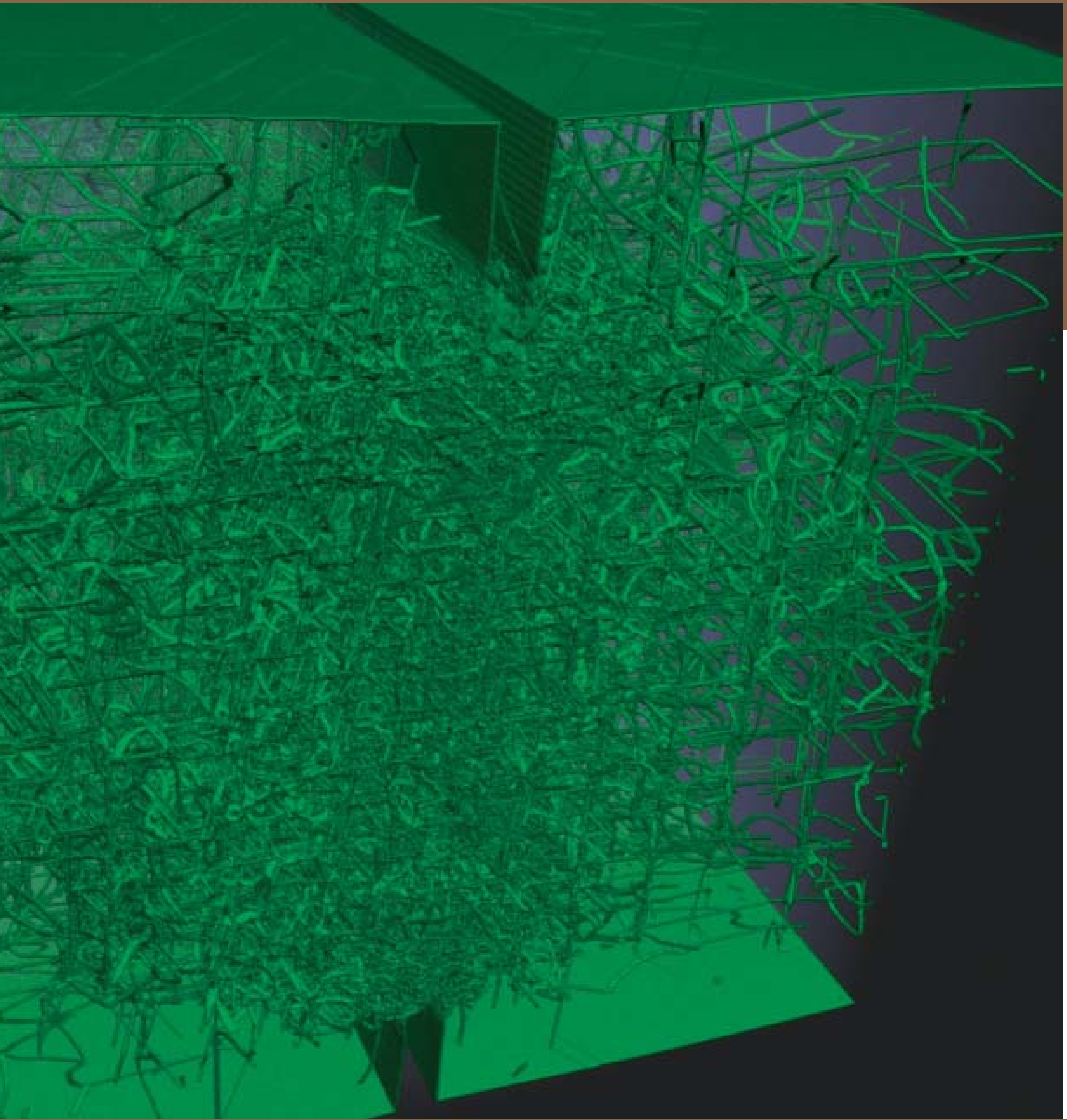


Dislocations lead to ductile failure in a simulation of copper metal under strain.

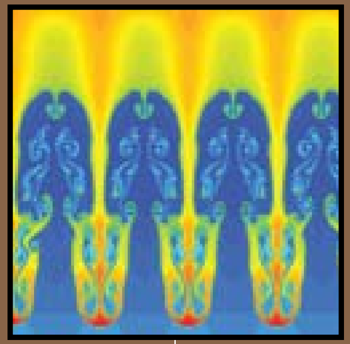
MEETING ENDURING *National Needs*

As part of its overarching national security mission, the Department of Energy pursues research and development in areas of enduring importance to the nation. DOE mission priorities in energy and environment, bioscience, and fundamental science and applied technology are supported by Laboratory researchers. Livermore seeks challenges that reinforce its national security mission and have the potential for high-payoff results.

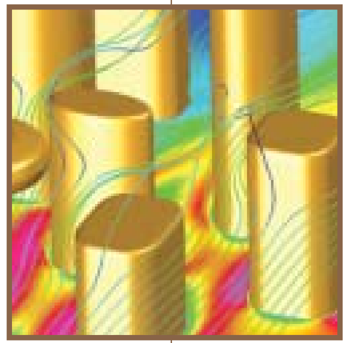
Long-term research is needed to provide the nation with abundant, reliable energy as well as a clean environment. Livermore's energy and environmental programs contribute to the scientific and technological basis for secure, sustainable, and clean energy resources for the U.S. and to reducing risks to the environment.

Bioscience research at Livermore enhances the nation's health and security. Projects in molecular biology, genetics, computational biology, biotechnology, and health-care research leverage the Laboratory's physical science, computing, and engineering capabilities. Research is directed at understanding the causes and mechanisms of ill health, developing biodefense capabilities, improving disease prevention, and lowering health-care costs.

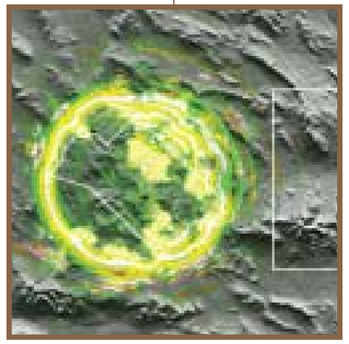
Livermore also pursues initiatives in fundamental science and applied technology that reinforce the Laboratory's strong research expertise. Many projects, sponsored by DOE's Office of Science and other customers, take advantage of the unique research capabilities and facilities at Livermore. Other work, supported by Laboratory Directed Research and Development funding, extends the Laboratory's capabilities in anticipation of new mission requirements.



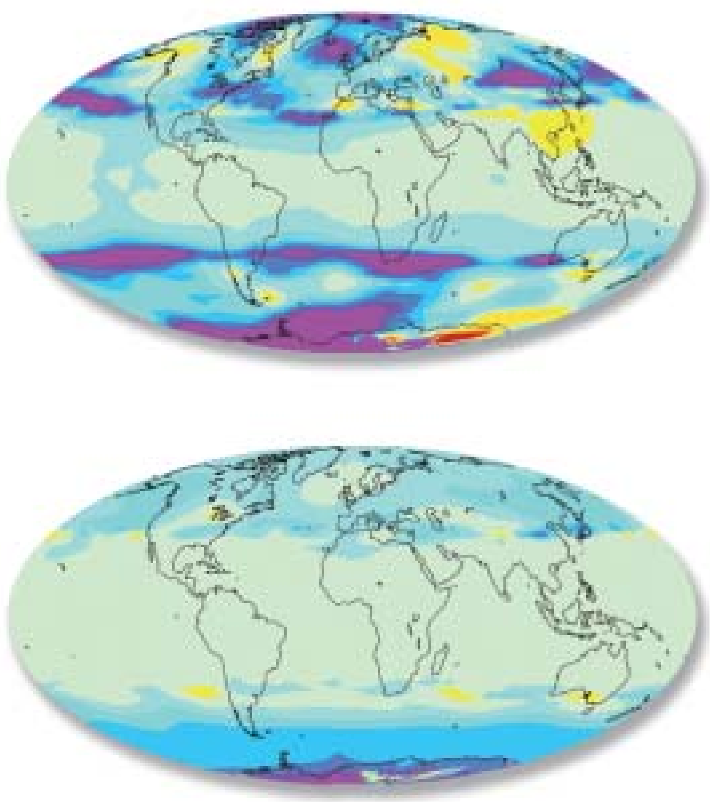
Hydrodynamic instability calculation.



Model of atmospheric dispersion in a cityscape.



Model of seismic energy moving in a complex geology.



Data for change in tropopause height (top) resemble simulation for the same period (bottom).

Modeling Human Effects on Global Climate Change

Computer simulations and data gathering by Livermore researchers are contributing to worldwide efforts to better understand the history of the Earth's climate, changes due to human activities, and methods for mitigating the harmful effects.

An international team of scientists, led by researchers from Livermore, has discovered that emissions from human activities are largely responsible for a significant increase in the height of the tropopause, the boundary between the troposphere and the stratosphere. Their results appeared in *Science*. The research was based on advanced climate models showing that human-induced changes in ozone and well-mixed greenhouse gases are the primary causes of the approximately 200-meter rise in the tropopause that has occurred between 1979 and 1999. Another team has discovered that satellite data used to measure temperature changes in various layers of the atmosphere contain uncertainties that may hamper the detection of human effects on climate change.

An article in *Nature* describes Livermore research on the effects of carbon dioxide on Earth's oceans. Models revealed that continued release of carbon dioxide during the next several centuries would increase ocean acidity more rapidly than during the past 300 million years, resulting in damage to marine life. Oceanic absorption of carbon dioxide had been viewed as beneficial because it removed greenhouse gases from the atmosphere. However, the increased acidity may damage marine organisms such as coral reefs, calcareous plankton, and sea life with calcium carbonate skeletal material. Organisms living in the deep sea may be particularly sensitive to increased ocean acidity.

A Year for Celebration in Genomics

In May 2003, the Human Genome Project, including DOE, the National Institutes of Health, and other laboratories around the world, declared its task of sequencing the human genome complete. The largest biological project ever undertaken, the Human Genome Project determined the sequence of the genome's three billion DNA base pairs. DOE's Joint Genome Institute (JGI) in Walnut Creek, California—a consortium formed by Lawrence Livermore, Lawrence Berkeley, and Los Alamos national laboratories—sequenced chromosomes 5, 16, and 19, which together constitute 11 percent of the human genome. JGI is currently sequencing about 2 billion base pairs per month for the study of a variety of organisms.

Also during the spring of 2003, celebrations around the world feted the 50th anniversary of Watson and Crick's discovery of the double helix structure of DNA, the "molecule of life." And Livermore marked the 40th anniversary of its Biology and Biotechnology Research Program, which has been an active participant in genome sequencing and the many research endeavors that have spun off from that effort.

Analysis at JGI of the genomes of several microscopic ocean-dwelling organisms is providing new insights into how the planet's oceans affect its climate. Comparative studies of four types of cyanobacteria—"photosynthetic" microbes that derive energy from sunlight, just like plants—were published in *Nature* and the *Proceedings of the National Academy of Sciences*. Three of the microbes were among the first organisms to have their DNA sequenced at JGI in the late 1990s and were the first ocean bacteria to be sequenced. Cyanobacteria are the smallest, yet most abundant photosynthetic organisms in the oceans, and they play a critical role in regulating atmospheric carbon dioxide, a major contributor to global climate change. Two of the cyanobacteria remove about 10 billion tons of carbon from the air each year, or two-thirds of the total carbon fixation that occurs in oceans.

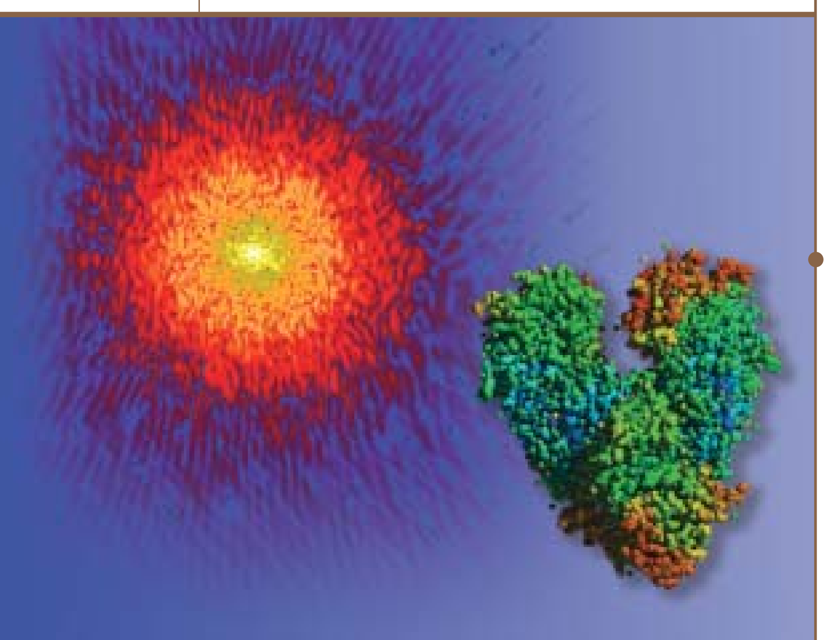
Measuring and Understanding Radiation Dose

New Laboratory research reaffirmed the accuracy of a 1986 study of radiation absorbed by survivors of the atomic bombs dropped on Hiroshima and Nagasaki. The controversial study had determined an absorbed dose that was much higher than earlier estimates. A computer-based search of Livermore's nuclear data libraries revealed that the reaction of neutrons on copper to produce nickel-63, which has a 100-year half-life, could still be detected and quantified today, more than 50 years after the event. But because the nickel-63 content is less than one million atoms per gram of copper, it first took Livermore scientists three years to develop a method that could isolate the nickel-63. Lightning rods, rain gutters, and copper roofing materials collected as far as 5,000 meters from the epicenter of the Hiroshima blast provided samples that were analyzed by the highly sensitive mass spectrometer at Livermore's Center for Accelerator Mass Spectrometry. The quantities of

Joint Genome Institute.

Center for Accelerator Mass Spectrometry.

Prototype focusing lens for the Linac Coherent Light Source.



Simulated diffraction pattern and model of the lethal-factor protein of an anthrax spore.

remaining nickel-63 revealed absorbed doses that were consistent with the 1986 findings, except at the closest distances. The study suggests that these results may be consistent with a slightly underestimated height-of-burst for the Hiroshima bomb.

Livermore has also performed some of the first research into the effects of low-level ionizing radiation. Using laboratory mice and human cell cultures, experiments show that a low-level dose causes cells to activate genes that specialize in repairing damaged chromosomes, membranes, and proteins and in countering cellular stress. The activity of these cells is not simply a reduced level of that seen in cells exposed to high doses of ionizing radiation. Rather, many genes are called into action in response only to low doses of radiation.

Developing Tools to Image Molecular Dynamics

Intense sources of light are essential for Laboratory advances on several fronts—from the imaging of biological molecules to the study of materials in weapons at extreme conditions. Innovations by Livermore researchers are contributing to the development of light sources that are brighter, faster, and more energetic than current capabilities.

A next-generation light source, the Linac Coherent Light Source (LCLS), is being designed for installation at the Stanford Linear Accelerator Center (SLAC). Livermore is part of the SLAC-led consortium to plan, design, and build the LCLS. When it becomes operational in 2008, LCLS will be the world’s first large-scale x-ray laser. Its x-ray beam will be as much as 10 billion times brighter than that of any x-ray light source available today. The light will last for only quadrillionths of a second, allowing the beam to capture the dynamic motion of molecules.

Livermore’s primary responsibility is to design and fabricate the optics that will transport the x-ray beam to experimental chambers and to diagnose the beam’s condition. Because of its extreme brilliance and ultrashort duration, a single x-ray pulse can melt many materials, which makes designing optical systems a challenge. Incorporating significant design innovations, Laboratory researchers are making great strides in developing a high-resolution camera for beam diagnostics, optical devices to redirect the beam, and focusing lenses that will not be damaged. Other Livermore scientists are examining possibilities for LCLS experiments and developing techniques for analyzing the diffraction data that will be produced by experiments.

X-ray imaging is also the goal of the Picosecond Laser-Electron Inter-Action for the Dynamic Evaluation of Structures (PLEIADES) project. The PLEIADES team has succeeded in creating high-brightness x rays (known as Thomson x rays) by colliding an energetic electron beam with a high-intensity laser. In January 2003, the first 70-kiloelectronvolt light was produced in experiments using the Laboratory’s 100-megaelectronvolt linear accelerator and FALCON laser. Supported by Laboratory Directed Research and Development funding, work continued in 2003 to increase x-ray production by improving the quality of the laser and electron beams and to prepare to conduct diffraction experiments. The goal is to use the extremely short burst of x rays, from 1 picosecond (10^{-12} seconds) to 100 femtoseconds (10^{-13} seconds) long, to image a variety of physical, chemical, and biological dynamic phenomena. Of particular interest will be experiments in which a strong shock is applied to a sample of dense material whose properties are then probed.

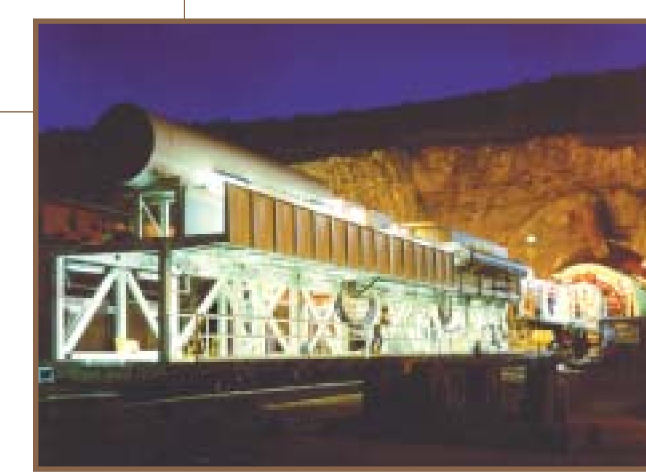
Other Laboratory scientists are using an extremely short pulse (10 trillionths of a second), high-power (100-terawatt) laser to create a focused beam of high-energy protons that could be used to rapidly heat and then image targets. These JanUSP laser experiments are described on p. 11.

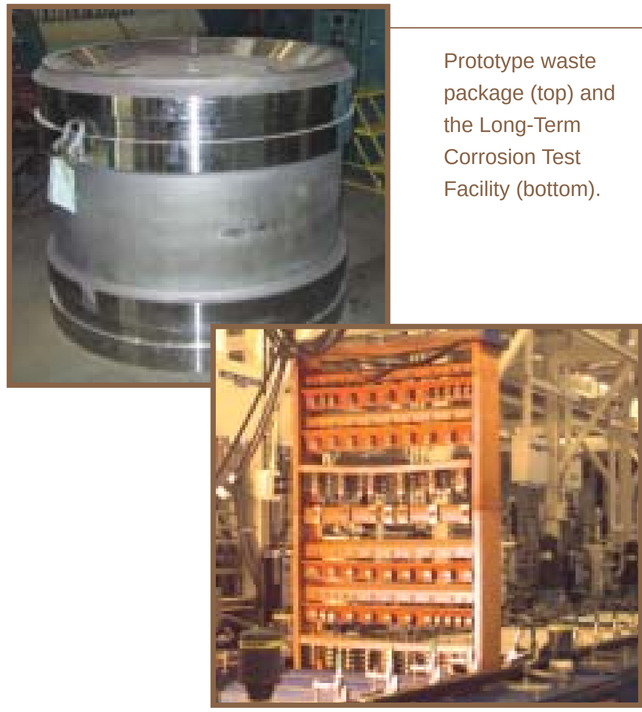
Materials Testing and Modeling for the Yucca Mountain Project

A team of Livermore researchers is testing and refining the design and materials for what may eventually be 12,000 nuclear waste packages as part of DOE’s program to design, license, and build an underground nuclear waste repository in Yucca Mountain, Nevada. Currently, DOE is preparing an application to obtain a Nuclear Regulatory Commission license to proceed with construction of the repository. The Laboratory is focusing on developing the engineered barrier system. This system consists of a waste package, drip shield, and supporting structures. The engineered barrier system is designed to work with the natural barriers of Yucca Mountain to contain the repository’s radioactive wastes and prevent them from seeping into the water table, which lies about 300 meters below the planned repository.

Linear accelerator used for PLEIADES.

Yucca Mountain Project.





Prototype waste package (top) and the Long-Term Corrosion Test Facility (bottom).

The Sustained Spheromak Physics Experiment.

In the current repository design, waste will be stored in a package consisting of corrosion-resistant metal (Alloy 22) and an inner canister made of a tough, nuclear-grade stainless steel (316NG). An overhanging drip shield made of titanium will give added protection from dripping water and any rocks falling from the repository ceiling. To gather information about how these materials will behave over thousands of years, researchers are conducting accelerated aging tests at the Laboratory's Long-Term Corrosion Test Facility. Some 20,000 test specimens are now being or have been exposed to the range of conditions expected to occur in the repository. In addition, in analyses that require the Laboratory's supercomputers, scientists are simulating the geologic evolution of the repository to predict the temperature evolution surrounding the buried waste and explore the possible means by which water could enter the repository tunnels over geologic time periods.

Progress in Magnetic Fusion Energy Science

In 2003, Laboratory researchers advanced magnetic fusion energy science through computational and experimental work performed primarily for DOE's Office of Science. Livermore collaborates in experiments using the DIII-D Tokamak at General Atomics in San Diego. Researchers also develop advanced computational models to study turbulence and other physical phenomena at the edge of the plasma. Building on the success achieved with these models, Laboratory scientists are undertaking the challenge of developing a first-principles model of the edge of high-performance tokamak plasmas, a region of steep temperature and density gradients. Results will have important implications for the performance of the International Thermonuclear Experimental Reactor (ITER), a major international project with significant U.S. participation.

In addition, Livermore is the site of the Sustained Spheromak Physics Experiment (SSPX), an alternative to the tokamak concept that may lead to lower-cost fusion reactors because of the spheromak's compact size and reduced complexity. Performance of the SSPX has increased significantly in the past few years. The pulse length has been extended to 4.5 milliseconds, and plasmas have been produced with low impurity content, high temperatures (over 240 electronvolts), and high plasma pressure. In 2003, SSPX researchers were selected to be part of the National Science Foundation Physics Frontier Center for studies in magnetic reconnection.

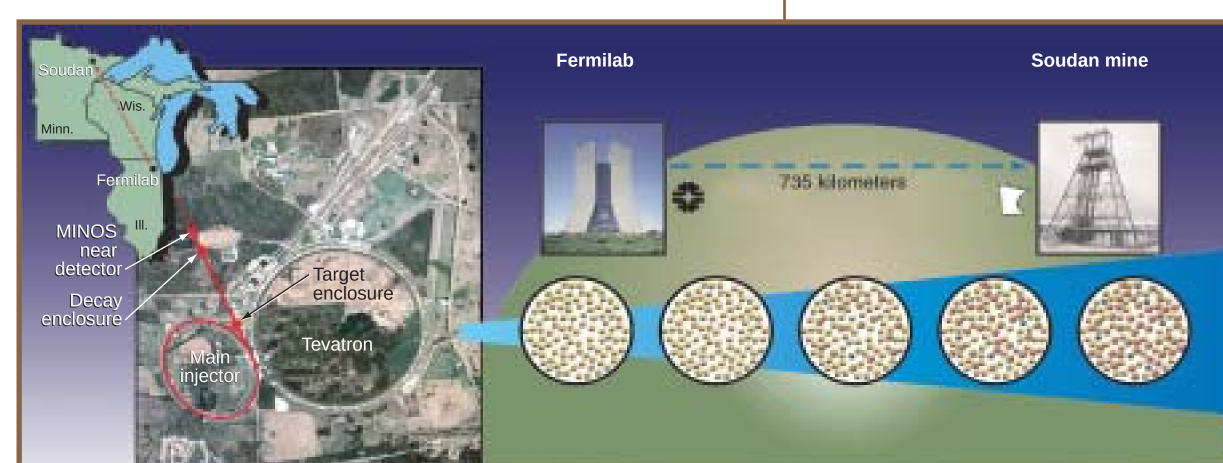
Experiments to Unravel the Nature of Matter

Livermore is engaged in a variety of large international physics projects, providing expertise in the underlying physics, sophisticated data analysis capabilities, and critically needed engineering solutions to challenging problems. For example, the Laboratory took the lead in design work—and devised the solution that was implemented—for steel detector planes for Fermi National Laboratory's Main Injector Neutrino Oscillation Search (MINOS) experiment. Because neutrinos are extremely difficult to observe, the detector required 450 steel planes, each 8 meters in diameter and weighing 10,000 kilograms. The planes had to be lowered 800 meters down a mine shaft only 2 meters across. In 2003, the detector system was assembled in a former iron mine in Soudan, Minnesota, and the MINOS experiment is expected to be up and running in early 2005.

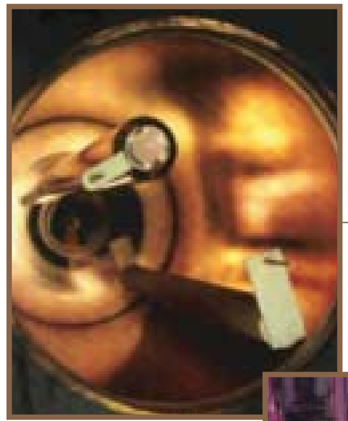
MINOS, which involves more than 200 scientists from many institutions, aims to look for neutrino oscillations (changes from one type of neutrino to another) as an explanation for why there are "missing neutrinos" in studies of cosmic rays and the energy output of the Sun. From Fermilab's home in Illinois, an intense beam of neutrinos will be directed toward Soudan, 735 kilometers away. Despite its immense size, the MINOS apparatus will be able to detect only about 9,000 of the 5 trillion neutrinos produced at Fermilab during each year of the experiment.

In more modest experiment, researchers at the Livermore site are engaged in the search for another elusive particle—the axion. This particle, if found to exist, would help "balance the budget" for the missing mass in the universe and clear up one of the thorniest issues in particle physics. The experiment is searching for the

Detector planes for MINOS neutrino detector.



From Fermilab to the MINOS detector.



Axion detection experiment.

Laser creates an artificial guide star at the Keck II telescope.

decay of an axion into a single photon in the presence of a strong magnetic field, which is provided by a 6-ton superconducting coil.

After Livermore's Laboratory Directed Research and Development Program provided the necessary groundwork, the Livermore axion experiment began in 1995 with funding from DOE's Office of Science. The team includes researchers from the Laboratory, the University of Florida, the University of California at Berkeley, and the National Radio Astronomy Observatory. No axion decays have yet been detected, setting an upper limit on the cosmic density of axions. The next generation of axion detectors at Livermore, which are being planned, should be able to answer the question of whether axions exist.

A Sharper View of the Universe

On September 20, 2003, scientists at the W. M. Keck Observatory on Mauna Kea, Hawaii, used a laser developed by the Laboratory to create an artificial guide star on the Keck II 10-meter telescope. With the guide star, researchers can make fuller use of the telescope's adaptive optics system, which was also developed by Livermore scientists and installed in 1999.

Adaptive optics allow astronomers to minimize the blurring effects of Earth's atmosphere, producing images with unprecedented detail and resolution. The system uses light from a relatively bright star to measure distortions caused by the atmosphere and then correct for them. But only about 1 percent of the sky contains stars sufficiently bright to be of use. By using a laser to create a virtual star, astronomers can study much fainter objects, increasing coverage to more than 80 percent of the objects in the sky. Laser guide stars have been used on smaller telescopes, but this is the first successful use on the current generation of large telescopes.

Major New Computers Augment Livermore's Capabilities

Since 1996, the Laboratory has made institutional investments, leveraging the ASC Program (see p. 12) to provide powerful computers for use by researchers in all programmatic areas. Because of this effort, called the Multiprogrammatic and Institutional Computing (M&IC) Initiative, Livermore has assumed a leadership position in the development and application of new classes of low-cost, reliable, high-performance production computers. Central to M&IC's achievements have been the development of strategic relationships with key vendors and the prototype application of their extraordinarily low-cost systems to scientific problems. Prior M&IC successes motivate vendors to bid new systems aggressively to the Laboratory, as success at Livermore becomes part of their marketing strategy. This further drives down cost, leads to more achievements, and gives the Laboratory options to explore additional paths to extremely low-cost computers that might operate in the petaops range. An important science and technology thrust area for the Laboratory is the development of petaops-scale simulations and the invention of better tools for mining data and integrating experiments and simulations (see p. 12).

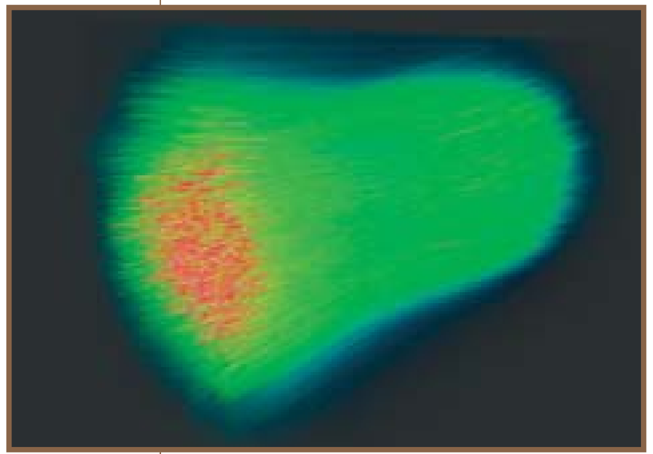
As an example of this strategy, M&IC has recently focused on acquiring low-cost Linux clusters. By leveraging ASC-developed software and technology, Livermore has been at the leading edge in using these as high-capability computers for production runs of science and engineering simulation models. The first such system to gain national recognition was the Multiprogrammatic Capability Resource (MCR) supercomputer, capable of 11.2 teraops. This system was integrated in Utah in summer 2002 and started running large-scale applications in December. In the June 2003 Top500 supercomputing list, MCR was ranked as the world's third fastest computer. The machine has been used as a production resource since August 2003 and dramatically increased Livermore's unclassified computing capability.

Competition for access to the MCR rapidly saturated the machine. In part because of this, Livermore is procuring a far more powerful system called Thunder. This machine, integrated by California Digital Corporation, features a peak speed of 22.9 teraops and uses 1,024 high-performance Intel Tiger-4 nodes with four Itanium 2 processors and 8 gigabytes of memory each. The Laboratory is partnering with Intel to improve the compiler, as this is a key element of achieving high performance. The machine is expected to move into full production in summer 2004.

First-Principles Simulations

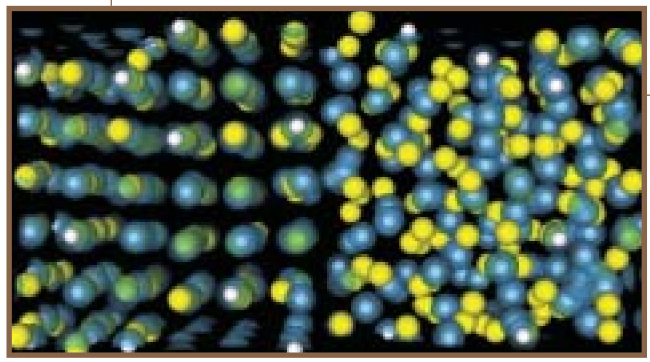
First-principles simulations, based on fundamental properties of matter derived from quantum mechanics, are providing a new avenue for exploring properties of condensed matter in extreme conditions. Because these simulations do not rely on any empirical or adjusted parameters, they are capable of making much needed

The 11.2-teraops Multiprogrammatic Capability Resource (MCR) supercomputer.



MCR simulation of a National Ignition Facility laser beam passing through a hot plasma.

First-principles simulation of lithium hydride shows coexistence of solid phase (left) with liquid phase (right).



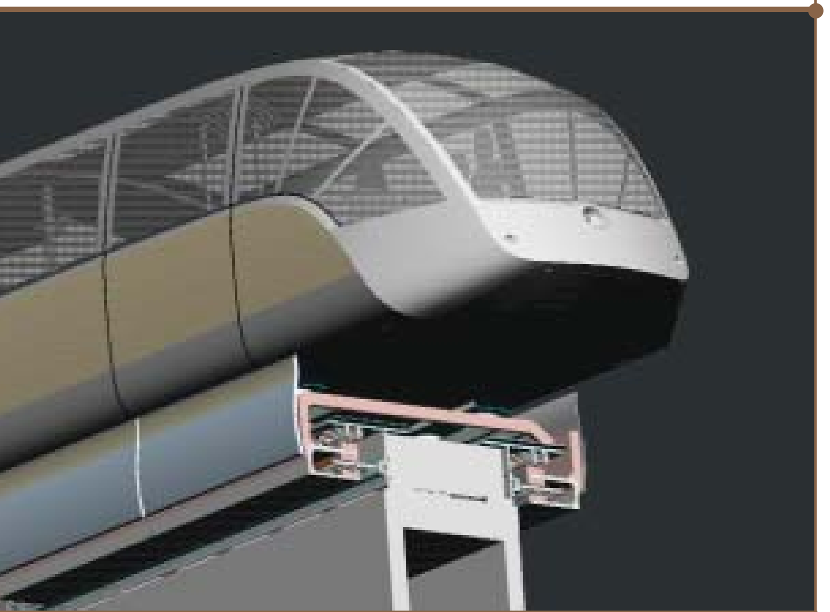
theoretical predictions. A substance's physical properties often change drastically when it is subjected to pressures reaching millions of atmospheres. Hence, an experimental determination of these properties is often complex and expensive.

The first-principles simulation code GP developed at the Laboratory has been used to study the properties of fluids at high pressure. In 2003, an important new capability was added to GP. For the first time, it was possible to accurately simulate the solid–liquid interface of a molecular substance at high pressure and high temperature with a first-principles approach. Using this new method, Livermore scientists were able to predict the melting properties of lithium hydride up to a pressure of 200 gigapascals. Results were published in *Physical Review Letters*.

Maglev on Track for Urban Transportation

Conceived by a Livermore physicist, the Inductrack magnetic levitation (maglev) system for urban and high-speed transportation is moving down the development track. In May 2003, General Atomics (GA) broke ground at its San Diego facility for a 120-meter-long track to conduct a full-scale demonstration. The project is sponsored by the federal government to showcase a new generation of urban transportation technology. GA and the Laboratory have signed a licensing agreement for use of the levitation technology in magnetic levitation train and transit systems.

Inductrack uses unique configurations of powerful, permanent magnets, called Halbach arrays, to create its levitating fields. It offers the promise of safer, cheaper, and simpler means to levitate urban and high-speed trains. While work on the demonstration effort proceeds in San Diego, the Livermore team is optimizing the design of the magnets and the track. In particular, the team is working on a revised design for the track, which is even simpler and should be less expensive to manufacture than the original.



Front end of the urban maglev vehicle.

Award-Winning Laser Technologies Benefit Industry

Innovative laser technologies developed at Livermore are improving processes used to manufacture aircraft parts. In 2003, Livermore and its industrial partner, New Jersey–based Metal Improvement Company, Inc., received an R&D 100 Award for a laser process for forming thick, curved metal parts. Called Lasershot™ Precision Metal Forming, the technique is especially effective for forming pieces greater than 2 centimeters thick—pieces so thick that they are difficult to shape by other means without weakening the material structure.

Lasershot™ Precision Metal Forming shapes parts to exact curvature and contour specifications, preserves a smooth surface finish, and leaves the parts resistant to stress corrosion cracking and failure from fatigue. The technique uses a solid-state laser system that induces a deep level of compressive stress on a section of metal, which elongates the treated surface, effectively bending the metal within the processed area. The process can be applied to any metal or alloy and is particularly effective with the aluminum alloys used for structural aircraft components. It can also be used to precisely form the final shape of nuclear waste canisters, which could be used in the Yucca Mountain waste repository program.

Developers of Lasershot™ Precision Metal Forming, which won a 2003 R&D 100 Award.

Six R&D 100 Awards in 2003

Livermore scientists and engineers earned 6 R&D 100 Awards for outstanding achievement in research and development. Each year *R&D Magazine* presents awards to the top 100 industrial, high-technology inventions submitted to its competition. The Laboratory's award winners (listed on p. 44) will have applications in laser machining, computer-chip manufacturing, high-power lasers, health care, and the war on terrorism. They bring to 97 the number of R&D 100 Awards that Livermore researchers have won.

A team of scientists from three national laboratories—Livermore, Sandia, and Berkeley—and one company, Northrop Grumman Space Technology/Cutting Edge Optronics, also received one of three Editor's Choice awards for the most outstanding achievement among award winners. Their Extreme Ultraviolet Lithography (EUVL) Full-Field Step-and-Scan System was honored for making the "greatest improvement upon an existing technology" for advancing the field of lithography.

Front view of the EUVL Full-Field Step-and-Scan System.