopes to build on the Site 300 research to develop detection capabilities for radioisotopes, which would benefit the nation's nonproliferation programs.

Detecting Communicable Airborne Diseases

BAMS also has the potential to detect communicable diseases such as severe acute respiratory syndrome (SARS) or tuberculosis, which typically take about a week for clinical detection. Livermore researchers have used tuberculosis surrogates to test the system's ability in this area. The LDRD Program is funding an effort to analyze human sputum. Led by physicist Matthias Frank, the project includes researchers from the Laboratory's Chemistry and Materials Science; Physics and Advanced Technologies; Nonproliferation, Arms Control, and International Security; and Biosciences directorates. By learning which particles occur naturally, these scientists hope to find a method for detecting abnormal cells for various diseases. Riot says, "The idea is to have a person breathe into a mask, then let BAMS analyze the particles released from the lungs and identify them instantaneously."

Members of the BAMS development team: (left to right, back row) Paul Steele, Todd Weisgraber, Bruce Woods, Abneesh Srivastava, and Keith Coffee; (middle row) Vincent Riot, Jim Birch, Herbert Tobias, and Eric Gard; (front row) Matthias Frank and David Fergenson.

The current BAMS system, about the size of three lecterns, is available for licensing. The Livermore team continues to work on improving the system's capability and reducing its size to fit various needs. Whether used to detect biological agents or contagious diseases, BAMS shows great promise for identifying problems reliably when time is of the essence.

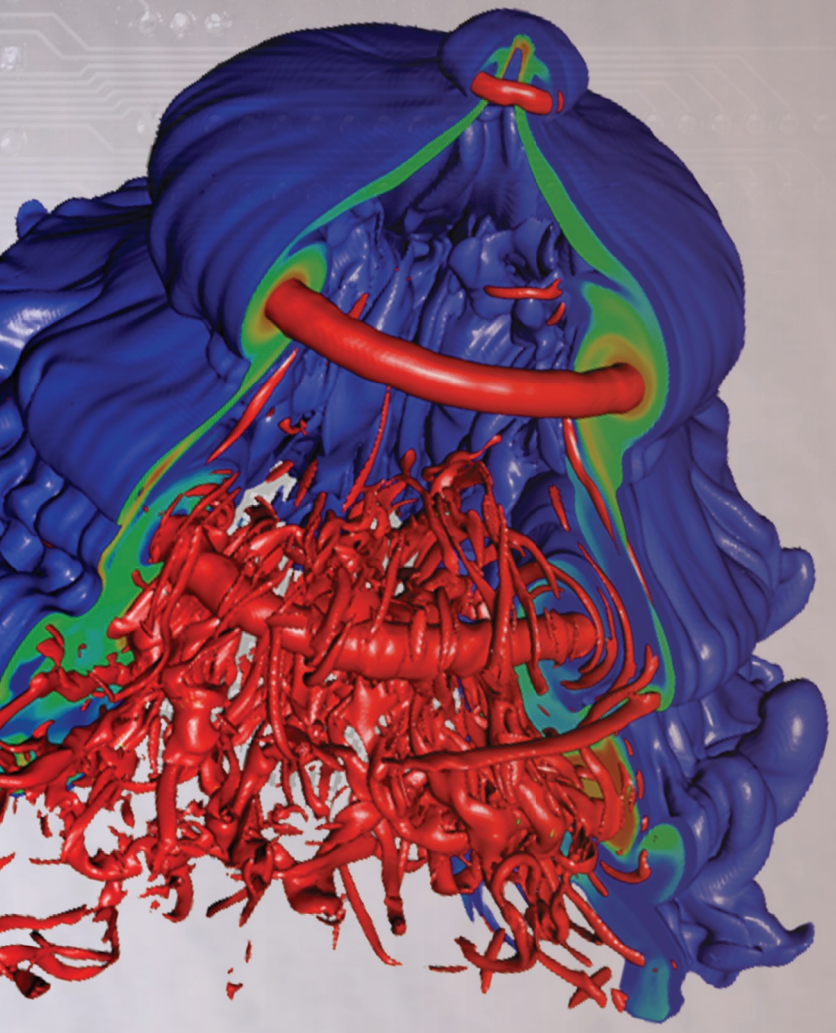
—Gabriele Rennie

Key Words: airborne pathogen, anthrax, bioaerosol mass spectrometry (BAMS) system, R&D 100 Award.

For further information contact Vincent Riot (925) 422-9798 (riot1@llnl.gov).

Picture Perfect with VisIt

COMPLEX simulations running on today's supercomputers can generate enormous data sets that contain trillions of bytes. To better understand these results, scientists and engineers often use visualization software to create pictures of the data that are far easier to interpret than reams of numbers. Problems that run for days or weeks on the world's most powerful supercomputers can now be visualized or analyzed in seconds using VisIt—a flexible visualization and analysis tool developed at Livermore.



With the visualization and graphics analysis tool called VisIt, scientists can create a three-dimensional image of a simulation. Here, results from a calculation using Livermore's RAPTOR code show the unstable growth of a dense spherical gas bubble subjected to a strong planar shock wave.

One of VisIt's strengths is that it has a scalable architecture, allowing it to process some of the biggest data sets ever generated. It also has a plug-in architecture, so additional capabilities can be easily added. VisIt is free as well, available as open-source software at: www.llnl.gov/visit.

VisIt is used to visualize data from a wide range of simulation codes including computational fluid dynamics, finite-element analysis, astrophysics, and hydrodynamics. The software was developed with funding from the Department of Energy's Advanced Simulation and Computing (ASC) Program by scientists in the Laboratory's Computation Directorate. The project team, led by computer scientist Eric Brugger, received a 2005 R&D 100 Award for this powerful application.

VisIt Is Flexible

Visual renditions of data sets range from the simple, such as basic plots, to the highly complex, such as three-dimensional (3D) volume renderings, with color frequently used to explain the data's characteristics. VisIt can produce images, movies, and statistical reports.

The visualization tool runs on various platforms from desktop computers to Livermore's Purple and Thunder supercomputers. Its three operating modes effectively use computing resources based on data-set size. For small- to medium-scale data sets, VisIt simply runs on a desktop machine. For larger scale sets, its work is distributed: Data are processed in parallel on a supercomputer, and surfaces are transferred back to a desktop machine for renderings. This mode leverages the best of both computing environments. On a supercomputer, large amounts of data are processed quickly through parallelization. The graphics card in a user's desktop computer provides the interactivity needed to examine data from different viewpoints. For the largest scale data sets, VisIt does all of the processing, including the rendering, on a supercomputer.

"Many visualization tools were originally implemented as serial applications that were later parallelized," says Brugger. "As a result, those tools cannot process certain algorithms, such as parallel streamline generation. We designed VisIt to be parallel from conception, so it's well suited for processing such visualization

algorithms and handling their communication and execution requirements."

Many Rich Features

VisIt supports different kinds of data input, and it can be easily extended through its dynamically loaded plug-ins. It also has a powerful graphical user interface. VisIt can be used to visualize different types of variables: scalars such as temperature or pressure, vectors such as velocity, and many more. It also supports 2D and 3D meshes whether they are structured, unstructured, adaptively refined, or gridless.

The software's plug-in design allows new capabilities to be quickly implemented. Database plug-ins import data from new file types. Operator plug-ins manipulate the data, for example, by slicing them or performing rigid body transformations such as rotation. Plot plug-ins define how data should be colored and rendered. VisIt even includes a tool for creating plug-ins. With it, a user describes a set of desired properties. The tool then generates most of the code needed to implement the plug-in.

The software's graphical user interface allows novice users to begin visualizing data quickly, while experienced users can access its advanced features. VisIt creates time-based animations from data sets with multiple time steps and allows users to pan, zoom, and rotate objects interactively using a mouse or other tracking device. Users can also easily size and position geometric objects such as planes and spheres.

VisIt is frequently used to debug simulation codes and has many features that allow code developers to access all portions of their simulations. In addition, its analysis capabilities include regression testing, where the output of computer simulations can be compared with their expected results.

Drop By for a VisIt

Brugger notes that VisIt has been downloaded more than 25,000 times by users from 4,000 different locations. Over 250 Livermore scientists use VisIt to render results from simulations of hydrodynamic instabilities, the dispersion of airborne chemical releases, and other complex physics events.

VisIt has enthusiasts throughout the world, including at the University of California at Berkeley, the San Diego Supercomputer Center, the United Kingdom's Atomic Weapons Establishment, and the Leiden Observatory of the Universiteit Leiden in the Netherlands. Jelle Ritzerveld from Leiden notes that, after trying several available visualization software tools, the observatory's astrophysics group not only uses VisIt but also recommends it to others. At Livermore, physics code group leader Michael Zika says, "I regularly use VisIt to gain insight into a wide range of physics simulations. It is an essential component of our scientific computing environment."

VisIt has already had an important impact on visualizing the extreme data sets in computational modeling and continues to broaden its user base. Says Brugger, "We're adding support for many new file formats and expect that, as a result, even more users will turn to it for visualizing data sets, constrained only by the disk space and computational resources available to them."

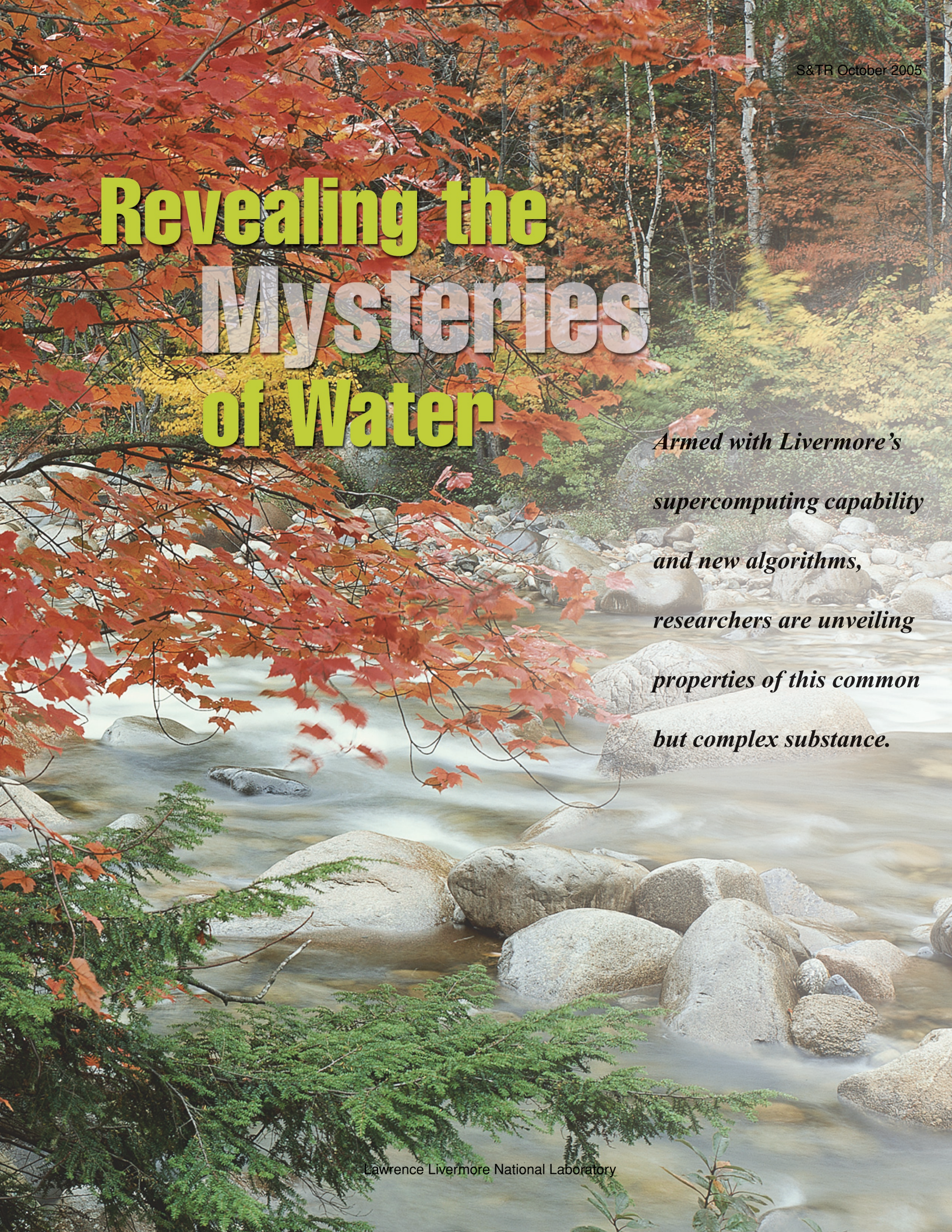
—Ann Parker

Members of the VisIt development team: (left to right, standing) Mark Miller, Sean Ahern, Eric Brugger, Kathleen Bonnell, and Brad Whitlock; (sitting) Hank Childs and Jeremy Meredith; and (kneeling) Linnea Cook.

Key Words: open-source software, R&D 100 Award, VisIt, visualization software.

For further information contact Eric Brugger at (925) 423-1293 (brugger1@llnl.gov).

Revealing the Mysteries of Water



Armed with Livermore's supercomputing capability and new algorithms, researchers are unveiling properties of this common but complex substance.

WATER would seem to be relatively easy for scientists to understand. It is the only natural substance on Earth that is found as a gas, liquid, and solid. It covers 70 percent of Earth's surface, makes up 60 percent of the human body, and constitutes 90 percent of a person's blood.

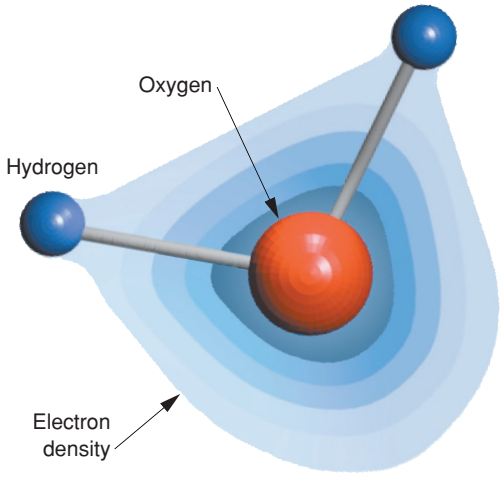
However, the water molecule is far from simple. Given its low molecular weight, water at ambient conditions should be a gas instead of a liquid. Its boiling point is nearly 200°C higher than expected compared with similar-size molecules. And, unlike most substances, when ice melts, the water molecules pack more closely together than they do when frozen, which is why ice cubes float. In addition to its familiar liquid phase, water has at least 3 other liquidlike phases and up to 14 solid phases.

Water's unusual properties have unexpected effects on the thermodynamic behavior of its phases. For example, temperature and pressure affect the molecules differently when water approaches its boiling point than when it is close to freezing. Heating already hot water increases its isothermal compressibility and heat capacity and reduces its density, but heating cold water has the opposite effect. Also, applying pressure reduces the mobility of the molecules in hot water but increases their mobility in cold water. Ice melts when slight pressure is applied, but under high pressure, liquid freezes.

Understanding water is important to a range of research areas from geosciences to biological systems to astrophysics. But explaining the anomalous properties of this mysterious molecule has challenged both theorists and experimentalists. Scientists began to simulate liquid water almost 40 years ago. Yet, they continue to pursue more accurate models so they can better analyze this surprisingly complex molecule.

The revolution in supercomputing has been a boon to such research. To simulate even a few hundred atoms requires supercomputing capabilities, such as those available with Livermore's unclassified supercomputer, Thunder. Funded by the Laboratory's Multiprogrammatic and Institutional Computing Initiative, Thunder can process 23 trillion operations per second. In June 2005, it ranked seventh on the Top500 List, the leading industry authority for high-performance computing.

By designing algorithms to exploit Thunder's capabilities, a team of Livermore researchers, led by chemist Christopher Mundy, has made important contributions to the study of water and its properties. With funding from the Laboratory Directed Research and Development Program, Mundy's team examined the behavior of water at the molecular level under changing conditions. The team's models reproduced



The average electron density around the oxygen atom in a water molecule is about 10 times that around the hydrogen atoms. This nonuniform distribution of positive and negative charges leads to the substance's unusual behavior.

the bulk properties of liquid water. With this improved capability, researchers can better understand the many phases of water and predict the behavior of more complex molecular fluids.

A First-Principles Approach to Water

The basis of water's unexpected properties is the electronic structure of the oxygen atom and the two hydrogen atoms that make up the V-shaped molecule. A water molecule's valence electrons (the electrons in the outer shell, which are thus the most reactive) spend more time around the oxygen atom than they do around the hydrogen atoms. Because electrons carry a negative charge, the oxygen end of the molecule develops a partial negative charge, and the hydrogen end of the molecule develops a partial positive charge. This nonuniform distribution of positive and negative charges is called an electric dipole.

The strong dipole present in water leads to its unique behavior. (See the box below.) The electrostatic attraction between the hydrogen and oxygen in adjacent molecules creates hydrogen bonding, a weak attractive force. Hydrogen bonds between water molecules are responsible for a tetrahedral structure that gives water many of its unusual properties.

Early simulations used classical molecular dynamics (MD) calculations to examine the liquid phase of water in bulk form. In classical MD, molecules move according to forces that are defined by empirical interaction potentials. These potentials are determined by observing how molecules behave in a given phase at a specific temperature or pressure. By integrating the Newtonian equations of motion, researchers can then compute the trajectory of molecules in small time steps.

A drawback to this method is the narrow range of information it provides because the calculation is specific to a set of parameters. To model the diffusion of a water molecule, researchers must limit the range of temperatures and pressures for the

A Common Substance with Unusual Properties

Water is indeed strange for a substance at neutral pH, midway between the hazardous acid and alkali extremes. The atoms in a water molecule—two hydrogen and one oxygen—are arranged at the corners of an isosceles triangle. The asymmetrical shape of the molecule occurs because the four electron pairs in the outermost shell of oxygen tend to arrange themselves symmetrically at the vertices of a tetrahedron around the oxygen nucleus. When water molecules are close enough, each oxygen atom attracts the nearby hydrogen atoms of two other water molecules, forming hydrogen bonds. These hydrogen bonds are responsible for many properties of water, some of which are unusual. For example, solids are usually the densest form of a substance, followed by liquids and then gases. As temperature increases, a substance's density generally decreases. But pure water is an exception to this rule—it is the only known substance that has its highest density as a liquid. At low temperatures, water has a higher density than ice, which is why ice floats.

Water has an unusually large heat capacity, requiring a lot of energy to increase its temperature. This characteristic prevents Earth from getting too hot or too cold, and it slows the temperature changes in oceans, biological cells, and tissues, making conditions possible for life. Water also has a high heat of vaporization, so a lot of energy from the Sun is needed to turn liquid water into vapor. It takes four times as much energy to heat a given mass of water by 1°C as it does to heat the same mass of dry air.

Water's dielectric constant—that is, its tendency to interact with applied electric fields—and its ability to neutralize the attraction between electric charges enables it to buffer or weaken the forces between dissolved ions and molecules. Thus, water is a powerful solvent and a medium for biochemical reactions.

Water is crucial for all life. Liquid water absorbs radiation of all wavelengths, except a narrow window in the visible (photochemical) waveband. This window is critical for photolysis and directly or indirectly influences the development of all life on Earth. Water's high thermal conductivity speeds up heat redistribution in living tissues, which helps protect the body from uneven heating and cooling, whether such changes are caused by metabolic processes or external mechanisms. In biochemical reactions, water plays a passive role as a solvent for minerals, organic solutes, and gases, but it can play an active role in such vital processes as photosynthesis and respiration.

simulation. Water's strong dipole moment and highly directional hydrogen bonds that participate in chemical and physical processes pose a great challenge in defining these parameters for dynamic simulations.

Another drawback is that classical MD does not capture bonds being made and broken. Instead, it approximates the real system by treating the entire molecule as a single unit. These calculations can provide useful information about water at low temperature and pressure, where chemical bonds rarely break. However, to study chemical reactions, especially at extreme temperatures and pressures, researchers need a more fundamental description of water that can only be obtained by a first-principles model.

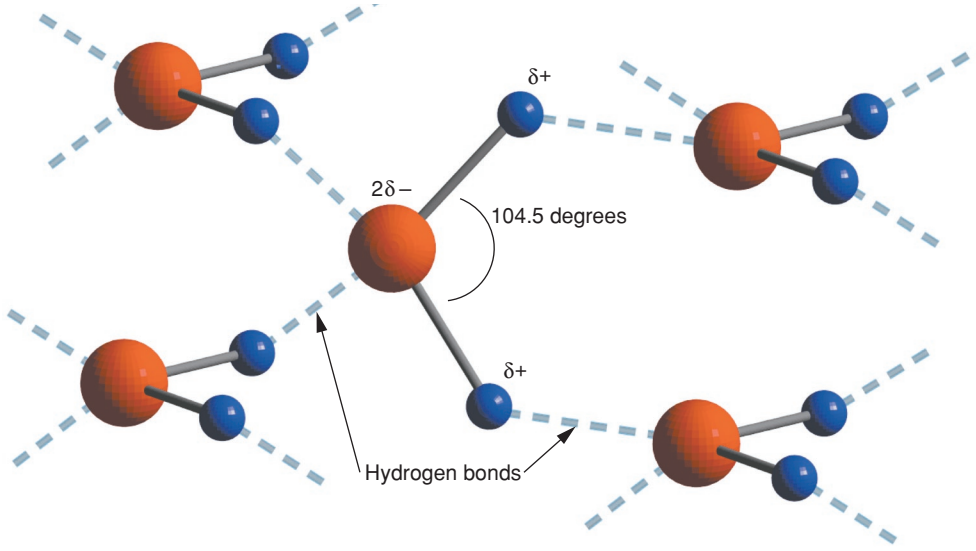
First-principles MD models do not include assumptions about the characteristics of interatomic and intermolecular interactions. Instead, the models use the laws of quantum mechanics to compute the forces that govern these interactions. These forces can be derived directly from the ground-state electronic structure of the molecules' chemical bonds.

One method used with first-principles models includes quantum mechanics based on density functional theory (DFT). Walter Kohn, a professor at the University of California at Santa Barbara, developed this approach and, in 1998, won a Nobel Prize in Chemistry for his work on DFT. Instead of using the many-body wave function to describe all the electrons in a molecule, DFT defines a molecule's energy and electronic structure in terms of the electron density in the molecule. Electron density is a simpler quantity to handle computationally, especially with a large number of electrons. Once scientists have defined the electronic structure of a material's molecules, they can, in principle, calculate all of the material's chemical and physical properties.

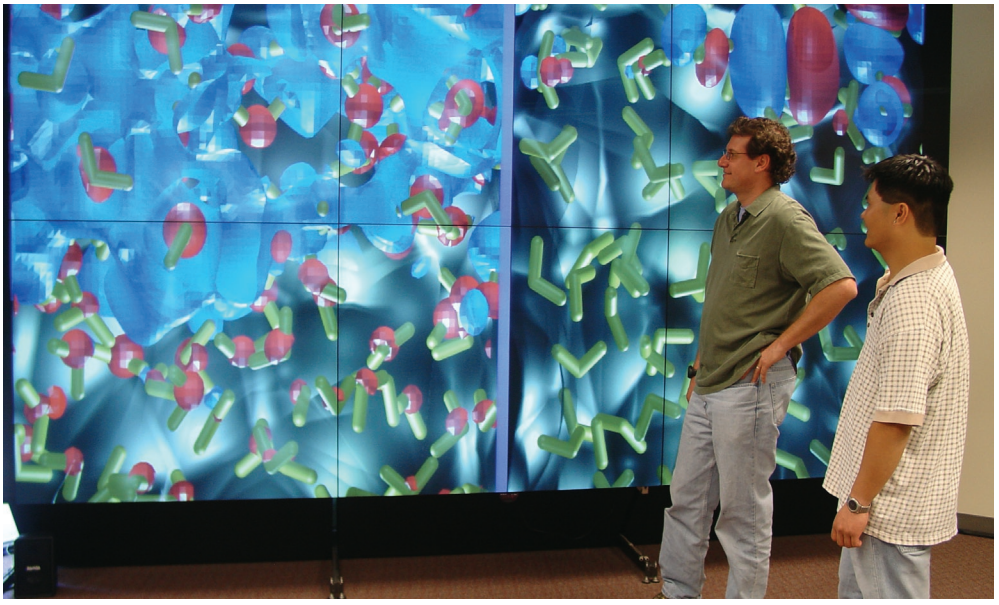
Finding Stable Phases of Water

To model the trajectories of water molecules, Mundy and his colleagues used a method called Car-Parinello molecular dynamics (CPMD). Developed in 1985 by Roberto Car and Michele Parinello, CPMD applies classical Newtonian principles to model nuclei and DFT principles to model electronic structure.

In the early 1990s, when CPMD was first used, computing capability limited the system being modeled to 32 water molecules and 1 to 2 picoseconds (a picosecond is 10^{-12} seconds). These size and time scales provided insufficient resolution for studying properties that arise from statistically rare interactions. With Thunder's capabilities,



In liquid and solid water, hydrogen (blue) and oxygen (red) molecules form so-called hydrogen bonds between the positive hydrogen atoms (δ+) and negative oxygen atoms (δ–). This bonding results in a relatively strong tetrahedral structure.



Livermore chemists Christopher Mundy (left) and Will Kuo view a simulation of water molecules.

the Livermore team can follow the trajectories of 64 water molecules for more than 10 picoseconds or 216 molecules for about 5 picoseconds.

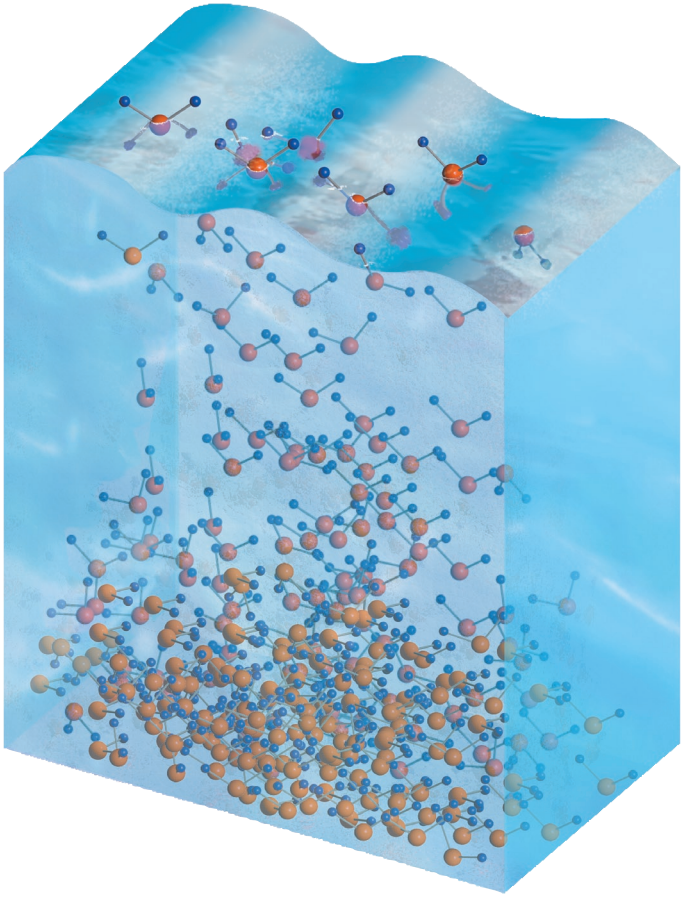
Mundy's team used CPMD and its successor, CP2K, to model the liquid–vapor coexistence curve in water's phase diagram. A coexistence curve is the boundary that separates two phases in equilibrium, such as the liquid and vapor phases. The model produces a phase diagram—a map showing the regions of pressure, volume, and temperature over which various phases are thermodynamically stable. Until now, no thermodynamic characterization of water could be obtained from first-principles methodologies.

Computing coexistence curves from first principles is important to physical chemistry research. "The phase diagram is central to thermodynamics," says Mundy. "Only by understanding thermodynamic properties can we properly compare experiments to theory and simulation."

First-principles calculations also provide a means for exploring the properties of water under conditions that are difficult or impossible to attain experimentally. "Having the capability to predict the thermodynamics of water will help us develop more accurate quantum mechanical models," says Mundy. "Once we can demonstrate that our codes accurately model the chemical and physical changes that occur in water, we can use them to fully characterize other complex molecules."

In the water simulations, Mundy's team ran calculations of 64 molecules at 323, 373, 423, 473, and 523 kelvins. Every simulation required 500 cycles. Each of those cycles ran for about 4 hours and used 192 of Thunder's 4,096 processors. The team then calculated averages from 200 production cycles. The results were in agreement with experiments, yielding two coexisting phases between 323 and 523 kelvins.

Mundy cautions that, to date, no model of water has been universally accepted. However, he says, "Our code is the first to predict the liquid–vapor coexistence curve using interaction potentials based on density functional theory. That's an important success that supports the Laboratory's national security mission. Many of the chemicals we want to study at Livermore are too hazardous to be tested experimentally. If our codes and models can fully characterize a fluid as complicated as water, we are hopeful that they can be used in Livermore's national security research. We need to better understand the physical and chemical properties of chemical warfare agents that might be used against the U.S. and develop technologies to protect the nation from their use."



The liquid–air interface of water has an abundance of molecules whose hydrogen atoms are oriented into the air. The phenomenon, known as surface relaxation, may increase the reactivity of molecules in this region of water.

Water's Behavior at the Surface

First-principles simulations also provide a virtual laboratory, allowing researchers to better examine how the structure of water changes at the air–liquid interface. Understanding the thermodynamic properties at the interface of bulk liquid and air is crucial to controlling chemical reactions in various applications, from biology to atmospheric science to homeland security.

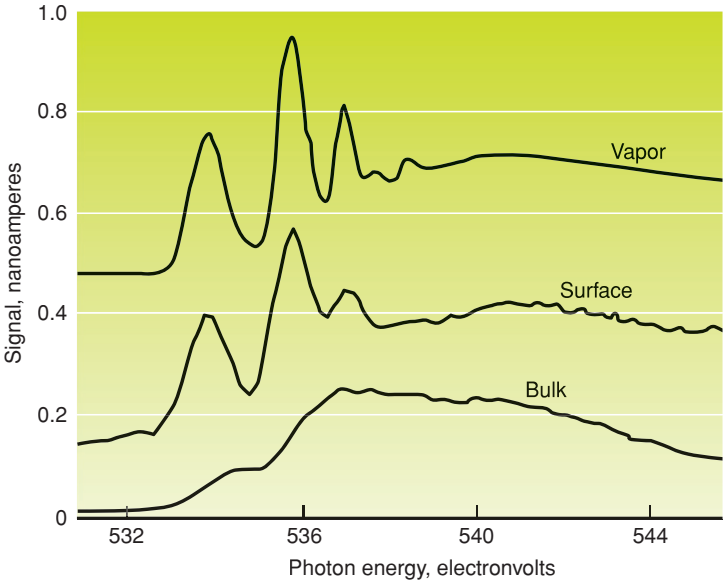
For example, scientists have long pondered the orientation of water molecules at the surface of liquid water. They have observed that water's density decreases as it approaches the liquid–vapor interface. The phenomenon, known as surface relaxation, could increase the reactivity of molecules in this interfacial region. Scientists previously believed the interfacial region had an abundance of water molecules whose hydrogen atoms "dangled" or were oriented toward the interface as so-called single donors.

A research collaboration involving Lawrence Livermore and Lawrence Berkeley national laboratories and the University of California at Berkeley provided the first experimental evidence that both hydrogens in a molecule were oriented out of the liquid. (See *S&TR*, November 2001, pp. 20–23.) This team developed a method using extended x-ray absorption fine structure (EXAFS) and near-edge x-ray absorption fine structure (NEXAFS) to probe the water molecule's electronic structure. Previously, x-ray techniques had difficulty characterizing the molecular-scale structure of liquids at interfaces, particularly for liquids containing hydrogen atoms. Another problem was that to perform x-ray spectroscopy, the sample had to be in a vacuum, so the liquid had to be placed behind a barrier. The barrier would interact with the surface of the liquid and absorb most of the x-ray signal.

To overcome these problems, the team replaced the barrier with liquid microjet technology in experiments conducted at Lawrence Berkeley's Advanced Light Source. Using this technology, the team made the first definitive EXAFS measurement on hydrogen and determined that the covalent oxygen–hydrogen bond length in water vapor is 0.095 ± 0.003 nanometer. This research showed that hydrogen bonds could be directly detected in water, paving the way for future studies of intermolecular hydrogen bonds.

In another experiment, NEXAFS spectra obtained for the water surface were intermediate between the spectra for water's bulk and vapor phases. These results indicated that the hydrogen atoms in a large fraction of the water molecules at the interface are not hydrogen-bonded to other molecules. Therefore, they must be oriented outward toward the interface.

Capturing these surface phenomena in theoretical models is more complicated than simulating water in bulk. Livermore chemist Will Kuo explains, "For one thing, we need many more molecules in the system than we do for simulations of bulk water because at the interface, we are studying particles, such as those released in ocean spray. Therefore, we must account for both interfacial and bulk properties within a single simulation."



Near-edge x-ray absorption fine structure spectra show the electronic structure of water in vapor form, at the surface of its liquid form, and in its bulk form.

To simulate a circular area about 10 nanometers in diameter on the surface of a water droplet, researchers need 216 water molecules—a model size that is three to four times larger than current first-principles MD models of bulk liquid water. Calculations with the CPMD code confirmed that the distance between oxygen molecules increases near the interface, which indicates surface relaxation and an increased potential for chemical reactions relative to bulk water. Kuo says, "The states with the highest energy, which are most likely to be involved in chemical reactions, are clearly located at the surface."

Mundy's team is encouraged by the results, not only for the information they provide about water but also because the methods can be applied to other molecules. "Once we establish the methods to simulate the interface for a system, we can look at any interface to see how the molecules will interact," says Kuo. "The techniques can be used in various applications, from studying environmental toxins to biothreats to biological systems."

Water in Extreme Conditions

Livermore researchers are also studying the dynamic properties of water under extreme conditions, where water is even more reactive. In one study, Laboratory chemists Larry Fried and Nir Goldman simulated the theoretically predicted superionic phase of water. In this phase, oxygen atoms form a lattice structure, but hydrogen atoms diffuse freely. The predicted superionic phase of water is unusual because it involves elements that form strong covalent bonds under ambient conditions. It is thus a striking example of how extreme pressure can disrupt covalent interactions.

Research indicates that the superionic phase of water could exist in giant planets such as Neptune and Uranus. In fact, scientists speculate that the magnetic field observed emanating from these planets may involve superionic water in the planets' interiors. Water is a highly reactive solid under these conditions. Inside a giant ice planet, superionic water would be hard as steel and would glow yellow at a temperature of more than 2,000 kelvins.

To re-create the extreme conditions inside these planets, Livermore researchers Alex Goncharov, Joe Zaug, and Jonathan Crowhurst compressed samples of ice and

liquid water in a laser-heated diamond anvil cell to pressures between 5 and 56 gigapascals and temperatures between 300 and 1,500 kelvins. Raman spectroscopy indicated a phase transition as temperature and pressure increased.

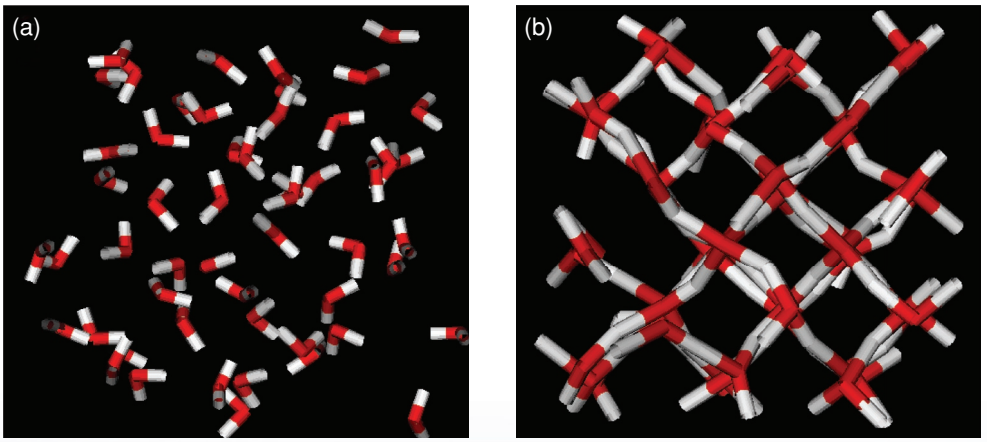
Fried and Goldman then ran the CPMD code on Thunder to simulate the same conditions, modeling a system with 54 water molecules for 5 to 10 picoseconds. In the simulations, they looked at properties such as bond lifetimes, the speed of proton diffusion through the system, and the chemical species present.

Their results explained the phase transition reflected in the Raman spectra. Above 47 gigapascals and 1,000 kelvins, the molecules transition to water's superionic phase. The simulations further showed that from 40 to 70 gigapascals and 1,000 to 2,000 kelvins, water consists of very short-lived molecules. Above 75 gigapascals and 2,000 kelvins, the water molecules are too short-lived to even be considered true molecules. Goldman says, "In this phase, the oxygen atoms form a lattice surrounded by a sea of mobile hydrogen atoms."

The superionic phase of water is important not only to planetary science but also to geosciences, fundamental chemistry, and weapons research. For example, Livermore researchers use computer codes to model detonation processes, which occur at similar conditions to those in planetary interiors. Goldman says, "The superionic phase could possibly result from a detonation process, however short-lived the phase would be."

Because water is involved in nearly every aspect of life, scientists want to completely understand the thermodynamic properties of its many phases. Equipped with the power of Thunder and new algorithms using first principles, Livermore researchers are revealing the secrets of this ubiquitous substance.

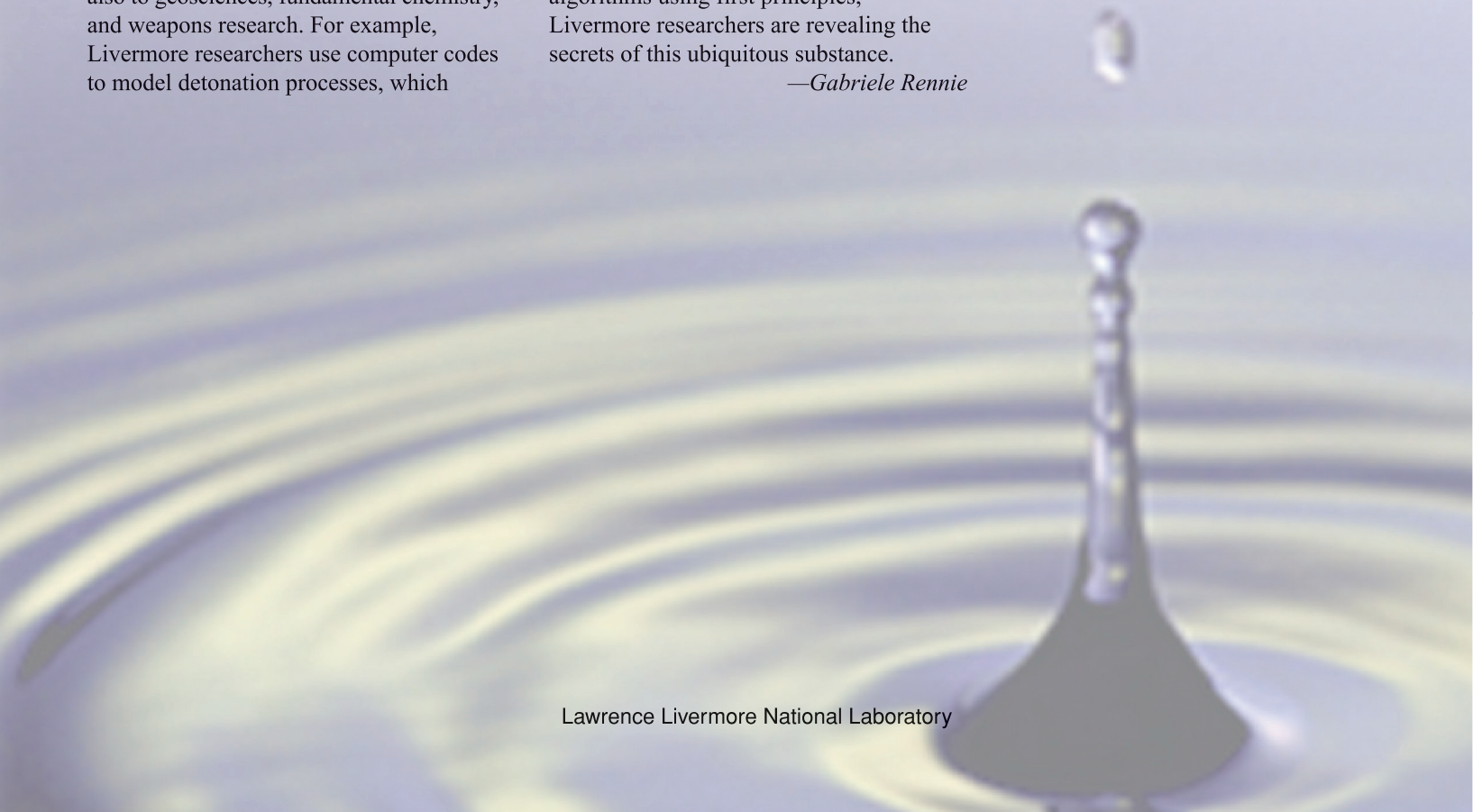
—Gabriele Rennie



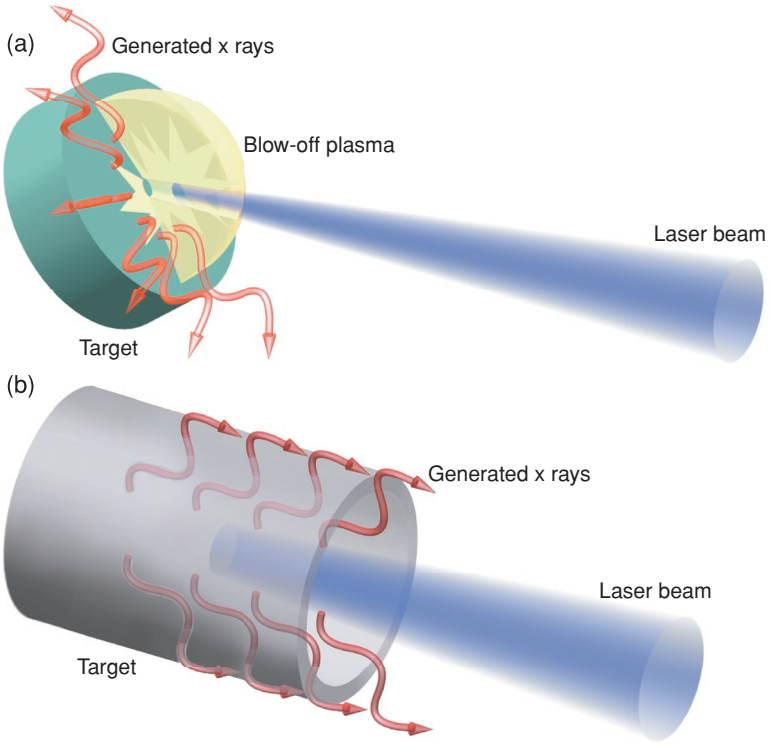
(a) At room temperature and atmospheric conditions, hydrogen (H) and oxygen (O) atoms in water exist predominantly as traditional H_2O molecules. (b) At 2,000 kelvins and a million times atmospheric pressure, the atoms begin to cluster, and water is in a superionic phase.

Key Words: Car-Parinello molecular dynamics (CPMD) code, classical molecular dynamics, density functional theory (DFT), first-principles molecular dynamics, hydrogen bonds, superionic phase, Thunder, water research.

For further information contact Christopher Mundy (925) 422-9571 (mundy2@llnl.gov).



Lightweight Target Generates Bright, Energetic X Rays



(a) In solid targets, the laser energy is deposited far from the emitting region of the target and in the plasma that is blown off. (b) In underdense targets, the laser beam deposits its energy volumetrically (as a whole), and x-ray emitting atoms are ionized supersonically by a laser bleaching wave.

RADIOGRAPHY with x rays is a long-established method to see inside objects, from human limbs to weapon parts. Livermore scientists have a continuing need for powerful x rays for such applications as backlighting, or illuminating, inertial confinement fusion (ICF) experiments and imaging still or exploding materials for the nation's Stockpile Stewardship Program.

X-radiography is one of the prime diagnostics for ICF experiments because it captures the fine detail needed to determine what happens to nearly microscopic targets when they are compressed by laser light. For example, Livermore scientists participating in the National Ignition Facility's (NIF's) 18-month-long Early Light experimental campaign, which ended in 2004, used x rays to examine hydrodynamic instabilities in jets of plasma. In these experiments, one laser beam irradiated a solid target of titanium, causing it to form a high-temperature plasma that generated x rays of about 4.65 kiloelectronvolts (keV). These x rays backlit a jet of plasma formed when two other laser beams hit a plastic ablator and sent a shock to an aluminum washer.

Livermore physicist Kevin Fournier of the Physics and Advanced Technologies Directorate leads a team that is working to increase the efficiency of converting laser energy into x rays so the resulting images provide more information about the object being illuminated. The main characteristics of x-ray sources are energy and brightness. "As experimental targets get larger and as compression of the targets increases, the backlighter sources must be brighter and more energetic," says Fournier. The more energetic the x rays, the further they penetrate an object. The brighter the source—that is, the more photons it has—the clearer the image.

Historically, researchers have used solid targets such as thin metal foils to generate x rays. However, when photon energies are greater than a few kiloelectronvolts, the conversion efficiency of solid targets is only a fraction of 1 percent. Solid targets have low efficiencies because much of the laser energy is deposited far from the target's x-ray emitting region, and the energy is carried by the relatively slow process of thermal conduction.

"The laser beam ablates material from the massive target, and that material moves away from the target's surface," says Fournier. "With a nanosecond pulse or longer, the laser interacts with the blow-off plasma rather than the remaining bulk sample. As a result, much of the laser's energy goes into the kinetic energy of the blow-off material, not into heating the bulk of the foil.

Heating Supersonically

Fournier worked with colleagues in Livermore's ICF Program, which is part of the NIF Programs Directorate, and in the Nonproliferation, Arms Control, and International Security (NAI) Directorate to test gas-filled, thin plastic bags as an alternative to the metal-foil targets. A gas bag is attractive because a laser beam can heat the gas molecules all at once, a process called volumetric heating. X rays are then produced by a so-called laser bleaching wave, in which the laser wave front passes through the gas supersonically.

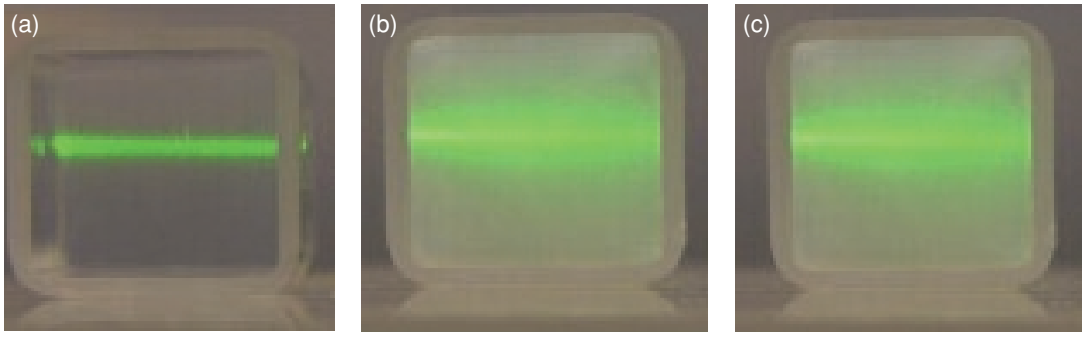
Materials that interact supersonically with a laser are said to be underdense. "Underdense targets allow the laser to propagate as

fast as possible to ionize all the gas molecules," says Fournier, "so they generate x rays more efficiently than solid targets can at comparable energies."

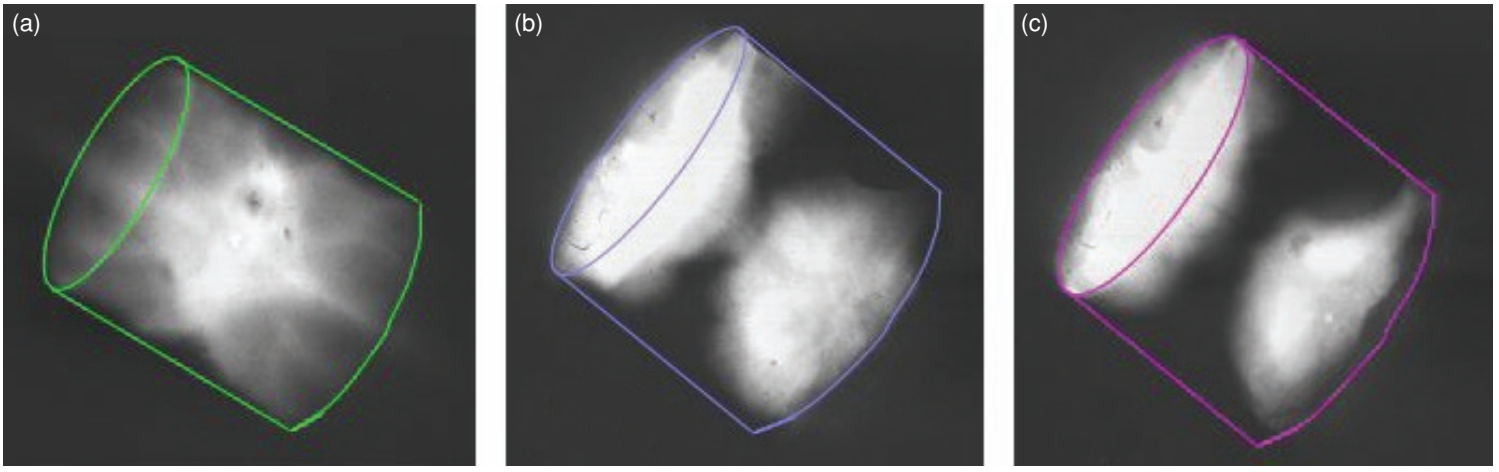
To examine the underdense targets, ICF physicists Christina Back and Carmen Constantin led experiments at the OMEGA laser facility at the University of Rochester's Laboratory for Laser Energetics. The team analyzed x rays produced by gas-filled bags struck simultaneously with 40 of OMEGA's 60 beams. When the bags were filled with krypton, the x rays generated ranged from 1 to 3 keV; with xenon, they ranged from 4 to 7 keV. Although the experiments were successful, gaseous targets have significant disadvantages. For example, gas can leak from the bag; bags can pop if filled too much; and only noble gases such as argon, krypton, and xenon can be used.

As an alternative, Fournier's team began testing aerogels—materials that, unlike gas-filled bags, are solid at room temperature and can be less dense than air. In addition, aerogels are robust materials and have a long shelf life. To develop aerogel targets, the team took advantage of the Laboratory's expertise in solgel chemistry, in which nanometer-sized particles form and then connect with one another to create a three-dimensional solid network in the aerogel. (See *S&TR*, May 2005, pp. 24–26.)

Fournier's team used the HELEN laser at the Atomic Weapons Establishment (AWE) in the United Kingdom to test aerogel targets of silicon dioxide (SiO_2) with a density of 1 milligram per cubic centimeter, about one-third the density of air. The team also used OMEGA to test aerogels with a density of 3.1 milligrams per cubic centimeter, about the same density of air. "Because the aerogel



Livermore scientists are developing lightweight aerogels to use as x-ray sources. Shown here in a 1-centimeter cube of Pyrex and illuminated by a laser pointer are (a) an aerogel doped with 20-percent germanium atoms, (b) an aerogel doped with 3-percent titanium atoms, and (c) a pure germanium dioxide aerogel, which contains 33-percent germanium atoms.



In experiments with the aerogel targets, the Livermore team placed samples in beryllium cylinders and heated them with laser beams. The aerogel samples had densities of (a) 3.1, (b) 4.8, and (c) 6.5 milligrams per cubic centimeter. The lowest density aerogel (a) is heated volumetrically and more uniformly than the other two (b, c).

density is so low, the laser sees the aerogel as a gas, not a solid, so it travels through the material at supersonic speeds," says Fournier.

By themselves, SiO_2 aerogels are poor x-ray radiators. In 2003 and 2004, Fournier worked with scientists from ICF, NAI, and the Chemistry and Materials Science Directorate to introduce a heavy element in a low-density aerogel. The researchers developed a technique to suspend titanium or zinc homogeneously in a SiO_2 aerogel. The titanium-doped SiO_2 aerogel generated 4.7-keV x rays, and the zinc-doped aerogel generated 9-keV x rays. "With this approach, we can theoretically tune the aerogel to produce the x-ray energy we need by substituting one dopant for another," says Fournier.

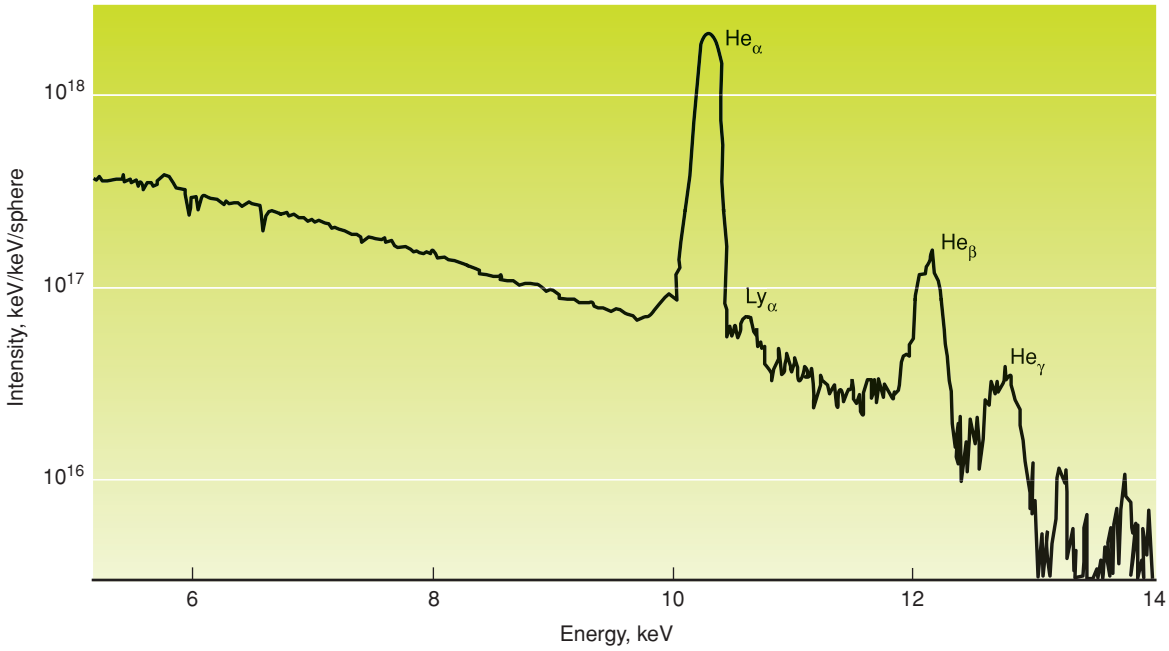
However, dopants affect how an aerogel forms. "If we make the dopant concentration too high, the aerogel can't support it, and the structure collapses," Fournier says. The team successfully introduced 3-percent titanium atoms into a SiO_2 aerogel with a density of about 3 milligrams per cubic centimeter. The titanium remained suspended after the aerogel solvent was removed and stayed uniformly dispersed. The doped aerogel was cast in cylindrical beryllium tubes that had walls 80 micrometers thick and were 2.2 millimeters long, with a 2-millimeter inner diameter.

For tests of the titanium-doped aerogels, the researchers used 40 OMEGA beams with 7 to 14 terawatts of power to illuminate the target's two cylindrical faces. The titanium within the aerogel target converted the blue laser light into 4.7-keV x rays with a conversion efficiency between 1 and 2 percent, performing three to four times better than a titanium foil target and with minimum scattering. The walls allowed 90 to 95 percent of the x rays to pass through, and researchers observed strongly supersonic propagation of the laser bleaching wave.

After the titanium-doped aerogel experiments, the team developed aerogels doped with germanium, which produces x rays at 10.3 keV. Germanium is a better dopant than titanium or zinc because it is chemically similar to silicon. Therefore, germanium atoms can be incorporated directly into the aerogel matrix, resulting in much higher concentrations. In March 2005, the team used OMEGA to successfully shoot germanium silicon dioxide ($[GeSi]O_2$) targets that contained 20-percent germanium atoms at densities of 4.8 and 6.5 milligrams per cubic centimeter. Again, the lower density doped-aerogel targets output significantly more 10.3-keV x rays than similarly irradiated germanium foils. By replacing the silicon atoms with germanium, the Livermore team also made a germanium dioxide (GeO_2) aerogel containing 33-percent germanium. Tests on the GeO_2 targets will be conducted in the near future.

Testing for X-Ray Effects

Another important application for doped aerogels is in radiation-effects testing. Military experts are interested in such testing to determine how x rays may affect different components of a ballistic



This x-ray spectrum shows results from radiation-effects tests using a germanium silicon dioxide target (keV = kiloelectronvolts). The three heliumlike lines (He_α, He_β, and He_γ) were generated by germanium ions with all but two electrons stripped by the laser energy. The Lyman-series (Ly) lines were produced by germanium ions with all but one electron stripped.

missile defense system. For example, an intercept of a nuclear-tipped missile might inadvertently trigger a high-altitude detonation. Such a detonation would generate x rays that might damage space- and Earth-based structures, optics, and electronics. "The radiation threats to a ballistic missile defense system create stringent hardness requirements because the systems must operate in especially stressful environments," says Fournier. "We need adequate simulators to validate the systems under these different scenarios.

Typically, scientists conduct radiation-effects tests using pulsed-power facilities such as the Z-pinch accelerator at Sandia National Laboratories in Albuquerque, New Mexico. Pulsed-power machines generate substantial debris, which increases costs. "Our radiation-effects testing with a laser produced fewer x rays than the Z-pinch but with no debris," says Fournier. "It's a complementary technology to pulsed-power testing."

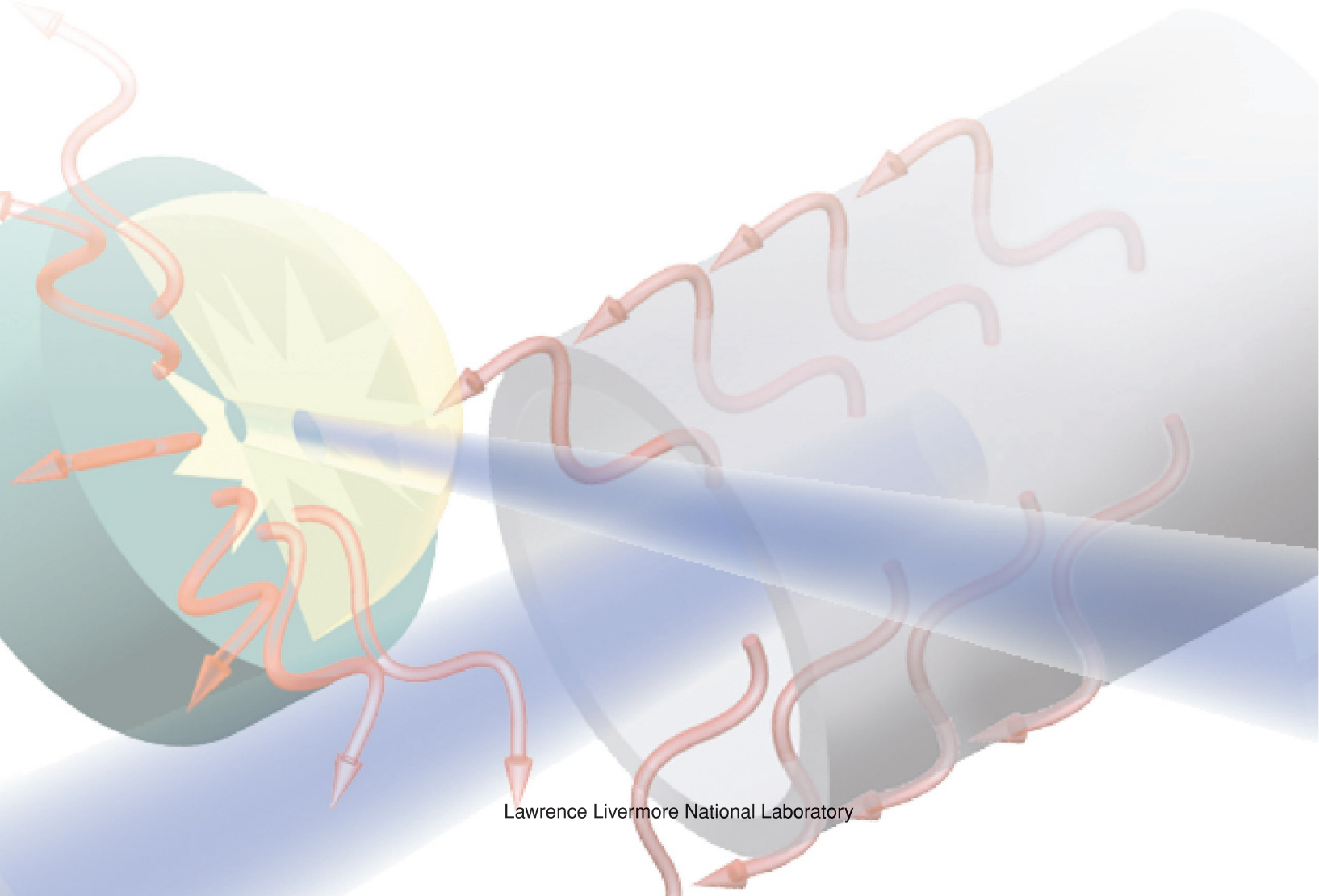
To determine the effectiveness of $(GeSi)O_2$ aerogel targets in radiation-effects tests, Fournier and his collaborators from Sandia, AWE, and Ktech Corporation used 40 OMEGA beams with nearly 20 terawatts of laser power. As part of the experiments, they placed different objects close to the doped aerogel and measured each object's response to the generated x rays. They obtained an average spectral energy of 7 keV and a 1- to 1.5-percent conversion efficiency, much better than in tests with solid targets that generate x rays in this energy range. The x rays produced thermomechanical shocks in aluminum plates and induced electrical currents in some test objects.

Much work remains to optimize the low-density, doped aerogels as efficient x-ray sources. In particular, the team looks forward to testing GeO_2 targets and wants to adjust the SiO_2 aerogel formation process to increase the percentage of titanium atoms. More experiments are planned in the quest to make x rays as bright and energetic as possible.

—Arnie Heller

Key Words: aerogels, doped aerogels, HELEN laser, inertial confinement fusion (ICF), National Ignition Facility (NIF), OMEGA laser, radiation-effects tests, x rays, Z-pinch accelerator.

For further information contact Kevin Fournier (925) 423-6129 (fournier2@llnl.gov).



Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Vapor-Deposited Porous Films for Energy Conversion

Alan F. Jankowski, Jeffrey P. Hayes, Jeffrey D. Morse
U.S. Patent 6,913,998 B2
July 5, 2005

Metallic films are grown with a spongelike morphology in the as-deposited condition using planar magnetron sputtering. The deposit's morphology is characterized by metallic continuity in three dimensions with continuous and open porosity on the submicrometer scale. The stabilization of the spongelike morphology is found over a limited range of the sputter-deposition parameters, that is, of working gas pressure and substrate temperature. This spongelike morphology is an extension of the features as generally represented in the classic zone models of growth for physical vapor deposits. Nickel coatings were deposited with working gas pressures up to 4 pascals and for substrate temperatures up to 1,000 kelvins. The morphology of the deposits is examined in plan and cross-sectional views with scanning electron microscopy. The parametric range of gas pressure and substrate temperature (relative to the absolute melt point) under which the spongelike metal deposits are produced appears universal for other metals, including gold, silver, and aluminum.

Magneto-Radar Detector and Method

Thomas E. McEwan
U.S. Patent 6,914,552 B1
July 5, 2005

A varying magnetic field excites slight vibrations in an object, and a radar sensor detects the vibrations at a harmonic of the excitation frequency. The synergy of the magnetic excitation and radar detection increases the detection range compared with the range of conventional magnetic metal detectors. The radar rejects background clutter by responding only to reflecting objects that are vibrating at a harmonic excitation field, thereby significantly improving detection reliability. In one arrangement, ultrawideband micropower impulse radar can be used to improve materials penetration and provide range information. The magneto-radar may be used to screen patients before they have magnetic resonance imaging, to detect land mines, and to find hidden treasures.

High Average Power Laser Gain Medium with Low Optical Distortion Using a Transverse Flowing Liquid Host

Brian J. Comaskey, Earl R. Ault, Thomas C. Kuklo
U.S. Patent 6,914,926 B2
July 5, 2005

A high-average-power, low-optical-distortion laser gain medium is based on a flowing liquid media. A diode laser pumping device with tailored irradiance excites the laser active atom, ion, or molecule within the liquid media. A laser active component of the liquid media exhibits energy storage times comparable to or longer than the liquid's thermal optical response time. A closed-loop system for mixing and circulating the lasing liquid into and out of the optical cavity includes a pump, a diffuser, and a heat exchanger. A liquid-flow gain cell includes flow straighteners and flow-channel compression.

Protein Crystallography Prescreen Kit

Brent W. Segelke, Heike I. Krupka, Bernhard Rupp
U.S. Patent 6,916,455 B2
July 12, 2005

A kit for prescreening protein concentration for crystallization includes multiple vials, reagents, and sample plates. The reagents and protein samples in solutions of varying concentrations are placed on the sample plates and incubated. After incubation, the plates are examined to determine which sample concentrations are too low and which are too high. The optimal concentrations for protein crystallization are selected and used.

System Using a Megawatt Class Millimeter Wave Source and a High-Power Rectenna to Beam Power to a Suspended Platform

Malcolm Caplan, Herbert W. Friedman
U.S. Patent 6,919,847 B2
July 19, 2005

A system for beaming power to a high-altitude platform is based on a high-power millimeter gyrotron source, optical transmission components, and a high-power receiving antenna—that is, a rectenna. This system can rectify received millimeter energy and convert it into usable electrical power.

Combined Advanced Finishing and UV Laser Conditioning Process for Producing Damage Resistant Optics

Joseph A. Menapace, John E. Peterson, Bernardino M. Penetrante, Philip E. Miller, Thomas G. Parham, Michael A. Nichols
U.S. Patent 6,920,765 B2
July 26, 2005

This finishing and ultraviolet (UV) conditioning method reduces the density of sites that are prone to laser-induced damage on the surface of fused silica optics. The resulting optics have far fewer catastrophic defects and can better resist optical deterioration when exposed to a high-power laser beam.

Fiber Optic Micro Accelerometer

Steve P. Swierkowski
U.S. Patent 6,921,894 B2
July 26, 2005

This accelerometer has a wafer with a proof mass integrated into it and an optical fiber. At least one spring member is connected to the proof mass. A Fabry–Perot cavity is formed by two partially reflective surfaces, one on the proof mass and another on the end of the optical fiber. The two surfaces, which form part of an optical detection system, are used to detect movement of the proof mass through the optical fiber.

Awards

Wei Cai, an assistant professor of mechanical engineering at Stanford University, was honored with a **2004 Presidential Early Career Award for Scientists and Engineers** (PECASE) for work he did while serving as an Ernest O. Lawrence Fellow at the Laboratory. The award was presented on June 13, 2005, by Presidential Science Adviser John Marburger in a White House ceremony. Cai was nominated for the award by the National Nuclear Security Administration's Office of Defense Programs in recognition of his role in developing Livermore's Parallel Dislocation Simulator, a supercomputing model that simulates the dynamics of crystals as they deform. Laboratory Director Michael Anastasio says Cai's computational theory of dislocation dynamics "after many years has been able to unify dislocation physics and crystal plasticity in a new computational discipline."

PECASE recognizes outstanding scientists and engineers who show exceptional potential for leadership at the frontiers of knowledge. The award is the highest honor bestowed by the U.S. government on scientists and engineers beginning their independent careers. Cai was one of 58 PECASE winners in 2004.

A team of researchers from Carnegie Mellon University, including Livermore researcher Bassem El-Dasher, received the **2005 Henry Marion Howe Medal** from the **American Society for Metals International**. The award recognized the team's paper "Statistically Representative Three-Dimensional Microstructures Based on Orthogonal Observation Sections," which appeared in *Metallurgical and Materials Transactions A*.

Established in 1923, the Henry Marion Howe Medal recognizes the authors of the best paper published in the journal for a given year and volume. In the 2005 award-winning paper, the researchers reported on a method they developed for modeling a polycrystalline microstructure in three dimensions using only two perpendicular sides of the material.

El-Dasher, who was completing graduate school at Carnegie Mellon at the time, is now a postdoctoral researcher for the Yucca Mountain Project in Livermore's Chemistry and Materials Science Directorate. Using techniques associated with his research at the university, he is characterizing the phases that can form over time in the outer barrier of nuclear waste packages.

Abstracts

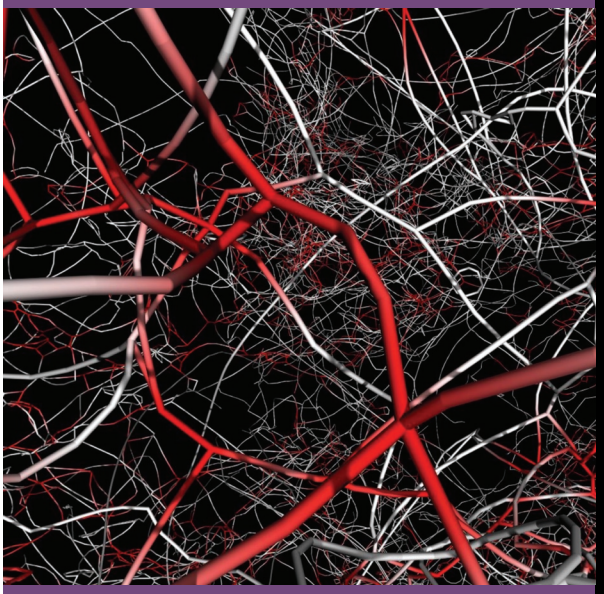
Revealing the Mysteries of Water

Livermore researchers are developing algorithms that use the power of the Laboratory's Thunder supercomputer to better understand water's unusual properties. Huge computational requirements and the limits of classical models previously prohibited scientists from obtaining a thermodynamic characterization of water, which is necessary for predicting an accurate phase diagram of this essential substance. First-principles simulations help researchers study the changes that occur in water's electronic structure at the interface between water's liquid and vapor phases, which affects its chemical reactivity. Laboratory researchers are also modeling the properties of water under extreme conditions, where it is even more reactive. They are using such simulations to study the predicted superionic phase of water, which may exist in giant planets such as Neptune and Uranus.

Contact:
Christopher Mundy (925) 422-9571 (mundy2@llnl.gov).

U.S. Government Printing Office: 2005/783-059-10012

Examining Metals Under Stress



A Livermore supercomputer code helps scientists simulate the changing properties of metals as they are deformed.

Also in November

• An automated, wide-field-of-view telescope promises to change astronomy forever.

• A Laboratory team is examining whether graphics processing units—the processors at the heart of the electronic gaming industry—can be adapted for national security applications.

• New calculations performed by Livermore physicists improve the accuracy of plasma density measurements using x-ray interferometry.

Coming Next Month

University of California
Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551