Science & Technology Review

March 2001

U.S. Department of Energy's
Lawrence Livermore
National Laboratory

R&D in the Superblock

Also in this issue:

- **Challenges of Computer Simulation**
- **Plutonium at the Atomic Level**
- **Lasers Strengthen Metals**

About the Cover

The area of Lawrence Livermore known as the Superblock is off limits except to those specially authorized to work within its secure perimeter. That's because research on plutonium, uranium, and tritium is occurring inside, requiring enforcement of the highest levels of safeguards and security. The missions: constantly improving the means of assuring the safety and reliability of the U.S. nuclear stockpile, and finding safe ways to dispose of surplus plutonium. The article beginning on p. 4 describes work in the Superblock and the rules and procedures that are followed for worker safety and accountability.

Cover photos by Michael Anthony

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy. At Livermore, we focus science and technology on assuring 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.

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Lawrence Livermore National Laboratory

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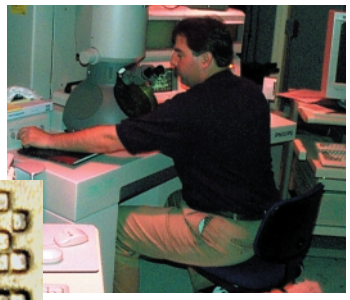

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Lab scientists revoke status of space object

A space object found near the Big Dipper, formerly thought to be a galaxy, was stripped of its status as the "most distant object known" by Laboratory astrophysicists Wil Van Breugel and Wim De Vries and colleagues from several universities and observatories. They published their findings in the November 30, 2000, issue of *Science*, showing that the initial distance estimate for the object, also known as STIS 123627+621755, was not correct. In fact, Van Breugel says that "It is even optimistic to say it is a galaxy—it could be a star in our own galaxy."

A group at the State University of New York at Stony Brook earlier had reported observations of this object using the National Aeronautics and Space Administration's Hubble Space Telescope. Based on the extremely red colors of the object and a single emission line in its spectrum, thought to be hydrogen, they had deduced the object was a galaxy approximately 12.5 billion light years away. If it were a very distant galaxy, it should essentially be invisible in the optical wavelengths and relatively bright at the near-infrared.

Contrary images were obtained by the Laboratory astrophysicists and their collaborators. Using the Keck telescopes in Hawaii to take their own images of deep space, they detected the object in optical light at a level 100 times brighter than expected and did not find it visible in the infrared. These results meant that the emission line, thought to be based on hydrogen gas, is more likely to be based on oxygen. Accordingly, the object's distance should be revised to a much closer 9.8 billion light years, and its classification to that of a small dwarf galaxy, similar to Earth's neighboring Magellanic Clouds visible from the Southern Hemisphere.

With STIS 123627+621755 no longer the most distant object, the title apparently belongs to a quasar, an active black hole that is 12.4 billion light years away. And the most distant galaxy would be one first observed by Livermore researchers in December 1998, designated as TN J0924-2201.

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Maglev technology may be used for urban transit

Livermore senior scientist Richard Post is working with a General Atomics–led team investigating the use of magnetically levitated (maglev) trains in urban settings. Post's Inductrack technology is one of the levitation techniques being evaluated for such trains. Inductrack is based on a system of magnets called the Halbach array, which produces a magnetic field underneath the train to induce strong currents in circuits on the track. Those currents repel the magnets, thereby creating a levitation effect (see *S&TR*, June 1998, pp. 20–22).

The transit project is a comprehensive study of propulsion and levitation technologies for low-speed, maglev systems. It is being performed under a contract from the Department of Transportation's Federal Transit Administration. On the team, besides Lawrence Livermore, are Carnegie Mellon University and Booz Allen & Hamilton, Inc., among others.

The information gathered in the study is to assist in technology choices and decisions for siting urban maglev systems anywhere in the U.S. A pilot program is being proposed for Pittsburgh, Pennsylvania, which, with its challenging terrain and established infrastructure, is a good place to prove the workability of such a system. The proposed Pittsburgh Airborne Shuttle System, or PASS, would run 10 miles through the city to connect Carnegie Mellon University, hospitals, shopping centers, and the downtown area.

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Smart Probe detects breast tumors instantly

At selected sites in northern California this spring, human studies will begin on a device that promises to provide early and accurate detection of breast cancer. A collaboration of Lawrence Livermore and San Jose–based BioLuminate, Inc., has developed the Smart Probe, a tool that can detect malignancies in a minimally invasive way and approach the accuracy of surgical biopsies. It provides several specific measurements of known cancer indicators in real time, thereby improving diagnosis and treatment.

The Smart Probe device is smaller than a needle used in routine blood tests. It is inserted into breast tissue after an initial screening indicates a suspicious area. Sensors at its tip measure optical, electrical, and chemical properties that are known to differ between healthy and cancerous tissue. The probe can detect multiple (five to seven) known indicators of breast cancer.

From the moment the probe is inserted into tissue, the sensors begin gathering information that a computer program then compares against known, archived parameters that indicate the presence or absence of cancer. The results are instantly displayed on the computer screen.

"The key technology and experience that Lawrence Livermore has to offer will allow the Smart Probe to be much smaller than first conceived and acquire data more accurately," said Luiz Da Silva, Livermore's associate program leader for Medical Technology and primary investigator for the device.

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Safety and Security Are Enhanced by Understanding Plutonium

UNDER the Department of Energy's Stockpile Stewardship Program, Lawrence Livermore National Laboratory is working on this crucial mission: assuring the safety and reliability of the nation's nuclear weapons stockpile without underground nuclear testing. A critical task in this scientific endeavor is to determine the behavior of materials in the stockpile, in particular the behavior of plutonium.

Plutonium is a comparatively stable material in weapons; however, its properties are among the most complex of all the elements. Experiments on plutonium have revealed its unusual ground-state structure; seven distinct crystallographic phases; dimensional changes with temperature, pressure, and impurity content; pyrophoricity; a multitude of oxidation states; and a highly anomalous resistivity. These curious behaviors make plutonium the most interesting element in the periodic table.

One major accomplishment of the Stockpile Stewardship Program is a greatly improved understanding of plutonium's many unusual properties. The understanding of how plutonium ages and how that aging affects the performance of a stockpiled weapon is important. With it, we can better develop schedules for the remanufacture of plutonium parts so they are available if and when they are needed. Long lead times are required because of the limited capacity in today's DOE weapons complex for plutonium operations.

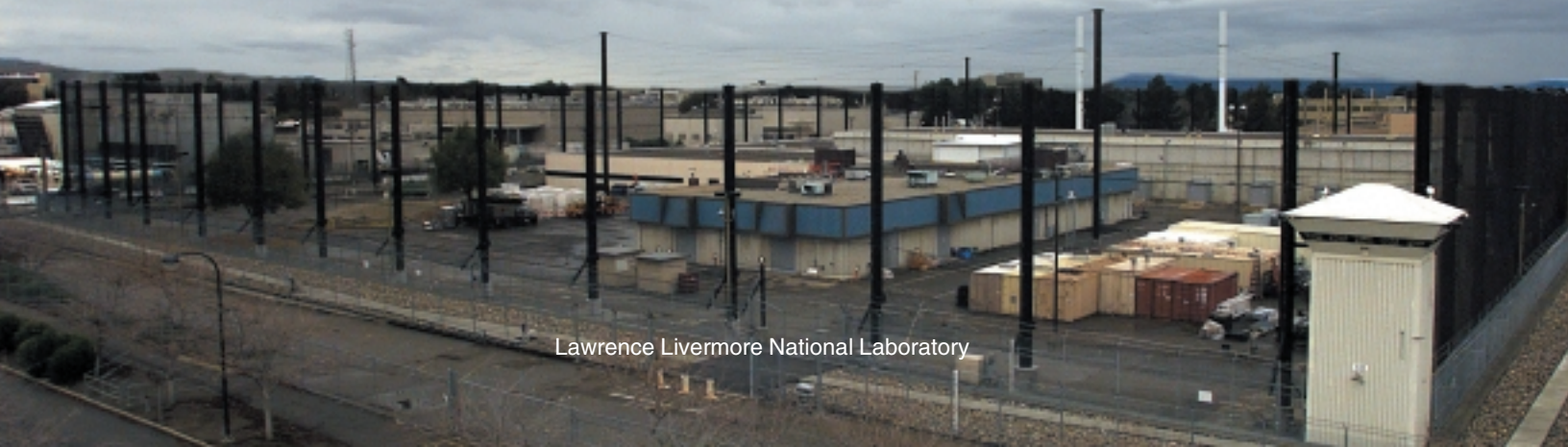
Inside Livermore's Superblock area is one of only two centers of plutonium expertise for stockpile stewardship science and technology in the U.S. The Laboratory will play an essential role over the next decade in preserving national competence in plutonium-related issues, material processing, advanced production technologies, enhanced surveillance, and material disposition. The article beginning on p. 4 describes the work being performed in the Superblock.

While nuclear testing was crucial for developing the stockpile, the integral nature of the test results could obscure important details. To study the subtleties of plutonium, Laboratory researchers use several scientific approaches. They are combining advances in theoretical modeling with many new nonnuclear research tools, now technically feasible and available because of investments by the Stockpile Stewardship Program. These tools include laboratory experiments to study the microstructure of plutonium, subcritical experiments at the Nevada Test Site to investigate the properties of plutonium shocked and accelerated by high explosives, and computer simulations of plutonium at the molecular and atomic scales. Through a combined theoretical, experimental, and computational approach, Laboratory scientists are solving a number of longstanding unknowns about weapon performance that arose from and remained unresolved through past nuclear testing.

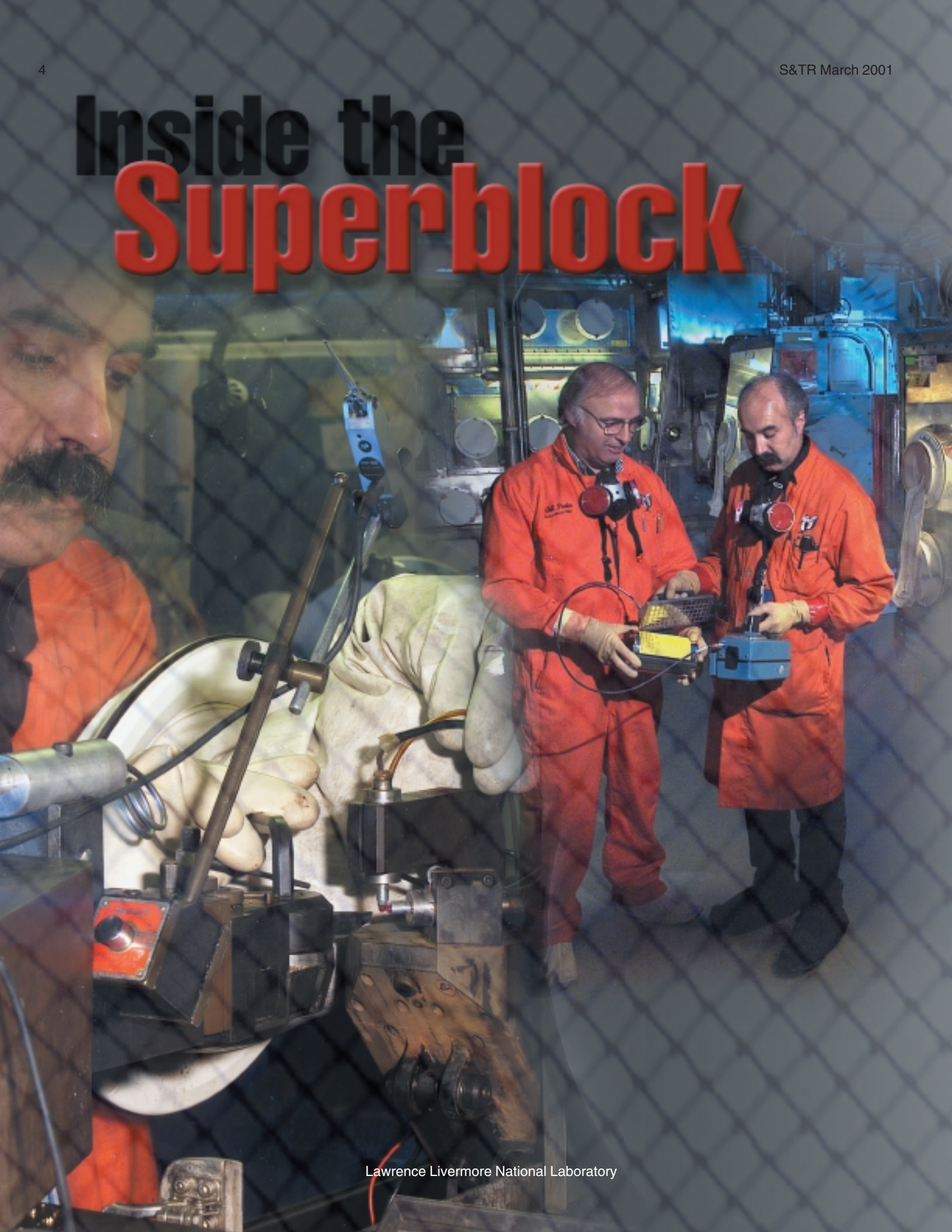
Plutonium aging is examined by fabricating new plutonium metallic samples and comparing them against samples cut from weapons stockpiled over several decades. The samples are subjected to dimensional inspection, surface analysis, tensile testing, mass spectroscopic analysis, transmission electron microscopy, and other tests to establish baselines for plutonium behavior. Livermore scientists have also devised a method for accelerating the aging of plutonium to learn more about how its properties change in weapons over time.

In the Superblock, Livermore is developing modern technologies to provide preproduction fabrication support, should this need ever arise, and also to serve as backup to the Los Alamos plutonium facilities, should they face a problem in their stockpile stewardship activities. But over and above meeting all their many stockpile stewardship responsibilities, Superblock personnel observe rules and procedures that assure the safety, security, and protection of those who work there and elsewhere at the Livermore site and who live in the surrounding community.

■ Michael Anastasio is Associate Director, Defense and Nuclear Technologies.



Inside the Superblock



Take a look behind the fences that surround Livermore's Superblock, where scientists are studying plutonium.

WELCOME to Lawrence Livermore's Superblock, home to one of just two defense plutonium research and development facilities in the U.S. Here, behind fences, guards, and ultrathick walls, scientists are developing ways to dispose of plutonium left over from the Cold War arms buildup. They are researching what happens to plutonium's physical properties over time, important knowledge in light of our aging stockpile of nuclear weapons. Technicians are machining parts for subcritical tests that help assure the safety and reliability of our nuclear stockpile. To a lesser extent, scientists and technicians in the Superblock also work with enriched uranium and tritium—a radioactive form of hydrogen.

To say that they work carefully is to put it mildly. They know what plutonium can do. One plutonium isotope, plutonium-239, releases huge amounts of energy when split (fissioned). A quick release of this energy drives a nuclear weapon. A slow, controlled release is what powers a nuclear reactor. The controlled release of another one of plutonium's isotopes can power a heart pacemaker or a deep space probe.

Only small quantities of any fissionable material can be together in one place in the Superblock at any time. If enough material is in the right configuration to form the critical mass needed to sustain a fission chain reaction, a criticality incident results. Joe Sefcik, leader of Livermore's Nuclear Materials Technology Program, which manages the Superblock, is pleased to note, "In our years of working with plutonium and other fissile materials, there has never been a criticality incident in the Superblock. We currently have one of the most robust criticality safety programs in the DOE complex."

The Department of Energy rules and regulations that govern operation of the Superblock are similar to those used by the Nuclear Regulatory Commission for nuclear reactors. Activities in the Superblock also come under the scrutiny of the Defense Nuclear Facilities Safety Board, an independent agency chartered by Congress and appointed by the U.S. president. It is charged with providing safety oversight of the DOE's defense nuclear facilities.

A safety analysis report has been developed for each facility in the Superblock, and all are updated annually. Worker safety during daily operations is key. In addition, a multitude of systems provides protection from fire and any other event that might threaten the public. The Superblock is a very safe place to work.

Security at the DOE facilities has been much in the news over the past year, and security at all DOE sites has been tightened as a result. Getting into the Superblock has always been a

challenge, even for those who work there every day. Entering the Radioactive Materials Area is even more complicated. Lists of allowed personnel, metal detectors, x-ray machines, and searches are the norm. Two fences around the Superblock with a "no man's land" in between, elaborate electronic security, a guard tower, and other precautions protect the Superblock from external threats.

A Look behind the Fences

The Superblock houses modern equipment for research and engineering testing of nuclear materials. The Plutonium Facility is the largest building in the complex and was the first to become operational, in 1961. As the place where plutonium expertise is developed, nurtured, and applied, it is the cornerstone of Livermore's plutonium capability. Research on highly enriched uranium also is performed here.

Engineering tests to simulate weapon environments are performed in the Hardened Engineering Test Building, which is a separate facility. That building also houses equipment for taking radiation measurements of plutonium- and uranium-containing assemblies. Two other buildings house the Tritium Facility, which will likely produce the tritium and deuterium targets for the National Ignition Facility, the 192-beam laser that will be an important experimental tool of DOE's Stockpile Stewardship Program to assure the safety and reliability of our nuclear stockpile.

Adjacent to the Superblock are a building for high-energy radiography of plutonium and plutonium-containing components and another for metallurgical characterization of small samples. Any work there, as well as the transport of parts and samples to and from the Superblock, is done under the watchful eye of armed security escorts and health and safety technicians.

In these facilities, the Nuclear Materials Technology Program has the capability to handle all phases of virtually any project related to plutonium or uranium. A typical project often begins with analysis, design, and perhaps some research. It proceeds through an in-depth analysis of any potential hazards that might result from the project and the development of appropriate measures to assure worker and public safety. Next comes the construction of necessary equipment, performance analysis, and demonstration of the project's product. A typical project often ends with deployment of a new process, sometimes throughout the DOE complex. Several projects discussed in this article typify this end-to-end capability.

Most work in the Superblock falls into one of two categories. It is related either to the stewardship of our nation's arsenal of nuclear weapons or to finding safe ways to dispose of surplus plutonium components from the Cold War. Physicist Booth Myers, deputy program leader for Programmatic Operations, oversees this work.

Behind the scenes, other activities support the ongoing work. Under the

Just How Dangerous Is Plutonium?

Most of the nuclear material in the Superblock is plutonium, a dense, gray metal. Yes, plutonium is dangerous. But it is by no means the world's most dangerous substance. Many common chemicals are at least as hazardous, if not more so.

Plutonium occurs naturally in trace quantities in uranium ore. But most plutonium is produced from irradiation of uranium in nuclear reactors. Plutonium is heavy, weighing 75 percent more than lead and nearly 20 times more than water. There are 18 different isotopes of plutonium, all of which are unstable and decay into other elements by emitting various types of radiation. Because of the radioactivity, a piece of plutonium is warm to the touch.

Plutonium-239 is an essential fuel for nuclear weapons and is the form of plutonium most often used at Livermore. When it decays, plutonium-239 emits a helium nucleus (two protons and two neutrons, also called an alpha particle) to become uranium-235, which then decays further, eventually into an isotope of lead. The alpha particle from plutonium-239 travels only a short distance before grabbing two electrons to become harmless helium. This range of the danger is just an inch or two in air. Alpha particles are easily shielded; they cannot penetrate a sheet of paper or even the thin dead layer of skin.

The danger from swallowing plutonium is not much greater than from other heavy metals such as lead or mercury. Very little plutonium is absorbed by the body. Most of it passes out in feces. In fact, accidentally swallowing a small amount of parathion, a widely used agricultural insecticide, would more likely result in death than ingesting a somewhat larger amount of plutonium.

The real danger from plutonium is from inhalation. If small particles of it or its oxide are inhaled into a person's lungs, they may become trapped there. Without any protective skin, the cells that line the lung can be damaged by the decaying plutonium, eventually resulting in lung cancer and perhaps death after many years. Inhaling chlorine gas would produce about the same effect.

Workers in the Superblock who handle plutonium are keenly aware of its hazards. Keeping it outside the body is the aim of the many health and safety rules that govern the handling of plutonium.

direction of engineer Alan Copeland, deputy program leader for Facility Operations, a staff of about 80 maintains the equipment and assures that all operations are carried out safely and securely. Health physicists, industrial hygienists, fire safety personnel, security professionals, and health and safety technicians are constantly reviewing procedures that control work in the Superblock. Any proposed new operation receives special attention. Detailed procedures that ensure safety and security are prepared before any new operation proceeds.

With the end of nuclear testing in 1992, most of the DOE's production facilities closed or had their operations cut back severely. The only other site in the DOE complex with facilities comparable to those in the Superblock is Los Alamos National Laboratory. The Nuclear Materials Technology Program is responsible for keeping the Plutonium Facility fully operational to ensure that work related to plutonium for the Stockpile Stewardship Program can proceed without interruption.

Safety First

Caution is always the watchword when working with or around fissile materials. A criticality incident, where a critical mass could produce a burst of radiation, would be the most serious safety problem for workers. A greater threat to the public would be a fire spreading contamination off the Laboratory site. As discussed in the box on p. 6, another danger from handling plutonium is breathing it. All manner of safety systems and work control procedures come together to protect workers in the Superblock's Radioactive Materials Area as well as the general public from any of these dangers. Considerable protection is also provided to prevent the theft of materials.

Depending on the specific work being done, there are 25 different sets of criticality controls to provide protection. Individual workers likely know four or five such controls that cover their authorized activities. Work controls cover handling of fissile material, industrial hazards, fire, and so on.

Virtually all handling of plutonium is done in a glovebox to protect workers from any airborne particles. The air pressure in the glovebox is slightly lower than the pressure in the room, which is lower than in the hall, and so on. This pressure control assures that the flow of air is always directed inward to contain and capture any plutonium that might escape the glovebox in an accident. A complex air handling system is needed that includes electrical power, fans, and a complete backup system. A filtration system prevents leakage of any potentially dangerous material into the atmosphere.

All fissile material must be accounted for. Following any operation that causes plutonium debris, such as cutting or machining, the waste crumbs are brushed into a tray and weighed. The weight for all material—both usable and residue—must be within a gram of the total weight prior to cutting. This system of weights and records, maintained by a dedicated computer network, verifies that all the Laboratory's plutonium can be accounted for at any time, day or night.

A two-person surveillance system is required when an operation involves more than a specified quantity of plutonium. The issue again is accountability. Two workers must together open the work room, and both must stay in the room, each within sight of the other at all times. If a visitor happens to be present, a fourth person must watch the visitor.

All Superblock workers must participate in the Laboratory's Personnel Security Assurance Program. It is aimed at assuring the highest levels of reliability and personal responsibility in all plutonium workers.

Implementation over the past year and a half of an integrated safety management system has increased attention to safety throughout the Laboratory. A similar program was put in place in the Superblock a full year ahead of the rest of the Laboratory, in the fall of 1998.

All of these procedures are only as good as the people implementing them. Says Copeland, "It takes a long time to get a skilled technician up and running in the Plutonium Facility. Acclimation and training take at least 12 to 18 months. At the same time, people tend to stay. We have very little turnover."

Machinist Bill Poulos, a trained fissile material handler, weighs a machined plutonium part in a glovebox in the Plutonium Facility's Radioactive Materials Area. He is using a certified balance that is part of the plutonium accountability system. Virtually all handling of plutonium is done in a glovebox such as this one.

Stewardship in Action

In the Superblock, work on stockpile stewardship includes nonnuclear testing of components of weapons that are now sitting in the stockpile (including fundamental physics and engineering experiments on plutonium) and investigating technologies for remanufacture of plutonium parts in nuclear weapons. Every year, the Livermore and Los Alamos national laboratories provide the technical basis for certification to the U.S. president that the nuclear weapons for which they are responsible are safe and reliable. Much of the research in the Superblock contributes to this annual process.

With no new weapons being designed to replace aging weapons in the stockpile, concern focuses on what is happening to existing weapons as they get older. Inside the Plutonium Facility, a "spiked" alloy of plutonium has been created that accelerates the metal's aging process.

Pyrochemist Karen Dodson leads the work on production of spiked plutonium, which incorporates more of the isotope plutonium-238 than would normally be found in weapons-grade plutonium, 7.5 percent rather than the typical 0.036 percent. Because plutonium-238 is more radioactive, the spiking process accelerates the formation of defects that occur within the metal during alpha decay of plutonium. The new alloy ages more quickly, on the equivalent of 16 years for every year of actual aging, which makes it perfect for experiments on plutonium decay. Information from experiments with the spiked alloy will be compared with and will supplement results generated from tests with naturally aged weapons material.

To produce the spiked alloy, plutonium-238 oxide is reduced to metal and combined with standard weapons-grade plutonium in molten salt. The metal is purified by electrorefining, and salt residues are filtered and/or scrubbed with calcium to recover all of the plutonium before disposal. The metal is then cast into "cookies" that are rolled, heat-treated, and machined to produce test samples for gas-gun experiments, tensile testing, examination by transmission electron microscopy, and other experiments (see "Plutonium Up Close . . . Way Close," pp. 23–25). Equipment for machining the samples was cold tested (that is, without plutonium) before actual machining of the spiked alloy began. This year, Dodson will be producing additional spiked plutonium alloys with varying amounts of plutonium-238.

Several steps in producing "cookies" of a spiked plutonium alloy are shown here, culminating in machinist Paul Benevento's work in a glovebox (photo at lower left). The spiked alloy has an increased percentage of the more radioactive plutonium-238, which accelerates the material's aging process. Experiments on aging plutonium are a critical part of Livermore's stewardship of the U.S. nuclear arsenal.

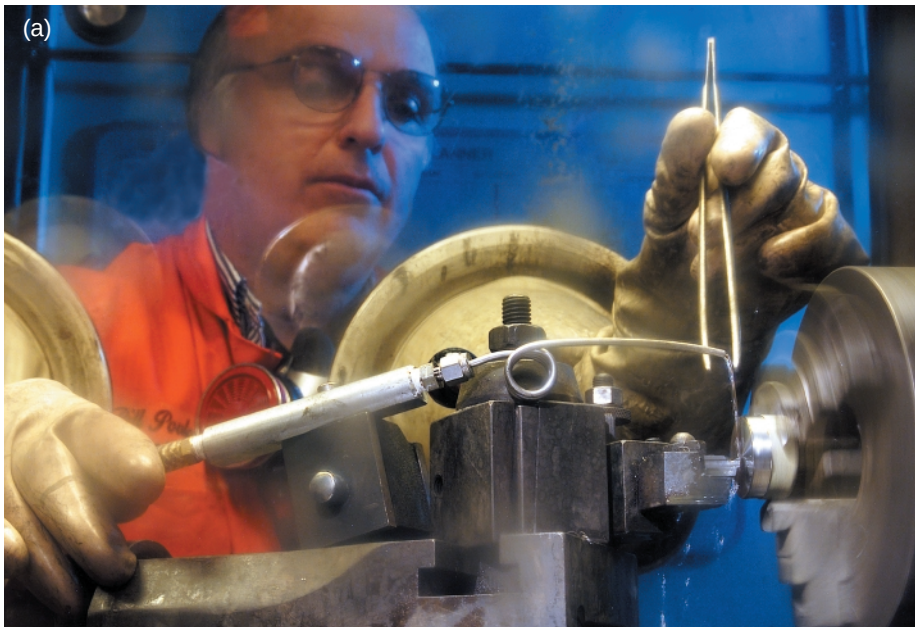
Subcritical tests of plutonium at the Nevada Test Site are another key feature of the DOE's Stockpile Stewardship Program. Subcritical experiments, which are tests that by design cannot create a fission chain reaction, provide a better understanding of the fundamental nature of plutonium and how aged plutonium affects the performance of a weapon (see *S&TR*, July/August 2000, pp. 4–11).

Engineer James Sevier oversees the production of plutonium samples in the Superblock for subcritical tests. Certified fissile material handlers cast a log of plutonium alloy and then slice it into disks that are machined and finished into the size and shape required for a particular test. The samples may also be heat-treated and put through a rolling mill to produce the grain structure needed. Says Sevier, "The resulting material looks and more or less behaves like weapons plutonium. The physicists who design a test must certify that the samples they have asked for do not contain enough material in the right geometry to go critical."

Plutonium test pieces are also used in experiments on the Los Alamos gas gun. And various alloys of plutonium, including spiked ones, will soon be used in Livermore's new, more powerful two-stage gas gun, JASPER (for Joint Actinides Shock Physics Experimental Research), at the Nevada Test Site (see *S&TR*, September 2000, pp. 12–19). The JASPER facility will be coming on line this year. Shock experiments help scientists determine the properties of materials at high pressures, temperatures, and strain rates.

Certifying a Weapon

Tests that shake, drop, heat, and cool samples of fissile materials take place inside the Superblock's Hardened Engineering Test Building. These tests are designed to duplicate as nearly as possible the likely environments for a weapon during its lifetime, known as its



(a) Bill Poulos machines a plutonium part to be used in an experiment. (b) Ed Thomas sets up a tool on a Moore T lathe in preparation for computerized machining of plutonium parts. (c) Dale Tumlin inspects the gold that has been deposited on a glass slide. The thickness of the gold is 1.5 micrometers. All of these technicians are trained fissile material handlers.

stockpile-to-target sequence. Such tests have been performed on weapons and their components since the early days of the nuclear weapons program. Mock high explosives and other carefully engineered materials stand in for many real substances to prevent potentially dangerous interactions with fissile materials.

Livermore engineers and technicians have performed several such tests as a service to Los Alamos. In 1999, Livermore vibration tested parts of Los Alamos's W76 weapon. In the spring of 2000, it shock tested part of the B61 bomb. This year, it is performing thermal and vibration tests of the W88 weapon. These tests at Livermore are a "critical step in the certification process," according to Sefcik.

Says Myers, "One version of the B61 bomb must penetrate the earth before it detonates, so it encounters severe shock. Our 4-meter-high drop test machine can simulate that tremendous shock." For this kind of test, mock high explosive is wrapped around a plutonium pit inside an aluminum case. The case has flanges that simulate the mounting to a warhead case. It is mounted to the test fixture, which in turn is mounted to the drop machine's carriage. When the test unit is dropped, the speed of its fall usually depends just on gravity. (Although in the testing of Los Alamos's B61, carefully arranged bungee cords pull the test fixture downward to create acceleration and velocities greater than those that could be achieved by gravity.) The unit comes down onto a chunk of steel that is suspended on hydraulic cylinders—to isolate the rest of the machine from the shock pulse. The steel is layered with felt to calibrate the shock pulse to known shock data for the test unit.

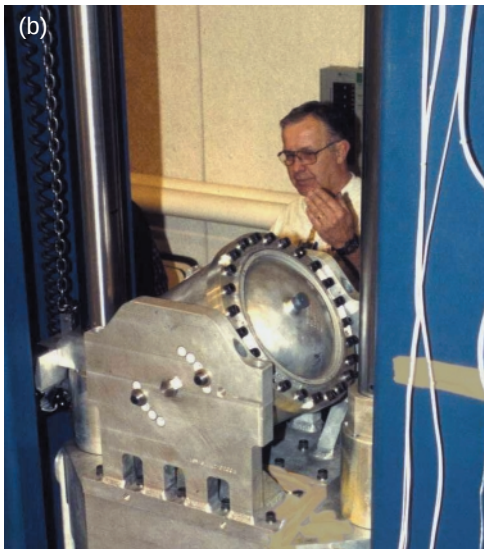
The test is performed just once with plutonium in the mock warhead, but practice runs assure that velocities, shock pulse, and other parameters are properly calibrated. The photos below show some activities of the calibration runs that preceded the shock test of the B61.

Before the shock test, the plutonium pit is radiographed. Afterward, the whole test assembly is radiographed to ensure there are no broken pieces. Then it is disassembled, and the pit is radiographed alone to see what changes, if any, occurred during the test. In the case of the B61, no change or damage resulted from the test. Says Alan Brooks, project engineer for these environmental tests, "Los Alamos's design work was indeed correct."

New Parts Needed

Some of the experimental work includes disassembly of a weapon to determine its continued safety and reliability. The plutonium pit is taken out for analysis and is often subjected to destructive testing. Because no new weapons are being produced, reassembly of the weapons may be required, and then a newly manufactured pit is needed.

The traditional method for manufacturing a pit includes casting a disk (blank) of plutonium, rolling and pressing it to the right size and overall shape, and machining it into its final shape. This was the process predominantly used at the Rocky Flats pit manufacturing plant in Colorado before it shut down in the early 1990s. While effective at producing parts, this method was expensive, generated considerable waste, and required a large amount of plutonium to be recycled in the plant. An alternative approach being developed in the Superblock is to cast the parts to their near-final shape in a precision mold, which avoids the rolling,



(a) Gerard Martinez of Los Alamos (left) and Richard Ring of Livermore remove the B61 test object from its shipping container. (b) The B61 test object is mounted on the carriage of the shock machine for a drop test. The shock test is part of the annual stockpile certification process.

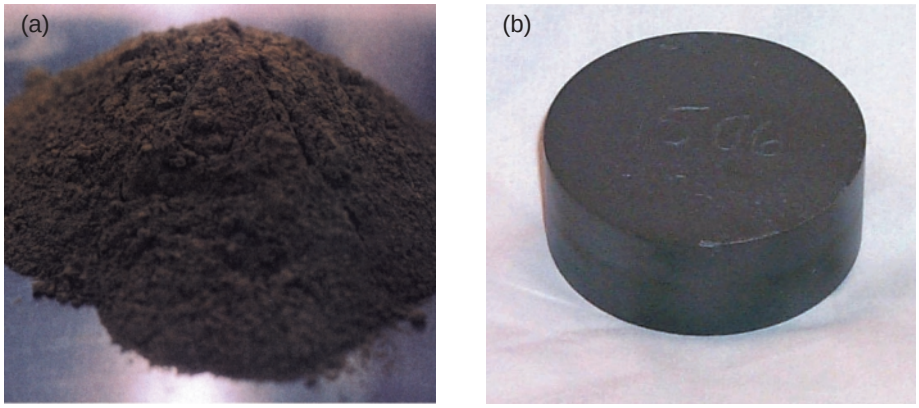
pressing, and extensive machining. This process also reduces waste generation in the machining process and thus the amount of plutonium that must be recycled.

Solutions for Surplus Plutonium

The other major facet of program work in the Superblock centers on disposal of surplus plutonium from dismantled U.S. nuclear weapons. Livermore researchers are continuing the development and demonstration of systems to bisect weapon pits, remove the plutonium, and convert the material into either plutonium oxide, which is suitable for disposal by immobilization, or into mixed oxide fuel for nuclear reactors (see *S&TR*, April 1997, pp. 4–13). The technology for plutonium oxide production will be transferred to DOE's Savannah River Site. As other DOE sites, such as Hanford, Rocky Flats, Livermore, and Los Alamos, process their surplus plutonium, they will ship it to the Savannah River plant where the oxide feed will be mixed with a ceramic material to produce inert, puck-shaped disks that immobilize the plutonium for long-term storage and, ultimately, underground disposal.

The Savannah River plant is expected to begin the immobilization effort late in this decade. In the meantime, a way is needed to store the oxide as well as any other excess plutonium metal from DOE sites. A method of "canning" plutonium has been developed by British Nuclear Fuels Limited, and Livermore is working to perfect it. Dodson is leading this effort.

In the method, processed plutonium oxides or metal are transferred into a "convenience can," which is itself sealed into an inner and then an outer can. Both inner and outer cans are laser welded. Says Dodson, "This canning process eliminates any organic materials that might react to produce unwanted gases in the package. In addition, the inner and outer cans are filled with helium that is used to check for any leaks." The laser welds must meet acceptance criteria established by the Savannah River Site, or the cans will not be allowed into storage. That qualification process was just completed earlier this year.



Livermore is developing the technology and the hardware to immobilize DOE's excess plutonium. (a) Plutonium oxide powder is blended into a ceramic material and then granulated, pressed, and baked to produce (b) ceramic "pucks" for long-term storage.

There are three configurations of the "convenience can" used for storing plutonium oxide and other excess plutonium metal. These three configurations are shown, from left, by the first stack of two cans, second can, and third can. Each convenience can will be crimp sealed or screw sealed and placed inside an inner can (fourth one from left), and it is then welded shut. The inner can is itself placed inside an outer can (fifth from left), which is also welded shut.

In another project, workers in the Superblock are recovering the plutonium from some weapon parts stored at Rocky Flats and destroying the shapes of the parts. The plutonium can then be processed and sent to Savannah River.

U.S. Needs Plutonium Facility

Livermore's Plutonium Facility and the Superblock in which it resides are one of the foundations of the DOE's research on plutonium. The National Nuclear Security Administration, the recently formed arm of the DOE for governing the national laboratories, has three missions: nonproliferation, stockpile stewardship, and meeting the Navy's needs for reactors. Livermore is home to active programs in two of these three missions. Says Sefcik, "The DOE's Stockpile Stewardship Program could not succeed without our Plutonium Facility and the research we do there. There is only one other plutonium R&D facility for defense programs in the country, at Los Alamos, and parts of it are not currently operating. So the experiments we do are key to certifying the weapons in the stockpile."

He continues, "The DOE also has to clean the plutonium out of Hanford, Rocky Flats, and other DOE sites housing a surplus of plutonium parts. We are taking the lead in research and development of technologies to dispose of the material. The Plutonium Facility and other buildings associated with it in and near the Superblock are essential to cleaning these sites up and preventing the material from falling into the wrong hands."

—Katie Walter

Key Words: fissile materials, material disposition, Plutonium Facility, plutonium immobilization, radiography, Stockpile Stewardship Program, subcritical tests, Tritium Facility.

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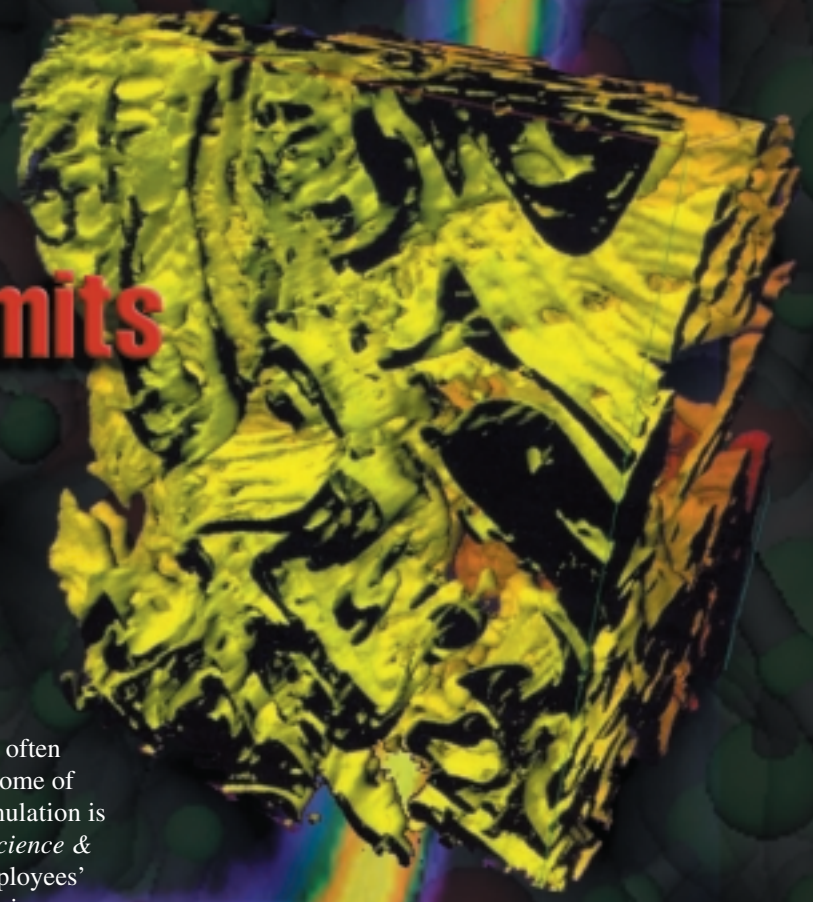
About the Scientist

JOSEPH A. SEFCIK is program leader for the Nuclear Materials Technology Program at Livermore. He is responsible for the research and development programs associated with special nuclear materials and for managing Livermore's Superblock complex. He received his B.S. in applied and engineering physics from Cornell University and his Ph.D. in nuclear engineering from the Massachusetts Institute of Technology. He joined the Laboratory in 1981 to work on issues in nuclear nonproliferation, export control, and strategic defense. Later, he participated in the design of thermonuclear devices shot at the Nevada Test Site and led one of the directed-energy weapons programs. With the moratorium on nuclear testing, he focused on applying Laboratory-developed defense technologies to commercial industry. Before his current assignment, he led the Advanced Design and Production Technologies (ADAPT) program to bring modern fabrication and integration technologies into the aging plants in the DOE complex. Sefcik is the recipient of two Department of Energy Awards of Excellence and shares an R&D 100 Award for the development of femtosecond laser materials processing. He is the author of numerous publications on nuclear nonproliferation, nuclear design, and directed-energy technology. His current focus is on nuclear facility safety and security.

Exploring the Fundamental Limits of Simulations



FROM aeronautical engineers designing passenger aircraft in virtual wind tunnels to molecular biologists designing anticancer drugs in a virtual laboratory, computer simulation is often the research tool of choice. At Lawrence Livermore, home to some of the most powerful supercomputers in existence, computer simulation is a growing part of every research effort. Indeed, the pages of *Science & Technology Review* are increasingly devoted to Laboratory employees' pioneering uses of simulation in fields as diverse as materials science, environmental remediation, and the safe stewardship of nuclear weapons.

But the increasing use of computer simulation has raised fundamental questions. Where is simulation taking science and engineering research? When, if ever, can simulation techniques replace experimental observation? Can scientists really describe "reality" with computer simulations?

Last October, some 60 of the nation's leading simulation experts gathered at Lawrence Livermore to try to answer these questions and explore ways to advance their craft. In discussions that ranged from the philosophy of science to the pitfalls of software, participants passionately cited the accomplishments and limitations of their rapidly evolving field (see boxes, pp. 14 and 17).

The workshop, called "Barriers to Predictive Simulation in Science and Engineering," was held at the University of California at Davis Department of Applied Science, a center of graduate research and training located adjacent to Lawrence Livermore. Laboratory physicist Giulia Galli Gygi, a workshop organizer, said the session was envisioned as a way for experts to explore the entire range of barriers to fully predictive simulations. "Although every discipline has its own simulation challenges, we wanted to bring together the best people in the different fields to look for areas where there were common challenges," she said.

Lawrence Livermore has been one of the leading simulation centers in the world since the 1950s. Laboratory computational biologist and workshop chair Mike Colvin notes, however, that simulation has become such an important tool for every industry and research field that Laboratory researchers have much to learn from other research centers. Consequently, they are seeking to strengthen their collaborations with colleagues nationwide. Colvin, who was a dynamic force behind this workshop, is at the forefront of such efforts.

Simulation experts from across the nation discover common barriers to modeling nature accurately.

Simulation Partners with Theory

Lawrence Livermore's Dave Cooper, associate director for Computation, told attendees that simulation has become a full partner with theory and experimentation. He pointed to the significant accomplishments of the Department of Energy's Accelerated Strategic Computing Initiative (ASCI), a vital element of its Stockpile Stewardship Program to assure the safety and reliability of the nation's nuclear weapons. Cooper said ASCI has demonstrated that high-resolution simulations of nuclear detonation can be performed efficiently on supercomputers using thousands of relatively simple microprocessors working in tandem.

He asked participants what would be required to make similarly revolutionary simulation advances in their disciplines. For example, he asked what barriers would need to fall to accurately predict the exact path of a hurricane.

Examples of Barriers to Simulation

- Not knowing the appropriate scientific questions to address with simulations.
- Not knowing the underlying equations to describe the phenomena of interest.
- Intrinsic limitations to computability.
- Inability to meaningfully analyze simulation data.
- Lack of experimental data to initialize or validate simulations.
- Inability to scale algorithms to increased model size and resolution.
- Limitations in the speed and efficiency of computer hardware.

Lawrence Livermore physicist Berni Alder, one of the founders of computer simulation, gave a personal perspective on the growth of the field. "There's too much emphasis on building new machines," said Alder, who did pioneering work in the 1950s using computers that could describe only 100 molecular collisions per hour. Alder's seminal simulations in the early 1960s on Lawrence Livermore's LARC (Livermore Advanced Research Computer, the supercomputer of its day) changed kinetic molecular theory, showing that simulations can significantly affect a scientific field.

Several speakers noted that experiment and theory must evolve together, with each needing the other. However, they described the challenge of comparing even closely related experiments and simulations. "There is not always an obvious relationship between the two—we don't understand all that is involved," said Galli Gygi. She said that setting up a good simulation is similar to setting up a good experiment in that "you have to ask the right questions."

Participants discussed the observation of famed British physicist Paul Dirac, one of the pioneers of quantum mechanics, that even if all of the relevant equations are known, a simulation is often impossible to conduct because it would require far too many supercomputers far too many years to complete. "The fact is," said Colvin, "to simulate a chemical or biological process, you can't simply throw a bunch of atoms together and try to use brute force computational approaches."

Multiscale Modeling

Instead of trying to describe a complex chemical or biological process entirely in terms of the underlying quantum mechanics equations, some simulations are broken into a hierarchy of size and time scales, each involving a different simulation method. Such multiscale modeling was discussed with considerable enthusiasm, although a number of major challenges remain. Under development at Lawrence Livermore (see *S&TR*, December 2000, pp. 4–11) and elsewhere, multiscale modeling was seen as essential because a "single numerical scheme is not feasible in materials and chemistry," according to Princeton University's Roberto Car.

"Multiscale is the only way to go," Car said, but integrating the different length and time scales represents a formidable barrier. As an example, he discussed the challenge of combining a simulation based on quantum mechanics with one based on classical physics. Lawrence Livermore physicist Tomas Diaz de la Rubia agreed that combining scales is vital for accurate materials models. He also noted that real materials contain impurities and other imperfections that are not addressed in ideal simulations.

David Ceperley from the University of Illinois said the multiscale approach was mandatory in part because the largest computers can now handle simulations of up to one billion particles, but real-world problems have vastly more particles. "We're never going to be able to do 10^{23} particles [10^{12} is a trillion], so we need to do multiscale," he said.

While it was clear that computer simulation is an important tool for both theorists and experimentalists, Galli Gygi asked if simulations could lead to a major scientific discovery. "Are computational tools an essential part of the discovery path, or will they be?" Most argued that it remained an important open question in most fields, but that with the steady advances in computers and software, the answer

would inevitably become "yes." Some, however, questioned whether simulation could ever discover a new field such as, say, superconductivity.

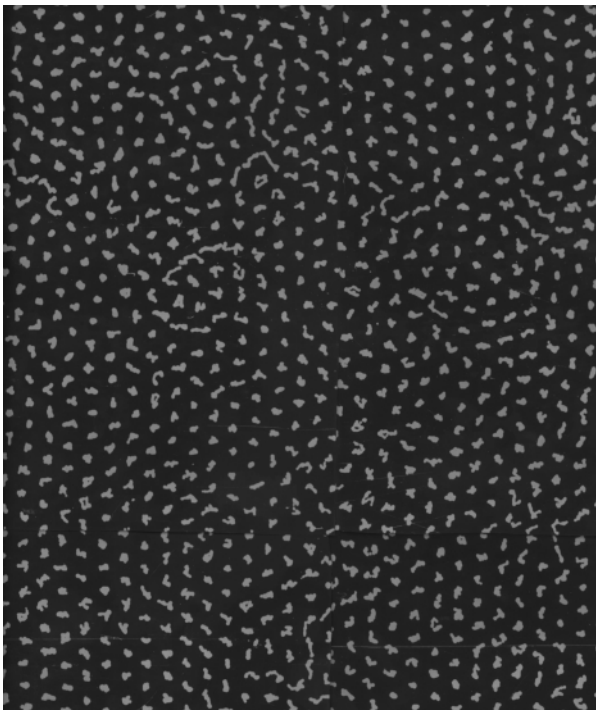
Lawrence Livermore engineer Kim Mish observed a distinction between scientific and engineering simulations when it came to discovery. "Science is concerned about fundamental truth, whereas engineering is an integrative process about systems you know a lot about," he said.

Simulations Still Have Limits

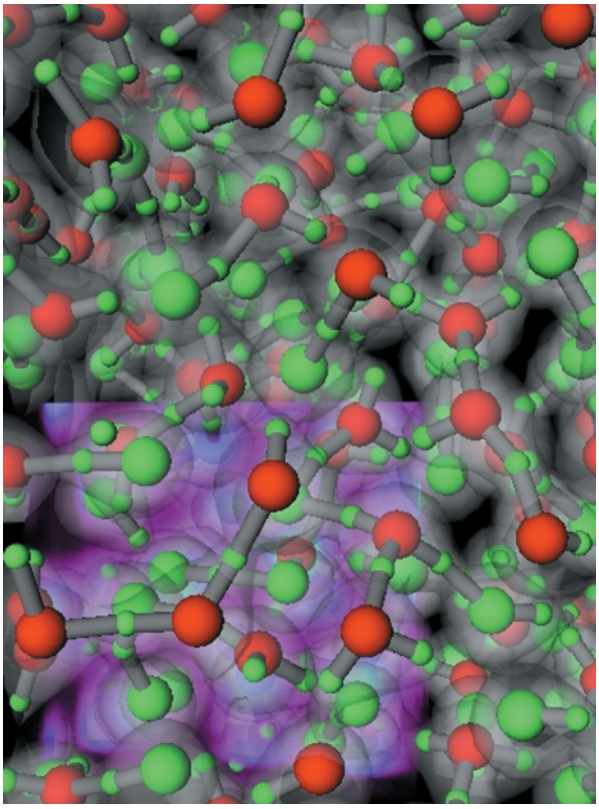
Several speakers discussed the limits of simulation validity, especially in simulations involving many phenomena. Paul Dimotakis, from the California Institute of Technology, noted that many things still cannot be computed, especially those containing heterogeneous materials and phases. Burning a piece of paper involves two phases of matter (soot particles and gases) and more than 2,000 chemical reactions involving more than 100 chemical species. Simulating such a system is probably beyond present capabilities, he said.

Another multiphenomena simulation is global climate modeling, which must take into account atmospheric physics, ocean physics, the effects of Earth's orbit, human activities, and the details of clouds, aerosols, water, and ice. UCLA's James McWilliams said climate modeling has matured as a simulation tool that involves many phenomena continually changing and affecting each other. He cited two grand challenges in the field: turbulence and pattern recognition. Although existing theories don't yet interface well with observed behavior, "We're learning an enormous amount from simulations," he said.

The University of Michigan's Joyce Penner, a former Lawrence Livermore scientist, traced the increasingly refined



Livermore physicist Berni Alder's pioneering computer simulation work was published in *Physics Review* in 1962. Shown here is an example of Alder's research performed on Lawrence Livermore's LARC supercomputer. This simulation tracked 870 particles over time and contributed to the understanding of matter.



This quantum-level simulation of a mixture of hydrogen fluoride and water molecules at high temperatures and pressures took 15 days on the Accelerated Strategic Computing Initiative machine at Lawrence Livermore. (Image by Francois Gygi, Lawrence Livermore.)

model of global warming that has been extended to include scattered radiation, aerosols, biomass burning, soot, and sulfates. How the subsystems combine is impossible to reconcile in full detail, she said. Nevertheless, climate modelers are closing in on the problem of long-term climate prediction.

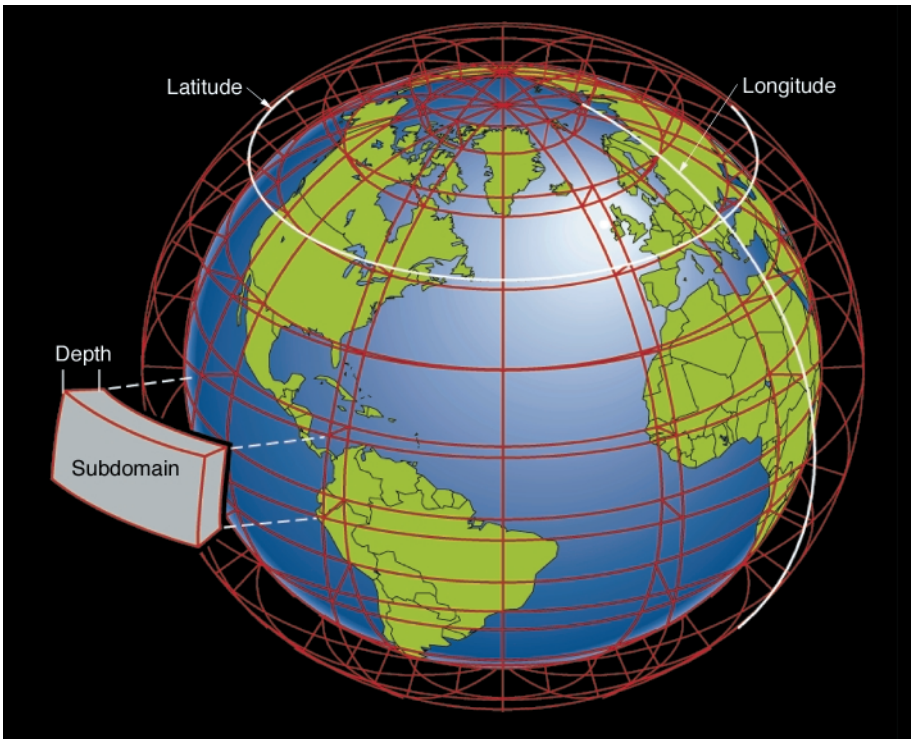
Lawrence Livermore's Philip Duffy explained the monumental task of simulating climate change that necessitates taking 1 million time steps to calculate grids of areas that are several hundred kilometers per side. Even with such a coarse resolution, it may take up to two months to complete a simulation. "Higher resolution is the holy grail of climate modeling," he said. Improvements will come, he suggested, from better computer designs and better representations of data, as well as better understanding how volcanic eruptions, solar variability, and aerosols affect the climate.

Biology: Simulation's New Frontier

Caltech's William Goddard predicted that in the next three years, advanced simulations would reveal the structure and function of many proteins and enzymes. Biologists worldwide, including those at Lawrence Livermore, are studying how proteins—polymers consisting of up to many thousands of atoms—fold in one-thousandth of a second into three-dimensional, functional structures measuring 2 to 3 nanometers in diameter.

Stanford University's Michael Levitt called biology "the ideal system for simulation" and drew similarities between mechanical engineering simulations and protein-folding simulations. Protein-folding studies have been influenced by experiments conducted in the Critical Assessment of Structure Prediction project, which is managed by a team in Livermore's Biology and Biotechnology Research Program Directorate. In those experiments, the amino acid sequences of proteins are posted on the Internet, and researchers from around the world predict the corresponding three-dimensional structures. The correct structures are concurrently determined experimentally by x-ray crystallography, and the predictions are revealed at a biannual conference. Workshop participants discussed whether this blind process could be valuable in other fields as a means to test different simulation software.

Lawrence Livermore biologist Elbert Branscomb, the first director of the DOE Joint Genome Institute, described a major challenge: simulating the regulatory control of genes. The genome's regulatory logic is "profound and complex," he said, with the locations of regulatory mechanisms seemingly "chaotic and crazy." He compared building a computer model



Climate models running on multiprocessor computers are divided into subdomains so that each processor handles a limited range of latitude and longitude and unlimited depth. This approach is typically the most efficient because it minimizes the amount of time spent exchanging information among processors, allowing the computer to perform the maximum number of calculations per second. (Image courtesy of Philip Duffy, Lawrence Livermore.)

of gene regulation to one describing the functioning of a computer chip. "The real barrier is the complexity barrier," he said.

Models Need Basis in Reality

Christopher Barrett from Los Alamos National Laboratory described novel software that his group has developed to help authorities better respond to emergencies. The software simulates a host of situations such as bioterrorism, earthquakes, or commercial power-grid outages. The software includes models to find how to reduce congestion, thereby allowing faster emergency response. "Computer simulations have become a commonplace, but artful tool for addressing these problems," he said.

Lawrence Livermore engineer Dave McCallen discussed what can happen when seismic engineering models are not based on real experiments: "Things can go bad when we don't fully understand the physics of the process." McCallen cited a newly constructed bridge that collapsed in the 1971 San Fernando Earthquake because "we didn't know then how bridges vibrate."

McCallen said engineers now have adequate computer power to model regional seismic activity and the response of structures. He pointed to a collaboration between the Laboratory and the University of California at Berkeley on the seismic response of long-span bridges (see *S&TR*, May 1999, pp. 17–19 and December 1998, pp. 18–20). The major 1999 earthquake in Taiwan provided a wealth of ground-motion data that validated the occurrence of huge ground displacements that were produced in Lawrence Livermore simulations. The predictions made by these simulations had originally been considered by many seismic experts to be unrealistically large. "Our ability to compute has vastly outstripped our ability to validate," he noted.

In that respect, participants drew a distinction between verification and validation: verification involves making sure models and equations have been implemented correctly while the process of validation ensures that the simulation represents reality.

K. K. Muraleetharan of the University of Oklahoma said it was difficult to get data on the material properties of soils for use in simulating the seismic response of new structures. Muraleetharan cited two other barriers to civil engineering simulations: a litigation-driven society and the reluctance of people in his field to try new approaches.

Workshop speakers made it clear that in some systems, predictive accuracy may always be limited by dependency on the precise details of initial conditions. For example, the propagation of a crack in a material is affected by what goes on at the crack's very tip. As a result, said Northwestern University professor Ted Belytschko, realistically predicting the formation of cracks is still problematic.

Simulations involving climate change also have a high sensitivity to starting conditions. UCLA's McWilliams noted that numerical weather prediction is 50 years old, but predictions are useful for only about one week in advance. "There is a fundamental limit of predictability because small disturbances become amplified," he said.

Nobel Prize–winning Livermore physicist and Stanford professor Robert Laughlin suggested that some physical properties seem to be protected from sensitivities to starting conditions and model details, and he encouraged the workshop participants to seek out such systems for simulation. One example of such a protected system is a phase transition, such as when water turns to ice.

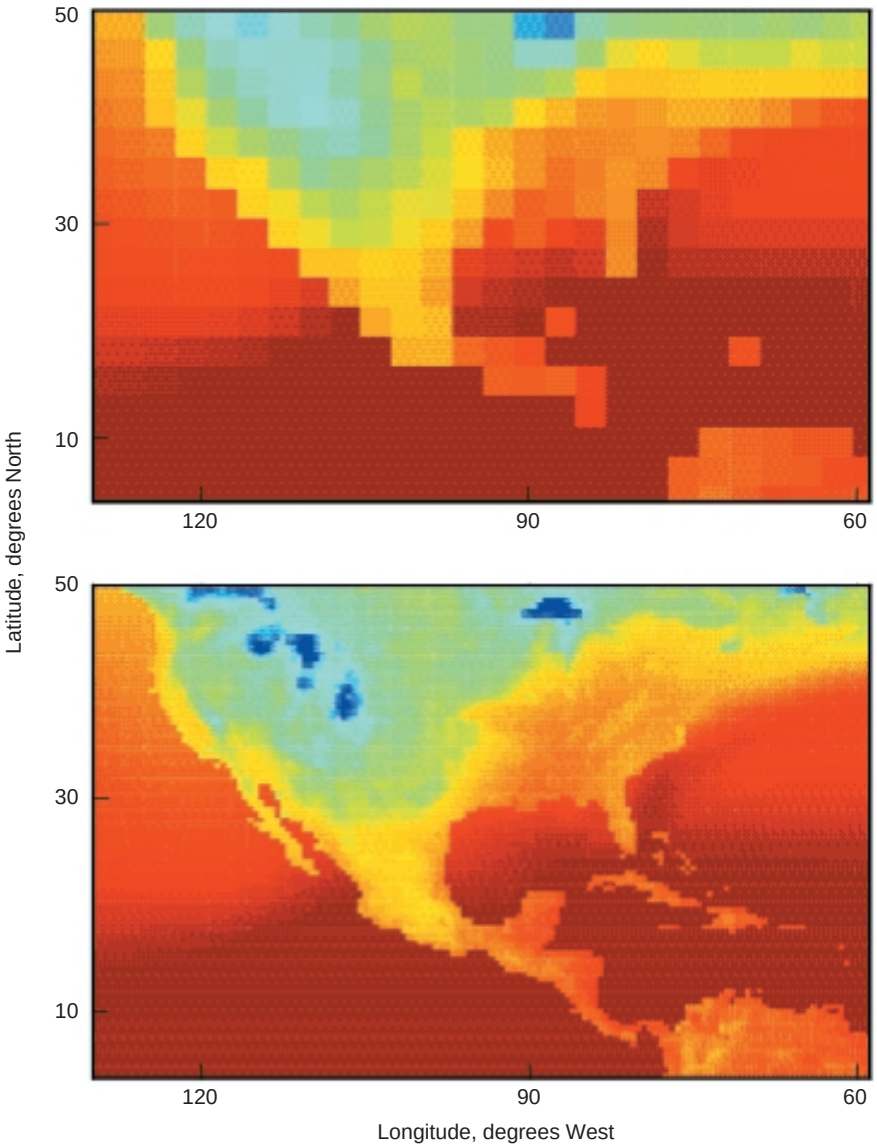
Virtual Proving Grounds

Belytschko also described the virtual proving grounds of U.S. car

Themes Arising from the Workshop

- Limitations in raw computer speed is not the sole barrier to progress in simulation.
- Expectation of outcome varies, ranging from discovering fundamental physical laws to determining the most efficient airfoil shape.
- The observation of Paul Dirac that all of the relevant equations are known but remain difficult to solve.
- Dependence on initial conditions (for example, crack formation, turbulence in some systems may limit results.
- Concept of robustness, in which many emergent behaviors are insensitive to model detail and starting conditions.
- Challenge of comparing even closely related experiments and simulations.
- Need to overcome limits of simulation, especially in multiphenomena simulations.
- Need of computers to do more than just numerics—they need to help set up grids, evaluate outputs, and analyze experimental data.
- Software development and management are major hurdles and perhaps lend themselves to interdisciplinary collaboration.
- The role of blind prediction experiments in protein folding could have valuable applications to other fields.
- Funding for solving problems with existing methods is easier to get than funding for developing better methods.
- Accurate material models are required for realistic computational simulations of macroscopic phenomena.

manufacturers that model, for example, a car's suspension system. A virtual car can be run over a pothole, with the resulting stress on the suspension system measured. A realistic simulation must include thousands of welds, some of which inevitably fail, sometimes because of poor workmanship. Predicting which welds will fail, when they will fail, and why is a tough challenge.



Higher spatial resolution is needed to accurately forecast both regional and large-scale climate change using global climate models. Typical global models (top image) use grid cells with horizontal sizes of 250 to 300 kilometers, preventing accurate forecasts for specific geographical regions (for example, California). The bottom image shows preliminary results of a simulation at 50-kilometer resolution performed at Lawrence Livermore on computers of the Accelerated Strategic Computing Initiative. At this resolution, much more accurate forecasts should eventually be possible. (Images by Philip Duffy, Lawrence Livermore.)

Scientist Jacqueline Chen of the Sandia National Laboratories Combustion Research Facility described efforts to simulate turbulent mixing and combustion found in diesel engines. Turbulent mixing, an irregular process of stirring and mixing, greatly enhances combustion by creating a flame area. Chen noted that in recent experiments by Sandia's John Dec, laser diagnostics of diesel combustion reactions involving 80 to 100 atmospheres of pressure and temperatures of 2,000 kelvins have significantly changed the conceptual understanding of diesel combustion. Further advances in the fundamental understanding of the relevant physics will be aided by first-principles numerical simulations.

One of the major keys to advances in simulation has been the rapid growth of computer capabilities, and a recurring theme during the workshop was the relative importance of computer speed. Laboratory physicist Malvin Kalos warned, "No one should assume Moore's Law [the law postulating that the power of computer processors doubles roughly every 18 months] will go on forever."

As Richard Freeman, chair of the UC Davis Department of Applied Science, pointed out, there is an absolute limit to Moore's Law. Quantum mechanics will begin interfering with the operation of semiconductor chips in 10 years if their features continue to shrink at the current rate. Participants cited the promise of optical computers that use pulses of photons instead of electrons, quantum computers that use quantum states of individual atoms, and DNA computers that take advantage of DNA "intelligence."

Beyond Computer Speed

Although speakers gave credit to the unprecedented power of current computers, raw computer speed was not identified as the sole barrier to progress in simulation. Livermore physicist Bill Nellis challenged the conventional

thinking that the key to better simulations was more powerful computers. He said that there are too many "brute force" simulations with not enough thought behind them. "The key to doing good science is using your head," he said. "You need as much intuition to do computation as you need to do experiments."

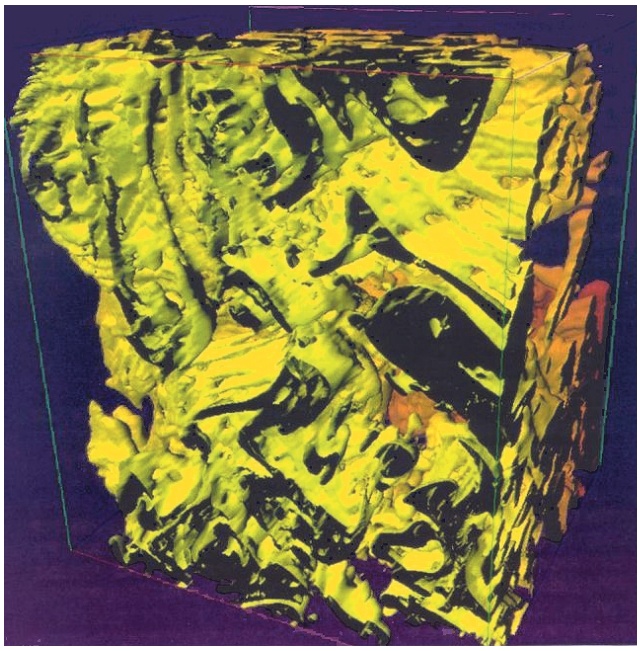
Alder said it made sense to focus more on developing advanced algorithms because the increased speed of computing has been as much due to improvement in algorithms as to new hardware. He also noted that it was easier to develop algorithms on personal computers than on larger machines.

Several speakers said there was plenty of room for both greater computational power and better algorithms. They voiced their concerns, however, that policymakers excessively emphasize multiparallel computing designs, such as ASCI machines using thousands of microprocessors. Different kinds of machines with fewer but more powerful processors would work better for some whole-system problems such as climate science, which involves interweaving data from physical, chemical, and biological processes.

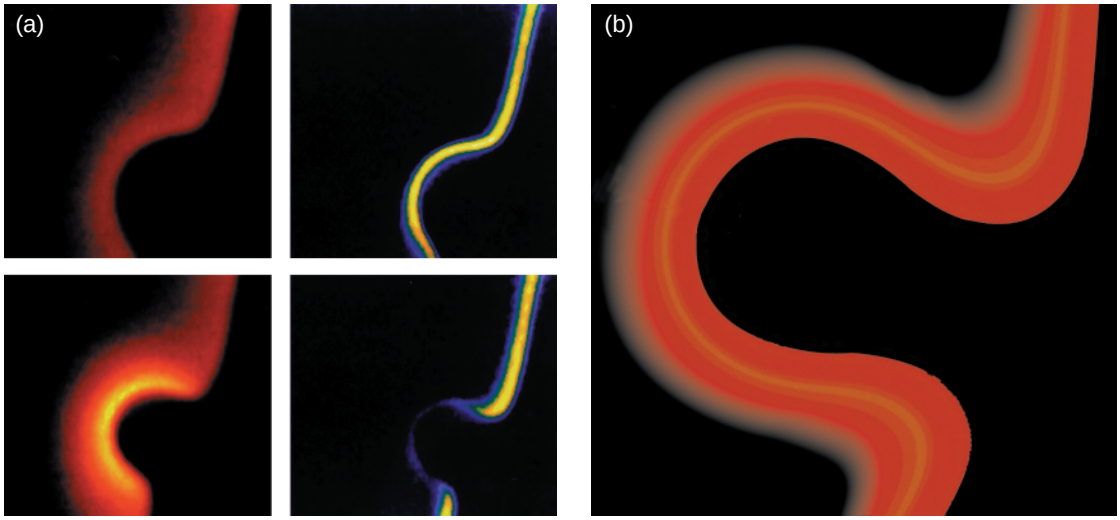
Many participants cited the development and management of simulation software as a key barrier. Several regretted that there is no Moore's Law for software. A common request was for robust software with intuitive interfaces that could be used by any engineering student or by a small engineering firm. Lee Taylor, from TeraScale LLC in Albuquerque, New Mexico, raised the issue of accessibility for small firms that may not be able to purchase an advanced computer, yet recognize that simulation "lets you design closer to the limits."

Collaborating on Software

A popular idea was to make software writing more efficient, perhaps by collaboration. UCLA's McWilliams said, "We all do everything for ourselves. We keep reinventing simple solutions that take lots of hours to develop and debug." Several participants



Simulating the chaotic nature of turbulence is one of computer simulation's great challenges. This three-dimensional image of laboratory data shows the tremendous complexity of a turbulent jet. (Image courtesy of Paul Dimotakis, California Institute of Technology.)



Modeling combustion in an engine demands close links to experiments. (a) Images of OH and CH in an actual flame–vortex interaction and (b) an image of OH from a simulation illustrate the complexity of modeling chemical response to fluid–chemistry interactions. (Image (a) is provided courtesy of The Combustion Institute, and (b) is by Jacqueline Chen, Sandia National Laboratories, Livermore.)

urged free exchange of software, but others cautioned that some institutions have cultural barriers against sharing software developed in-house.

One suggestion was an interdisciplinary collaboration on common software components. Although such an effort would necessitate going beyond rigidly defined academic disciplines, many felt that the time had come for researchers to have a broader knowledge of science and technology. In that light, Princeton's Car suggested creating new positions such as "software physicist" or "software chemist."

Participants also voiced concern that Silicon Valley was drawing off some of the best software minds. Lawrence Livermore's Krzysztof Fidelis commented, "We need better software, but we live in a world where software experts tend to go to industry."

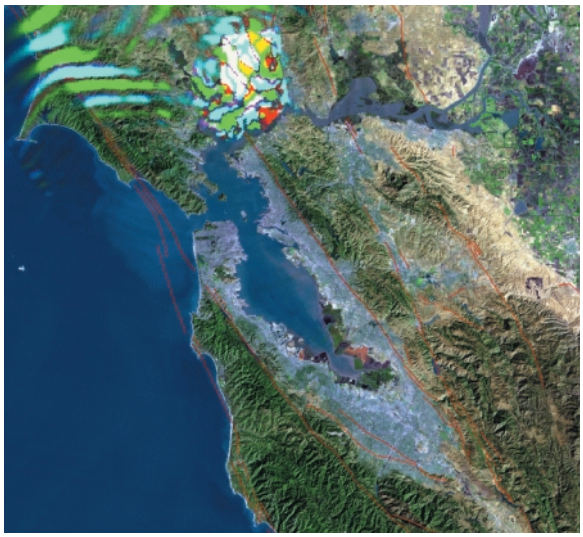
Several participants observed that it is much easier to get funding to solve problems with existing methods than to develop better methods. Many agreed with William Goddard of the California Institute of Technology that funding was needed to explore new directions that offered long-term but sizable payoffs. Unfortunately, funding sponsors want a particular problem solved and are not interested in funding better methods that may not directly solve their problem.

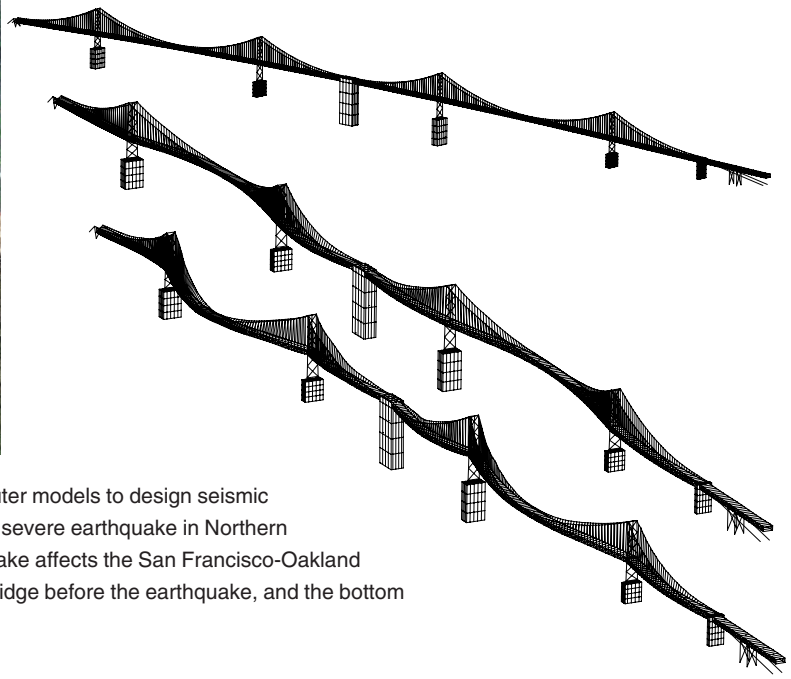
Simulating Extreme Conditions

Two areas of major interest to Lawrence Livermore are nuclear weapons physics and its close relative, astrophysics. Lawrence Livermore physicist David Nowak, ASCI program leader, said, "ASCI has led the U.S. to world leadership in high-performance simulation." The first major barrier to success, said Nowak, is resources, which include funding, hardware costs, and recruiting and retaining computational experts. The second barrier is technical, for example, validating new software that simulates imperfectly understood processes such as turbulence and materials properties. ASCI simulations, he said, must reflect a host of data that include engineering details, weapon designer comments from 30 years ago, information gathered in nuclear tests, and the results of equation-of-state experiments.

Because astrophysics is not a classical experimental science, simulation plays a strong role in that field. University of California at Berkeley's Christopher McKee said the primary barrier in astrophysics simulations is vast time and distance scales, ranging from atomic nuclear reactions to the formation of entire galaxies, with time scales ranging up to a billion years.

"People are stretching the ability of computers" with these problems, McKee said. He added that computer simulations can perform virtual experiments whose outcomes can be validated with observations. The





More and more, seismic engineers are using powerful computer models to design seismic retrofits to existing structures. The simulation above shows a severe earthquake in Northern California, and the simulations at right show how the earthquake affects the San Francisco-Oakland Bay Bridge. The topmost one of those simulations is of the bridge before the earthquake, and the bottom two show the aftermath.

grand challenge is to follow the simulated gravitational collapse of a molecular cloud to the formation of one or more stars.

Lawrence Livermore physicist Richard Klein said an important barrier to astrophysics simulation is the difficulty in obtaining enough data to validate models. A new testbed for validation is emerging in the University of Rochester's Omega laser and the National Ignition Facility, currently under construction at the Laboratory. Klein has used simulation to predict photon bubble oscillation, a new phenomenon on the surface of neutron stars, with structures the size of New York's World Trade Center.

Lawrence Livermore astrophysicist Dave Dearborn noted that astrophysics simulation incorporates lots of physics, some of it not well known. "We're still human," he said. "We need the brightest people to pose new questions."

Simulations are helping to reveal the three-dimensional structures of proteins. This image shows the structure of a protein determined by computational modeling. (Image by Ceslovas Venclovas, Lawrence Livermore.)

Workshop Speakers and Panelists

Simulations History
Berni Alder, Lawrence Livermore National Laboratory

Infrastructure Modeling
Christopher Barrett, Los Alamos National Laboratory
David McCallen, Lawrence Livermore National Laboratory
K. K. Muraleetharan, University of Oklahoma
Theofanis Theofanous, University of California at Santa Barbara

Mechanics
Richard Becker, Lawrence Livermore National Laboratory
James Belak, Lawrence Livermore National Laboratory
Ted Belytschko, Northwestern University
Lee Taylor, TeraScale LLC

Physics and Simulation
Robert Laughlin, Lawrence Livermore National Laboratory and Stanford University

Quantum Mechanics
Roberto Car, Princeton University
David Ceperley, University of Illinois at Champaign-Urbana
William Goddard, California Institute of Technology
Bill Nellis, Lawrence Livermore National Laboratory

Accelerated Strategic Computing Initiative (ASCI)
David Nowak, Lawrence Livermore National Laboratory

Astrophysics
David Dearborn, Lawrence Livermore National Laboratory
Richard Klein, Lawrence Livermore National Laboratory
Christopher McKee, University of California at Berkeley

Biology
Elbert Branscomb, Lawrence Livermore National Laboratory
Krzysztof Fidelis, Lawrence Livermore National Laboratory
Michael Levitt, Stanford University
John Moult, University of Maryland

Climate and Weather
Philip Duffy, Lawrence Livermore National Laboratory
James McWilliams, University of California at Los Angeles
Joyce Penner, University of Michigan

Fluid Dynamics
Jacqueline Chen, Sandia National Laboratories, Livermore
Paul E. Dimotakis, California Institute of Technology
Anthony Jameson, Stanford University

Next Steps

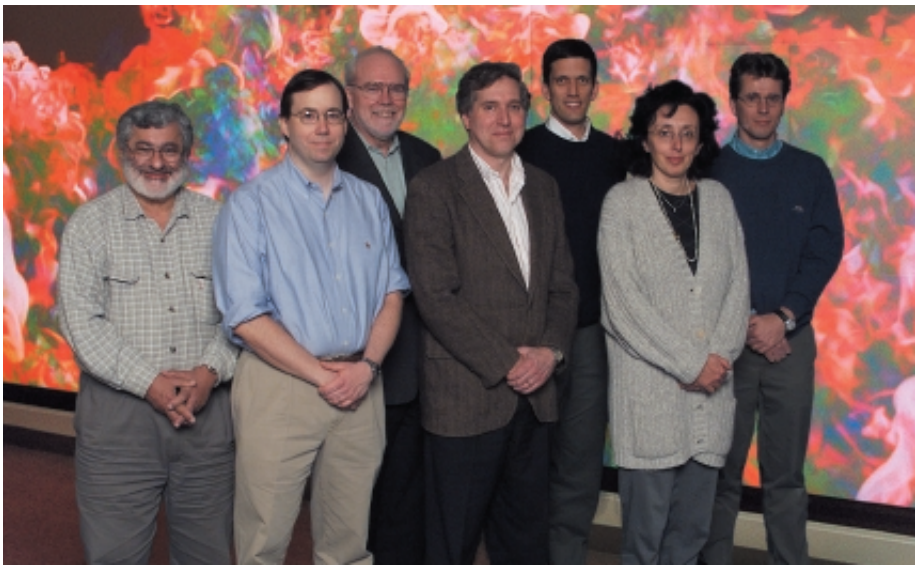
Colvin says the workshop was so successful that plans are under way for a number of follow-on meetings. Kalos will be chairing a simulation workshop this summer addressing a number of other simulation fields. Livermore's Materials Research Institute, under director Mike McElfresh, is holding a Computational Materials Science and Chemistry Summer Institute where graduate students can explore cutting-edge computational methods (see http://www.llnl.gov/mri/ for more information). A workshop on advanced simulation software is being organized by Mish for the summer of 2002.

Discussions are also continuing about extended programs involving visiting faculty and graduate students who would research a single topic. More informally, individual researchers are working on ways to build on existing collaborations and newfound friendships formed at the workshop. Fortunately, the barriers to lasting friendship are less formidable than those required for scientific and engineering simulations.

—Arnie Heller

Key Words: Accelerated Strategic Computing Initiative (ASCI), blind prediction experiments, computing speed, Dirac observation, model validation, multiscale modeling, predictive simulations, software.

For further information contact Giulia Galli Gygi (925) 423-4223 (galli@llnl.gov).



Members of the simulation workshop steering committee, from left, are Malvin Kalos, Mike Colvin (chairman), John Holzrichter, Steve Libby, Paul Miller, Giulia Galli Gygi, and Francois Gygi.

About the Scientist

GIULIA GALLI GYGI is a group leader for the Quantum Simulation Group in the Chemistry and Materials Science Directorate. She joined Lawrence Livermore as a staff physicist in 1998, after holding the position of senior scientist at the Swiss Federal Institute of Technology in Lausanne, Switzerland. She received a B.S. in physics from the University of Modena in Italy, and an M.A. and Ph.D. in physics from the International School for Advanced Studies in Trieste, Italy. Thereafter, she was a postdoctoral research associate at the University of Illinois at Champaign-Urbana and then at the IBM Zurich Research Center, Switzerland. Galli Gygi has published over 70 papers in refereed international journals. Her areas of interest are in systems and processes relevant to condensed-matter physics, physical chemistry and materials science, and quantum simulations. Current topics of investigation include modeling of fluids under pressure, DNA in solution, and complex surfaces and nanostructures.

Plutonium Up Close . . . Way Close

STOCKPILE Stewardship, the Department of Energy's program for assuring the long-term safety and performance of the nuclear weapons stockpile without underground testing, has created a heightened focus on better understanding plutonium.

At Lawrence Livermore, a number of experiments are under way to measure the structural, electrical, and chemical properties of plutonium and its alloys and to determine how these materials change over time. The measurements will enable scientists to better model and predict plutonium's long-term behavior in the aging stockpile (see "Inside the Superblock" beginning on p. 4 of this issue).

Plutonium's Peculiarities

"Plutonium is a complex and perplexing element," notes metallurgist Adam Schwartz. "For instance, plutonium has seven temperature-dependent solid phases—more than any other element in the periodic table. Each phase possesses a different density and volume and has its own characteristics. Alloys are even more complex; you can have multiple phases present in a sample at any given time."

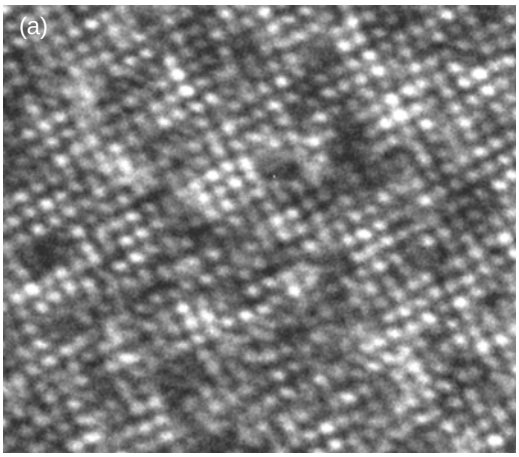
Because plutonium is so complex, surrogate materials cannot give a complete picture of plutonium's characteristics. With the importance of stockpile stewardship, the Laboratory has seen a resurgence of interest and research in plutonium and the other actinide elements (see *S&TR*, June 2000, pp. 15–22). One area that Schwartz, microscopist Mark Wall, and physicist Bill Wolfer are pursuing as part of their stockpile stewardship responsibilities is the evolution of damage to plutonium's structure. As with the atoms of all metals, plutonium atoms form structures on scales as small as a billionth of a meter. These microstructures are constantly changing because of plutonium's radioactive nature. When an atom of plutonium-239 (the isotope of plutonium used in nuclear weapons) decays, it splits into an alpha particle—a helium nucleus with two protons and two neutrons—and an atom of uranium-235. The heavy uranium atom recoils, displacing other plutonium atoms and disrupting the surrounding microstructure. Scientists are concerned that the buildup of gaseous helium atoms combined with other elements in the weapon's environment might gradually change the properties of the plutonium metal.

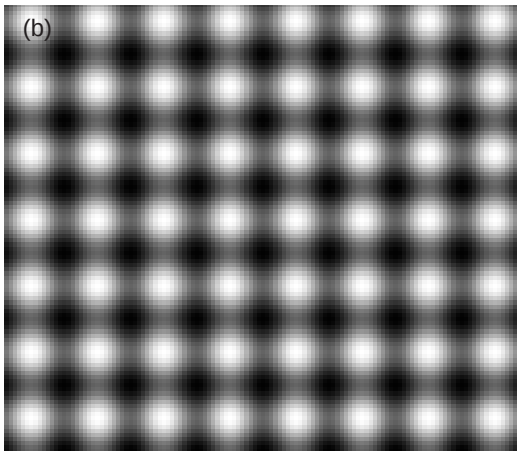
Seeing Beneath the Surface

To better understand the basic nature of this complex metal and search out the long-term effects of the weapon environment, scientists must know what goes on at the atomic level. To aid this endeavor, the Laboratory acquired a 300-kiloelectronvolt, field-emission transmission electron microscope (TEM) about one year ago. This remarkable instrument uses electrons instead of light waves to "see," so features can be resolved, or viewed at the atomic scale. Where most microscopes can only probe the surface of materials, a TEM looks directly at the internal structure of materials, explains Wall.

Microscopist Mark Wall uses the transmission electron microscope to image the microstructure of plutonium.

(a) An atomic resolution image of plutonium. Such an image was created for the first time ever by the team studying plutonium properties with a transmission electron microscope. (b) A high-resolution computed image of plutonium's atomic structure.





The Inside Scoop with the Transmission Electron Microscope

According to Mark Wall, the new 300-kiloelectronvolt transmission electron microscope (TEM) leased by the Laboratory is the best of its kind in DOE's weapon complex. "Having a high accelerating voltage allows us to see through thicker specimens, facilitating more microstructural observations and better image resolution," says Wall.

The TEM is used to characterize the internal structure of a wide variety of materials, not just plutonium. It not only can image the microstructure directly, but can also identify the phases present in a specimen. The TEM characterization techniques are cataloged here under headings that describe what they do (although there is some overlap among the techniques):

Characterization of Atomic Structure

High-Resolution Atomic Structure Imaging: Directly resolves the atomic structure of crystalline materials down to individual columns of atoms.

Characterization of Microstructure, Defects, and Phases

Bright Field: Images the internal microstructure of materials, including grain and defect structures such as dislocations and voids. Can also be used to observe precipitates or inclusions.

Dark Field and Weak Beam: Allows researchers to link diffraction information with specific phase regions in the sample. Weak-beam imaging is dark-field imaging at higher resolution and is primarily used for imaging closely spaced defect structures on the nanometer scale.

Electron Diffraction (Selected Area Diffraction) and Microdiffraction: Both techniques help researchers identify internal crystal structures. Selected area diffraction allows researchers to view and record the electron diffraction pattern from selected areas as small as 0.5 micrometer. Microdiffraction allows analysis of regions as small as 1 nanometer.

Convergent Beam Electron Diffraction: Reveals diffraction details that provide additional three-dimensional crystallographic and symmetry information.

Lorentz Microscopy: Images directional variations in the magnetic field within thin samples.

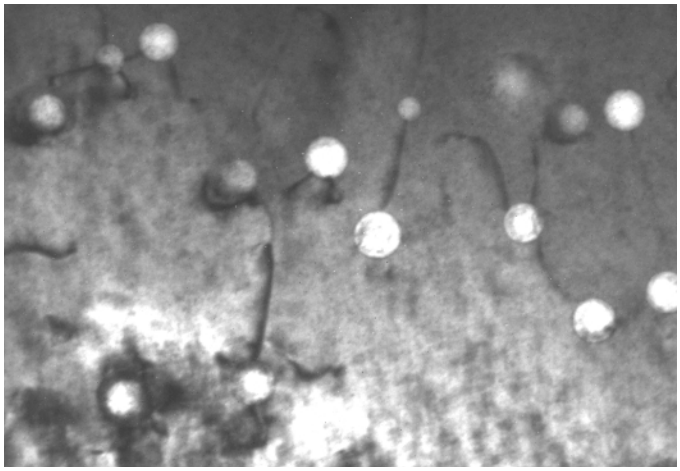
In Situ Microscopy: Allows researchers to record the evolution of a material's microstructure during heating, cooling, and mechanical deformation.

Characterization of Chemical Composition and Impurities

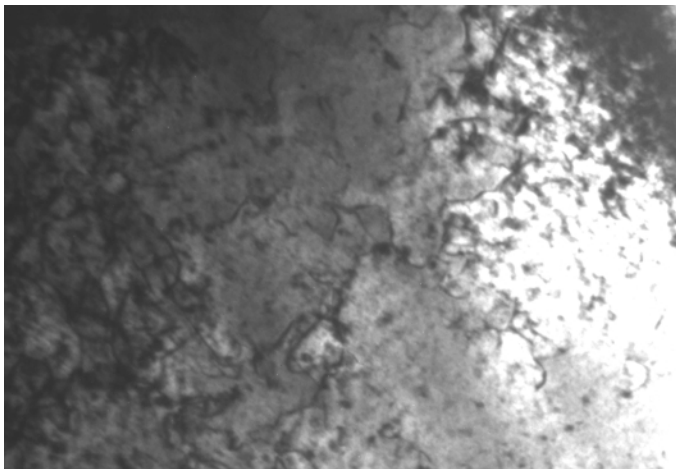
Energy-Dispersive Spectroscopy: Produces x-ray spectra that reveal the presence and amount of elements (for carbon and heavier elements).

Parallel Electron Energy Loss Spectroscopy: Complements energy dispersive spectroscopy, in that it is more sensitive to light elements, including lithium and heavier elements.

*Energy-Filtered Transmission Electron Microscop*e: Acquires real-time, quantitative chemical "maps" of a specific region with a resolution as small as 1 nanometer.



Voids or bubbles could be created by recoiling uranium nuclei and gaseous helium from alpha particles that result from plutonium decay. Here, an aged sample has been intentionally annealed to create bubbles.



A dislocation—an extra half plane of atoms—in the plutonium structure can create sinks or sources for radiation damage.

The primary strength of the instrument is that it can provide detailed characterization simultaneously over many length scales and at high resolution—from hundreds of micrometers to nanometers—and do this in either imaging, spectroscopic, or diffraction modes (see box on p. 24). "In principle, we can observe and measure the defects and composition of microstructural features in these materials down to the nanometer level," says Wall.

Schwartz and Wall start with plutonium samples measuring less than 3 millimeters in diameter and 150 micrometers thick. They then use special sample preparation techniques to thin each sample until it is transparent to high-energy electrons, that is, to between 10 to 100 nanometers in thickness. The specimens are then vacuum-transferred to the TEM for characterization experiments. The resulting electron micrographs reveal in unprecedented detail the nature of the material and any defects in it. During this work, Schwartz and Wall produced the first-ever image of plutonium at the atomic level.

Using samples of plutonium from old, disassembled nuclear warheads and comparing their resulting micrographs to those from newly cast plutonium, the researchers can better determine the kinds and amounts of defects and changes that occur over time. In particular, they look for voids or bubbles created by recoiling uranium nuclei and the gaseous helium from alpha particles. An example from an old material annealed to intentionally form bubbles is shown in the image directly above. Dislocations—which can be described as an extra half plane of atoms—can create sinks or sources for radiation damage (see image above right).

So Far, So Good

To date, the news for the stockpile is encouraging. Schwartz sums up the results as "So far, so good. We haven't seen any issues or surprises with the pit samples we've viewed." Last year, the team began another project, looking at special plutonium alloys that have been prepared to accelerate the rate of aging. For Livermore's Enhanced Surveillance Program (see *S&TR*, September 1999, pp. 3–11), scientists have made several alloys spiked with plutonium-238, which decays much faster than plutonium-239, to try to understand what will happen with stockpiled plutonium as it ages.

Schwartz and Wall also plan to conduct in situ microscopy of plutonium. Heating plutonium samples up to 400°C will allow researchers to see helium bubbles nucleate and for the first time see the early stages of nucleation. "In essence, we'll be speeding up the kinetics of the material and increasing the diffusion rate," said Schwartz.

—Ann Parker

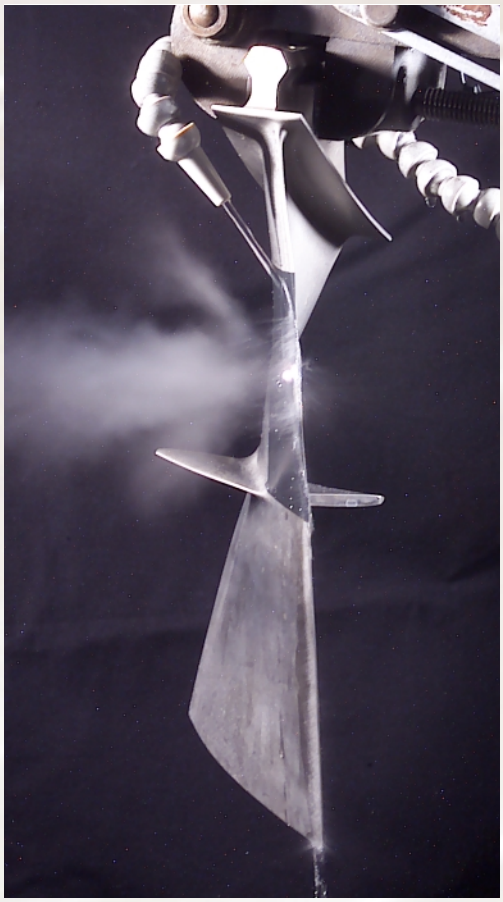
Key Words: plutonium research, stockpile stewardship, transmission electron microscope.

For further information contact Adam Schwartz (925) 423-3454 (schwartz6@llnl.gov).

Shocked and Stressed, Metals Get Stronger

PEOPLE who know their way around metalworking are no doubt familiar with peening—using a ball-peen hammer to pound a piece of metal into shape and strengthen it against fatigue failure. For the past 50 years, an industrialized equivalent has been shot peening, in which metal or ceramic beads as large as marbles or as small as salt and pepper grains pneumatically bombard a metal surface. Laser peening, a process based on a superior laser technology developed at Lawrence Livermore, replaces the hammer blows and streams of beads with short blasts of laser light. The end result is a piece of metal with significantly improved performance.

Lawrence Livermore and Metal Improvement Company, Inc., won a coveted R&D 100 Award for their laser-peening process in 1998 (see *S&TR*, October 1998, pp. 12–13). Since that time, they've been developing uses for the technology with a number of industries, including automotive, medical, and aerospace. They've also developed an offshoot technique—laser peenmarking℠—which provides a way to easily and clearly identify parts with a mark that is extremely difficult to counterfeit. Another outgrowth is a new peen-forming technology that allows complex contouring of problematic thick metal components such as the thick sections of large aircraft wings. There have also been spinback applications to the Department of Energy's programs for stockpile stewardship, fuel-efficient vehicles, and long-term nuclear waste storage.



A jet engine fan blade that is being peened by a laser shot.

Peening with Light

The concept of laser peening is not new, but it took a DOE Cooperative Research and Development Agreement (CRADA) between Livermore and Metal Improvement Company to develop a machine that makes laser peening a cost-effective option. The resultant Lasershot℠ Peening System uses a solid-state, high-energy (50-joule), neodymium-doped glass laser, which pulses at a rate 20 times faster than other available systems and can peen about 1 square meter of metal per hour. With each pulse of the laser, an intense shock wave is created over a roughly 5-millimeter by 5-millimeter area and drives in a residual compressive stress about 1 to 2 millimeters deep into metal. In conventional peening, this compressed layer is only about 0.25 millimeter deep. The added depth is key to laser peening's superior ability to keep cracks from propagating and extends the life of parts three to five times over that provided by conventional treatments.

For Fan Blades and Knee Implants

Shot peening has long been used on automobile springs and transmissions because the treatment increases resistance to cracks, corrosion, and fatigue. Physicist Lloyd Hackel, who heads the Livermore side of the joint development effort, says that the automotive industry is now interested in applying the depth compression afforded by laser peening to automobile frames.

Traditionally, automakers have added mass to the entire frame structure to achieve the required fatigue lifetime and keep high-stress areas in frames from cracking. Now, laser peening can extend fatigue

lifetime and allow manufacturers to cut back on the weight of the frame. By one company's calculations, laser peening would improve the fatigue lifetime of a 200-kilogram frame by a factor of two, allowing them to lessen the frame weight by about 20 kilograms. This 20-kilogram weight savings translates into gas savings as well. Laser peening 8 million automobile frames could save about 285 million liters of gasoline per year. "So this technology has two big benefits: it makes the car lighter and cheaper to build, and it results in more fuel efficiency," says Hackel.

Livermore is also working with the Biomechanics Department of the University of California at Los Angeles to use laser peening for knee implants. "The biggest concern in this area is pediatric knee replacement," says Hackel. "A surgeon puts in a small knee joint, the child grows, so the knee is loaded with more stress, which can lead to joint failure. What do you do? Until now, the answer has been to undertake a painful and risky operation every few years to replace the knee with a larger model." In contrast, a laser-peened metal joint would be strong enough to last nearly a decade.

The aerospace industry also sees major applications for laser peening, particularly in jet engines. "If you look at a modern turbo jet engine such as those used in a Boeing 777," says Hackel, "you'll see that it's essentially a giant propeller engine, with the fan blades in the front and the compressor blades inside." These blades get hit by a variety of debris including nuts and bolts, seagulls, sand, and rocks, that can cause cracks and failure. Laser peening adds safety while also lowering the life-cycle cost of each fan blade.

Another use of laser peening for aerospace and other industries involves metal shaping. For instance, the leading edge of an airplane wing is basically a big piece of curved metal. "Aerospace and other industries bend metal all the time, but it's difficult to bend very thick pieces and get certain complex shapes. And when you do bend metal, its surface is under tension—think of the metal as being 'stretched' around that bend. That stretching weakens it and makes it more vulnerable to cracking."

Laser peening just one side of a metal piece will make it naturally bend, which places both peened and unpeened sides under compression and makes the part more resistant to failure. The deep compressive stress and the precise placement of the stress afforded by the laser-peening process allows forming of thick, complex shapes never before possible.

Marking by Laser

Another recently developed application involving industries using or manufacturing metal parts is laser peenmarking℠, in which a high-resolution mark is imprinted into the metal. This identification mark can take any form, for example, as alpha numeric characters, a logo, or a data matrix. This development is particularly timely for aerospace industries facing a new marking requirement from the Aerospace Transportation Association, called the ATA 2000. An ATA mark, in a matrix form that can be read by barcode machines, must be set into each part early in the manufacturing process so that the part can be tracked throughout its lifetime.

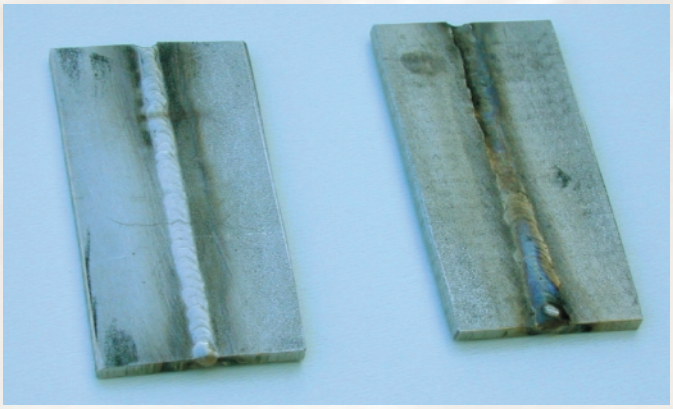
Normal marking methods—scribing, etching, or stamping—remove material or impart tensile stresses that can leave the part weakened at the marked spot. But laser peenmarking adds a strengthening residual compressive stress. Peenmarks are also of very high resolution, similar to the watermark on currency,

Laser peening a gear at the base of its teeth increases the strength of the gear and its fatigue lifetime.

and thereby provide a barrier to counterfeiting. Counterfeit, substandard parts are a major concern, notes Hackel. For example, the U.S. Coast Guard prosecutes approximately 20 cases each year involving the fraudulent use of counterfeit parts. "Laser peenmarking could be an enormous deterrent to criminals and really put a dent in the counterfeit metal parts racket," says Hackel.

Lawrence Livermore and Metal Improvement Company have been working with other organizations, including the National Aeronautics and Space Administration, to determine the efficiency of laser peenmarking. In June 2001, three laser peenmarked parts are tentatively scheduled to ride on the NASA shuttle to the international space station. The parts will be bolted onto the space station to face the slipstream solar wind. After three years, they'll be retrieved and examined to see how well they held up in the hostile space environment.

Laser peenmarking prints a complete high-quality, machine-readable matrix mark that could deter the counterfeiting of metal parts. This data matrix represents the number string "123456."



To test the resistance of laser-peened welds to corrosion, the team took two welded pieces of 304 stainless steel and bathed them in a 40-percent solution of magnesium chloride, a highly corrosive salt, at 160°C. Cracks developed in the unpeened weld within 24 hours, whereas the laser-peened weld showed no observable cracks after a week of exposure.

Spinback to DOE

The laser-peening technology is a spinoff of high-energy lasers developed in the DOE Inertial Confinement Fusion program. Those lasers were brought to high average power with Department of Defense funding. The technology is spinning back home as it becomes clear that peening has relevant applications for DOE's Yucca Mountain Nuclear Waste Disposal and Stockpile Stewardship programs.

For Yucca Mountain, laser peening could be used to prevent stress corrosion cracking in the final closure welds of 6-meter by 1.5-meter nuclear waste storage canisters. Such canisters must completely contain waste for a minimum of 10,000 years. Analyses show that stress corrosion in some of the canister welds could cause the canisters to fail prematurely. Experiments show that laser peening the welds would keep corrosion and cracking at bay, allowing the canister to remain intact for 10,000 years and more.

In the Stockpile Stewardship Program, one research area seeks to determine the effect of intense strain on various materials. The laser-peening team discovered that it could generate meaningful strain rates and effects through shock waves created by the laser-peening process. "We can give stockpile stewardship scientists 10 laser shots a minute, providing them with an enormous amount of data and information," says Hackel. The process, he adds, can give these scientists exquisite control over test parameters, including the intensity, duration, and profile of the desired shock wave.

As for DOE's efforts in promoting fuel efficiency in vehicles, Hackel says, "I see peening as another spinback for the DOE— particularly the Office of Transportation Technology—in terms of reducing the weight of vehicles. DoD would also benefit, from getting better fuel efficiency in the field and also for airlift capability."

Far-Reaching Technology

Going from ball-peen hammers to laser light takes a big jump in technology. The applications of laser peening—some known years ago, others newly discovered—are just as far-reaching. "What we've come to," says Hackel, "is an active CRADA that's working to field the technology for specific industries and spinning it back with important benefits to Laboratory and DOE work."

—Ann Parker

Key Words: Laser peening, Stockpile Stewardship Program, Yucca Mountain Nuclear Waste Disposal Program.

For further information contact Lloyd Hackel (925) 422-9009 (hackel1@llnl.gov)

Patents and Awards

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

Because of a layout error in the January/February 2001 issue of Science & Technology Review, the following four patents were attributed to the wrong inventors. The attribution below is correct, and the error has also been corrected in the online version of S&TR. The staff of S&TR sincerely apologizes for this mistake.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Joe N. Lucas	**Method for Isolating Chromosomal DNA in Preparation for Hybridization in Suspension** U.S. Patent 6,077,671 June 20, 2000	A method is provided for detecting nucleic acid sequence aberrations using two immobilization steps. A nucleic acid sequence aberration is present when one acid sequence has both a first nucleic acid sequence type (for example, from a first chromosome) and a second nucleic acid sequence type (for example, from a second chromosome). In the method, immobilization of a first hybridization probe is used to isolate a first set of nucleic acids from a sample of the first nucleic acid sequence type. Immobilization of a second hybridization probe is then used to detect and isolate a second set of nucleic acids from within the first set. The presence of the second set of nucleic acids indicates the presence of a nucleic acid sequence aberration. Chromosomal DNA in a sample containing cell debris is prepared for hybridization in suspension by treating the mixture with RNase. The treated DNA can also be fixed prior to hybridization.
Charles G. Stevens Norman L. Thomas	**Immersion Echelle Spectrograph** U.S. Patent 6,078,048 June 20, 2000	A small spectrograph containing no moving components and capable of providing high-resolution spectra of the mid-infrared region from 2 to 4 micrometers in wavelength. The resolving power of the spectrograph exceeds 20,000 throughout this region and at an optical throughput of about 0.00005 square centimeters per steradian. The spectrograph incorporates a silicon immersion echelle grating operating in high spectral order combined with a first-order transmission grating in a cross-dispersing configuration to provide a two-dimensional spectral format that is focused onto a two-dimensional infrared detector array. The spectrometer incorporates a common collimating and condensing lens assembly in a nearly aberration-free axially symmetric design. The spectrometer has potential uses in general research as well as in areas such as monitoring atmospheric constituents for air quality, climate change and global warming research, and monitoring exhaust fumes for smog sources or exhaust plumes for evidence of illicit drug manufacture.
Alan D. Conder	**Vacuum-Compatible Miniature CCD Camera Head** U.S. Patent 6,078,359 June 20, 2000	A charge-coupled device (CCD) camera head that can replace film for digital imaging of visible light, ultraviolet radiation, and soft-to-penetrating x rays, such as within a target chamber where laser-produced plasmas are studied. The camera head is small, is capable of operating both in and out of a vacuum environment, and is versatile. The CCD camera head uses PC boards with an internal heat sink connected to the chassis for heat dissipation, allowing for close (0.22 centimeters, for example) stacking of the PC boards. Integration of this CCD camera head into existing instrumentation provides a substantial enhancement of diagnostic capabilities for studying high-energy-density plasmas in a variety of military, industrial, and medical imaging applications.
Jesse D. Wolfe Norman L. Thomas	**Durable Silver Coating for Mirrors** U.S. Patent 6,078,425 June 20, 2000	A durable multilayer mirror that includes reflective layers of aluminum and silver and has high reflectance over a broad spectral range, from ultraviolet to visible to infrared. An adhesion layer of a nickel and/or chromium alloy or nitride is deposited on an aluminum surface, and a thin layer of silver is then deposited on the adhesion layer. The silver layer is protected by a passivation layer of a nickel and/or chromium alloy or nitride and by one or more durability layers made of metal oxides and typically a first layer of metal nitride. The durability layers may include a composite silicon aluminum nitride and an oxinitride transition layer to improve bonding between nitride and oxide layers.

(continued on p. 30)

(continued from p. 29)

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Joe N. Lucas	**Method for Obtaining Chromosome Painting Probes** U.S. Patent 6,132,974 October 17, 2000	A method for determining a clastogenic signature of a sample of chromosomes. The frequency of each of two types of chromosome aberration present in the sample is quantified. Then the frequencies are compared to each other. A method is also provided for using that clastogenic signature to identify a clastogenic agent or dosage to which the cells have been exposed.
Eberhard A. Spiller Paul B. Mirkarimi Claude Montcalm Sasa Bajt James A. Folta	**Method to Adjust Multilayer Film Stress-Induced Deformation of Optics** U.S. Patent 6,134,049 October 17, 2000	Stress-compensating systems that reduce stress in a multilayer without losing reflectivity and reduce total film thickness, compared to the thicknesses produced by the earlier buffer-layer method. The stress-free multilayer systems contain two different material combinations of opposite stress, both giving good reflectivity at the design wavelengths. The main advantage of this multilayer design is that stress reduction does not require the deposition of additional layers, as in the buffer-layer approach. If the optical performance of the two systems at the design wavelength differ, the system with the poorer performance is deposited first, and then the system with better performance is added, forming the top of the multilayer system. The components for the stress-reducing layer are chosen from among materials that have stress opposite to that of the preferred multilayer reflecting stack and simultaneously have optical constants that allow good reflectivity at the design wavelength.
James E. Trebes Perry M. Bell Ronald B. Robinson	**Miniature X-Ray Source** U.S. Patent 6,134,300 October 17, 2000	A miniature x-ray source using a hot filament cathode. The source is sized on the millimeter scale and is capable of producing broad spectrum x-ray emissions over a wide range of x-ray energies. The miniature source consists of a compact vacuum tube assembly containing the hot filament cathode, an anode, a high-voltage feedthrough for delivering high voltage to the cathode, a getter for maintaining high vacuum, a connector for initial vacuum pumpdown and crimpoff, and a high-voltage connection for attaching a compact high-voltage cable to the high-voltage feedthrough. At least a portion of the vacuum tube wall is fabricated from materials highly transparent to x rays, such as sapphire, diamond, or boron nitride.
Conrad M. Yu Jackson C. Koo	**System and Method for Preconcentrating, Identifying, and Quantifying Chemical and Biological Substrates** U.S. Patent 6,134,944 October 24, 2000	The system and method consist of an input valve that directs a volume of sample gas to a surface acoustic wave (SAW) device where a mass of a substance within it is preconcentrated and detected. Some of this sample gas containing the preconcentrated substance is directed through an output valve to a gas chromatograph (GC) where the preconcentrated substance is then identified. A shunt valve exhausts a volume of the sample gas equal to the volume directed to the SAW minus the volume sent to the GC.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Anthony M. McCarthy Robert J. Contolini Vladimir Liberman Jeffrey Morse	**Submicron Patterned Metal Hole Etching** U.S Patent 6,139,716 October 31, 2000	A wet chemical process for etching submicrometer patterned holes in thin metal layers using electrochemical etching helped by a wetting agent. In this process, the wafer to be etched is immersed in a wetting agent (such as methanol) for a few seconds before it is inserted into an electrochemical etching setup. The wafer is kept horizontal during transfer so that a film of methanol continuously covers the patterned areas. The electrochemical etching setup includes a tube that seals the edges of the wafer to prevent the loss of methanol. An electrolyte composed of 4:1 water:sulfuric acid is poured into the tube, and the electrolyte replaces the wetting agent in the patterned holes. A working electrode is attached to a metal layer of the wafer, with reference and counter electrodes inserted in the electrolyte and all electrodes connected to a potentiostat. A single pulse on the counter electrode, such as a 100-millisecond pulse at +10.2 volts, is used to excite the electrochemical circuit and perform the etch. The process etches uniform patterned holes in the metal layers (such as chromium and molybdenum) of the wafer without adversely affecting the patterned mask.
Joe N. Lucas	**Method for Detecting a Pericentric Inversion in a Chromosome** U.S. Patent 6,140,057 October 31, 2000	A method is provided for determining a clastogenic signature of a sample of chromosomes by quantifying a frequency of a first type of chromosome aberration present in the sample; quantifying a frequency of a second, different type of chromosome aberration present in the sample; and comparing the frequency of the first type of chromosome aberration to the frequency of the second type of chromosome aberration. A method is also provided for using that clastogenic signature to identify a clastogenic agent or dosage to which the cells were exposed.
Roger D. Aines Robin L. Newmark Kevin G. Knauss	**Thermal Treatment Wall** U.S. Patent 6,142,706 November 7, 2000	A thermal treatment wall emplaced to perform in situ destruction of contaminants in groundwater. Thermal destruction of specific contaminants occurs by hydrous pyrolysis–oxidation at temperatures achievable by existing thermal remediation techniques (electrical heating or steam injection) in the presence of oxygen or soil mineral oxidants such as manganese oxide. The thermal treatment wall can be installed in a variety of configurations, depending on the specific objectives, and can be used to clean up groundwater contamination in situ, rather than extracting contaminated fluids to the surface for cleaning. In addition, the thermal treatment wall can be used for both plume interdiction and near-wellhead in situ groundwater treatment. Thus, this technique can be used for a variety of groundwater contamination problems.
William M. Greenbaum	**Active Alignment-Contact Verification System** U.S. Patent 6,143,989 November 7, 2000	A system involving an active (that is, electrical) technique for the verification of (1) close-tolerance mechanical alignment between two components, and (2) electrical contact between mating through an elastomeric interface. For example, the two components may be an alumina carrier and a printed circuit board, two mating parts that are extremely small and high density and require alignment within a fraction of a millimeter, as well as a specified interface point of engagement between the parts. The system comprises pairs of conductive structures defined in the surface layers of the alumina carrier and the printed circuit board, for example. The first pair of conductive structures relate to item (1) above and permit alignment verification between mating parts. The second pair of conductive structures relate to item (2) above and permit verification of electrical contact between mating parts.

Awards

Four Laboratory scientists have been named **fellows** of the **American Physical Society**, an honor bestowed on those recognized by their peers for outstanding contributions to physics. The honorees are **Robert Cauble**, **James Hammer**, **Joseph Nilsen**, and **Ann Orel Woodin**.

Cauble, a senior scientist in the Laboratory's High-Energy-Density Physics and Astrophysics Division, was cited for "important contributions to the understanding of the equation-of-state of dense, strongly coupled plasmas." His work has included using a laser to shock matter to a million atmospheres of pressure to learn more about the behavior of hydrogen, laser fusion, and how stars and planets form and evolve.

Hammer was recognized for his pioneering work in developing novel approaches to fusion and high-energy-density plasma applications, including contributions to the fast igniter inertial confinement fusion (ICF) concept, acceleration of compact toroidal plasma rings, and the use of *z*-pinch x-ray sources for ICF.

Nilsen was cited for his contributions to the understanding and development of x-ray lasers. He demonstrated the world's shortest-wavelength, highest-energy x-ray laser and discovered the prepulse technique used to drive virtually all x-ray laser systems.

Woodin was honored for "pioneering the understanding and development of theoretical methods for studying excitation, ionization, and dissociation of polyatomic molecules." She divides her time between the Laboratory and the University of California at Davis, where she is a professor in the Department of Applied Sciences.

For the second consecutive year, **Bruce Curtis** of the Computation Directorate has been a member of a team receiving a **Gordon Bell Prize**, the most prestigious award in high-performance computing. The team comprises 13 members, and it won in the "special" category for its submission, "High-Performance Reactive Fluid Flow Simulations Using Adaptive Refinement on Thousands of Processors." The paper describes the largest and highest-resolution three-dimensional simulation of a detonation front propagating through stellar material. Curtis says, "This helps determine how a supernova explodes and aids in the understanding of the origin and evolution of the chemical elements."

Dave Cooper, Associate Director for Computation, says of Curtis, "Bruce is a person with almost unique skills. He is one of just a few people in the world who fully understand all of the details of a computer as well as how applications 'fit' on them and run." On Curtis's two consecutive wins, Cooper likens it to "winning back-to-back Oscars!"

Abstracts

Inside the Superblock

Livermore's Superblock is home to one of only two defense plutonium research and development facilities in the U.S. Research on uranium and tritium, a radioactive form of hydrogen, is also undertaken here, albeit to a lesser extent. In the Superblock facilities, the Nuclear Materials Technology Program has the capability to handle all phases of virtually any project related to these materials. Today, much work there is related to the stewardship of our nation's arsenal of nuclear weapons. Experiments in the Superblock are key to the annual process of certifying the safety and reliability of the nuclear stockpile. Livermore is also leading the research and development of safe ways to dispose of surplus plutonium from the Cold War.

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Exploring the Fundamental Limits of Simulation

Computer simulation has become an important tool in scientific and engineering research, especially at national research centers such as Lawrence Livermore. The growing use and influence of simulations, however, has raised important questions about its limitations. Last October, some 60 of the nation's leading simulation experts gathered at Livermore to discuss the wide range of barriers facing advanced computer simulations. Several basic issues, from computer architecture to software challenges, arose from the workshop that crossed major disciplines. The workshop was so successful that plans are under way for a number of future meetings.

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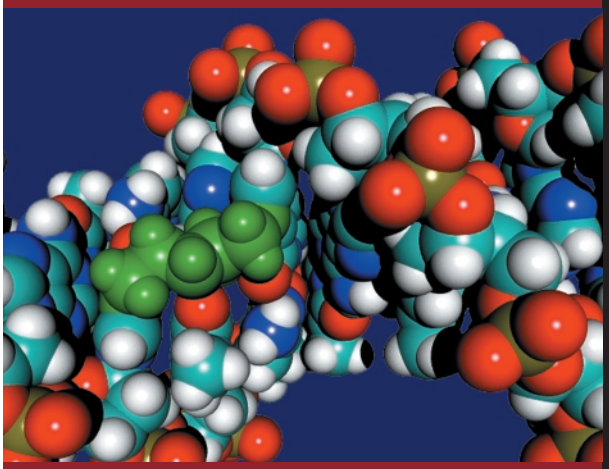
Coming Next Month

Computational Biochemistry

A New Dimension of Biological Research



Livermore scientists are linking advanced simulations with laboratory experiments to explain biological phenomena at an unprecedented level of detail.

Also in April

- *Livermore's Large Optics Diamond Turning Machine continues making large mirrors of extraordinary accuracy for NASA and advanced telescopes.*
- *Scientists from Livermore and the University of California at Davis Cancer Center have joined forces to discover better ways to prevent, detect, diagnose, and treat cancer.*
- *Improvements in stackable magnetic random access memory speed up information retrieval and delivery to supercomputing microprocessors.*

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