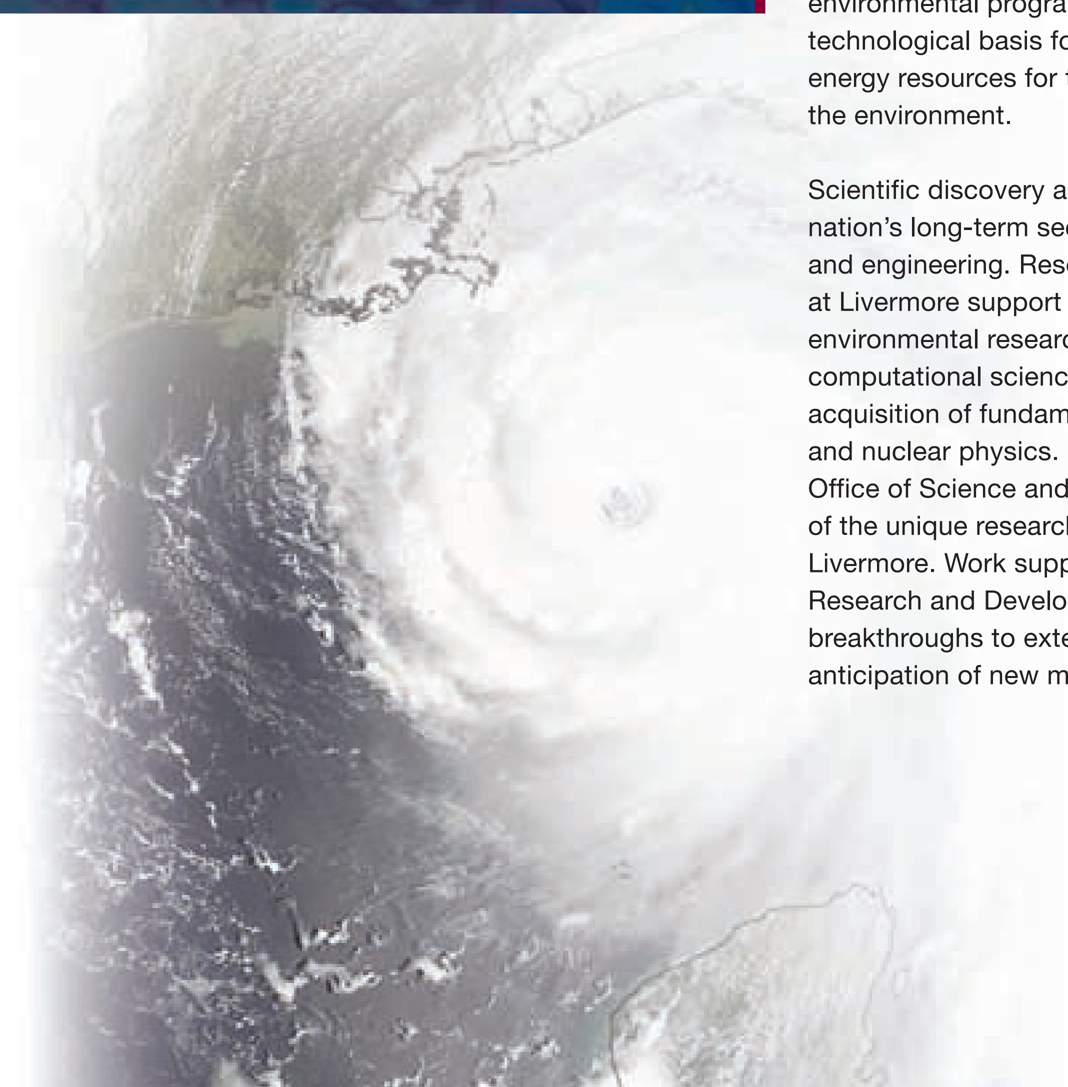
Enduring National Needs

As part of its overarching security mission, the Department of Energy (DOE) pursues research and development to provide reliable and affordable energy for the nation and to keep the U.S. at the forefront of international science and technology. Laboratory research programs support DOE priorities to meet these enduring national needs. Livermore continually seeks challenges that reinforce its national security mission and have the potential for high-payoff results.

Energy security is a central DOE mission, and long-term research is essential to ensuring abundant 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 for reduced risks to the environment.

Scientific discovery and innovation, also vital to the nation's long-term security, require leadership in science and engineering. Research and development activities at Livermore support DOE's goals in biological and environmental research, fusion and plasma science, computational sciences, basic energy sciences, and acquisition of fundamental knowledge in high-energy and nuclear physics. Projects sponsored by DOE's Office of Science and other customers take advantage of the unique research capabilities and facilities at Livermore. Work supported by Laboratory Directed Research and Development funding aims at scientific breakthroughs to extend Livermore's capabilities in anticipation of new mission requirements.



Stardust Surprises

Livermore researchers were on hand in January when samples from the Wild 2 comet first arrived at Johnson Space Center in Houston. The particles were captured in 2004 when the National Aeronautics and Space Administration's (NASA's) Stardust spacecraft flew through Wild 2's tail. Laboratory scientists have been involved in virtually all phases of the highly successful scientific mission—from the development of technologies for sample collection and extraction to the first analyses of the cometary materials, which were full of surprises.

As Stardust neared Wild 2 at a relative speed of more than six kilometers per second, the spacecraft briefly extended a collector filled with lightweight aerogel glass foam to capture thousands of tiny particles from the comet's tail. The 132 aerogel cells in the collector were designed to cushion the impact and prevent significant damage to the particles. With funding from NASA, Livermore had developed methods to produce the ultralow-density silica aerogel for Stardust. Laboratory scientists also played a major role in the technologies adopted by NASA to extract the particles from the aerogel cells, such as a tiny diamond-blade knife to smoothly cut aerogel, and they performed some of the first extractions at Johnson Space Center.

The biggest surprise is that although comets were formed a long distance from the Sun, far beyond the orbit of Neptune, Wild 2 appears to be full of material from the inner solar system, close to the Sun. This unexpected result means that vastly more mixing of material must have occurred while the Sun and planets were forming than previously thought. Preliminary results from the Wild 2 particle analyses were presented at the American Geophysical Union's fall meeting in San Francisco and simultaneously published in the December 15, 2006, issue of *Science*. Laboratory researchers were coauthors on all seven *Science* papers detailing first findings.

Scientific Discovery with Supercomputers

The Laboratory purchased a next-generation supercomputer powered by Linux cluster technology consisting of three clusters, called Atlas, Zeus, and Rhea, for a total of 77 teraflops. The largest cluster, Atlas, at 44 teraflops, will serve as the mainstay of the Laboratory's Multiprogrammatic and Institutional Computing Program, which is a resource for unclassified, high-end computing across the Laboratory. Atlas will greatly

John Bradley (left) celebrated when Stardust returned to Earth, and Hope Ishii (above) showed an aerogel cometary dust collector to the media. Analyses of Wild 2 particles used the Laboratory's unique capabilities, including the super scanning transmission electron microscope (SuperSTEM), the world's most powerful electron microscope. It allows atomic-scale analyses of a particle's composition.

augment the capabilities of Thunder, a 23-teraflop cluster that was the world's second fastest computer when it was introduced in 2004. Thunder runs unclassified "grand challenge" problems—large calculations that promise breakthrough science. Thunder results have helped Laboratory scientists solve problems ranging from high-resolution climate modeling and seismic simulations to protein folding and molecular dynamics.

Several grand challenges lie in the area of material properties. Whether studying an organic material, such as a protein, or an inorganic material, such as a metal, scientists must understand the origin of its microstructural features to predict the material's properties. In metals, atoms stack in an orderly fashion, forming a crystal lattice. However, some regions have impurities or misaligned planes of atoms, called dislocations. In large-scale simulations of dislocation dynamics—the interaction of dislocation lines under conditions of stress—Laboratory scientists found the common presence of three or more intersecting dislocation lines. These knots greatly add to a stressed metal's strength. Results were reported in the April 27, 2006, issue of *Nature*.

Laboratory scientists and collaborators also simulated the folding of the 1BBL protein, which has also been studied in experiments. The simulations, comprising about 65,000 atoms, most of them water molecules, were replicated 256 times at temperatures ranging from 250 to 600 kelvin. The calculations confirmed experimental results that the folding is a "downhill" energy process. However, an initial energy barrier has to be overcome for a synthesized protein to collapse into a globular package that then loses energy as it folds into its native state. These simulations were three times larger and four time longer than any done previously.

In addition, Livermore scientists continue to advance the state of the art in scientific simulations, software development, and data visualization and interpretation. More than 40 Laboratory researchers are working on 14 multi-institutional scientific computing projects as part of the DOE Office of Science Scientific Discovery through Advanced Computing Program. Two R&D 100 award winners in 2006 exemplify the capabilities developed by Livermore computer scientists: Babel, a program that allows software written in different programming languages to seamlessly pass scientific data back and forth, and Sapphire, a sophisticated tool for mining scientific information from terabytes of data.

Tom Arsenlis (left) and Vasily Bulatov used the Parallel Dislocation Simulator (ParaDIS) code to study how metals deform and fail.

Climate: Volcanoes, Hurricanes, and California

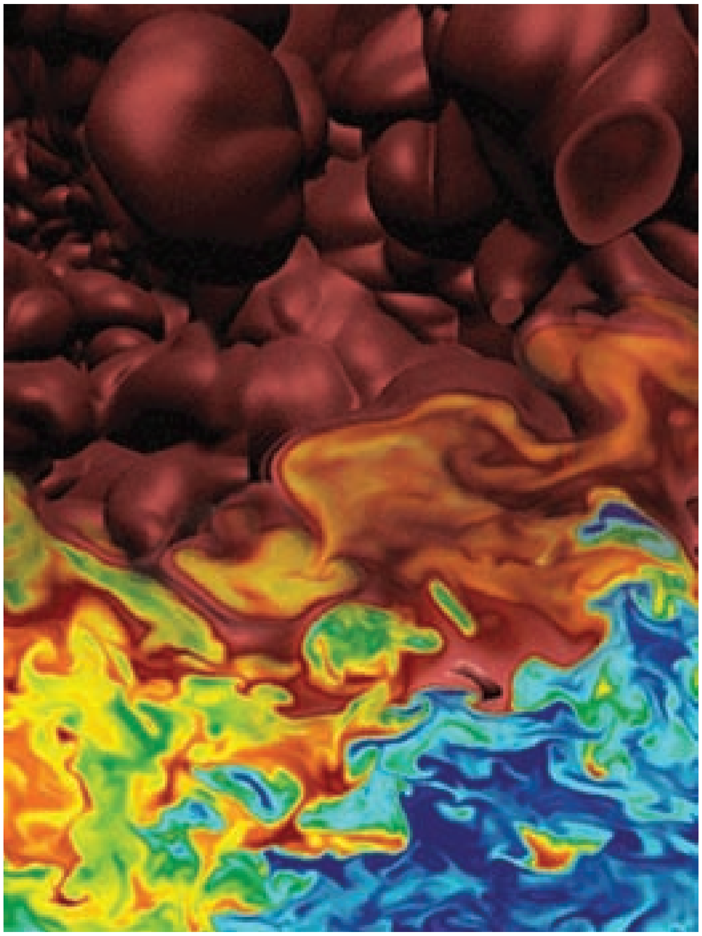
Livermore is contributing to a variety of efforts to better understand factors affecting global and regional climate. In May 2006, the U.S. Climate Change Science Program released *Trends in the Lower Atmosphere: Steps for Understanding and Reconciling Differences*. Laboratory scientist Benjamin Santer, who was awarded a Distinguished Scientist Fellowship by the DOE Office of Science last year, was one of the report's lead authors and made important contributions to the underpinning research.

In 2006, Livermore scientists (including Santer) and collaborators showed that ocean warming and sea level rise in the 20th century were reduced substantially by the 1883 eruption of the volcano Krakatoa in Indonesia. Volcanic aerosols scatter sunlight and cause the ocean surface to cool. The more recent 1991 Mt. Pinatubo eruption in the Philippines, which was comparable to Krakatoa in size and intensity, resulted in minimal net cooling because it was countered by human-induced warming.

A team of researchers from Livermore and ten other institutions also studied sea surface temperature in hurricane "breeding grounds" of the Atlantic and Pacific oceans. Using 22 different computer models of the climate system, they showed that the warming of these tropical oceans over the last century is directly linked to human activities. These findings complement earlier work that uncovered compelling scientific evidence of a relationship between warming sea surface temperatures and increases in hurricane intensity.

California is another region of special interest. Research indicates that global warming may dramatically change river flows in the state. California's water infrastructure is efficient at providing

Research shows that the warming of the tropical oceans over the last century is linked to human activities, adding to evidence of a link between warming sea surface temperatures and increases in hurricane intensity, as exemplified by Hurricane Katrina.



Researchers used BlueGene/L for this high-resolution simulation of Rayleigh–Taylor instability in supernova thermonuclear burning.

an adequate water supply and minimizing flood risk when there are large amounts of mountain snow. If winter temperatures warm, more rain than snow will fall at higher elevations, and where snow does accumulate, it will melt sooner. Higher river flow rates during winter and lower rates during spring and summer would reduce the overall water supply for the entire year. Other studies examined the impact of temperature rises on California crops.

Astrophysics Discoveries through Simulation

Running advanced simulation models on some of the fastest computers in the world, Laboratory researchers are making exciting discoveries in stellar and planetary astrophysics. One puzzle in stellar evolution has been the fate of helium-3 produced in low-mass stars (one to two times the size of the Sun). The observed amount of helium-3 in the universe is less than that predicted to have been created by the big bang and stellar evolution. By modeling red-giant evolution with a fully three-dimensional hydrodynamic code, Livermore researchers identified a new mixing phenomenon that leads to the burning of excess helium-3. As reported in the October 26, 2006, edition of *Science Express*, predictions now agree with observations.

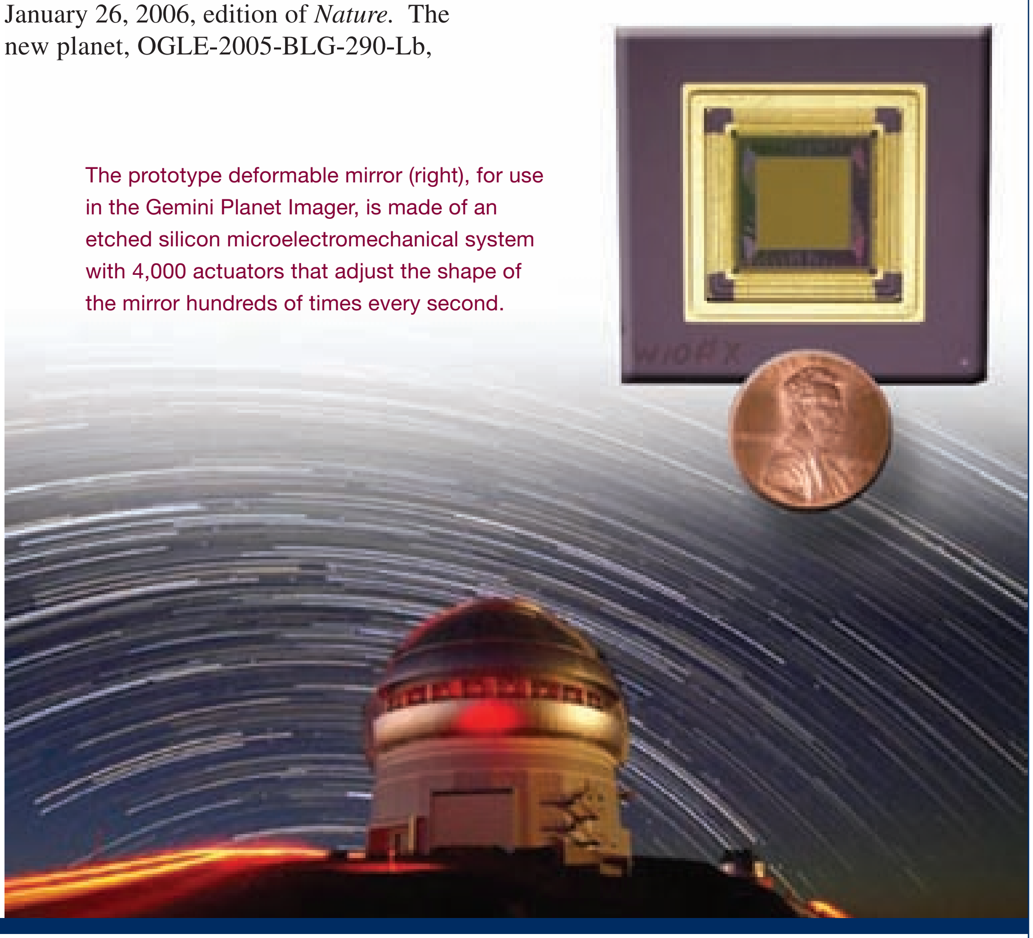
The cover of the August 2006 issue of *Nature Physics* featured a simulation of Rayleigh–Taylor instability—the same phenomenon that mixes a top layer of oil into water. The turbulence of a fluid flow is described by the Reynolds number; when it is above about 2,300, eddies of varying scales are present. The Livermore simulation achieved a Reynolds number of 32,000 and is the first to reach past the turbulent mixing transition at the necessary resolution. These results offer new insights into the dynamics of turbulent combustion in type Ia supernovae. Eddies affect the propagation of thermonuclear burning and the brightness of supernova "standard candles," which are used to guide estimates of distances and the expansion rate of the universe.

Yet another set of simulations revealed important aspects of the behavior of carbon at high pressure and temperature. In particular, they showed the solid–liquid and solid–solid phase boundaries for pressures up to 20 million atmospheres and temperatures of more than 10,000 kelvin. The physical properties of carbon in this regime are of great importance for devising models of Neptune, Uranus, carbon-rich planets in other solar systems, and white dwarf stars.

Finding Distant Planets

An international collaboration of astronomers, including a Laboratory scientist, discovered a small, rocky or icy planet similar to Earth, as reported in the January 26, 2006, edition of *Nature*. The new planet, OGLE-2005-BLG-290-Lb, is the smallest planet yet detected outside our solar system. It has about 5.5 times the mass of Earth and orbits a dim star about 390 million kilometers away. The discovery was made by the Probing Lensing Anomalies Network (PLANET) using microlensing, a technique developed nearly two decades ago by Livermore astrophysicists as part of the Massive Compact Halo Object (MACHO) Project that searched for evidence of dark matter. PLANET observatories in the Southern Hemisphere tracked anomalies in the light from a more distant star. The gravitational pull of the red dwarf and the orbiting Earth-like planet caused the bending of light rays and indicated the presence of a planet.

Livermore scientists are also at the forefront of new technology to directly image distant planets. The Laboratory has been selected to lead the project to build the Gemini Planet Imager for the



The prototype deformable mirror (right), for use in the Gemini Planet Imager, is made of an etched silicon microelectromechanical system with 4,000 actuators that adjust the shape of the mirror hundreds of times every second.

8-meter-diameter Gemini South Telescope in Chile. The Gemini Planet Imager will be the most advanced adaptive optics system in the world. Through the use of adjustable mirrors, adaptive optics allow ground-based telescopes to produce clear images by correcting for atmospheric turbulence, which causes stars to twinkle and appear blurry to astronomers. The system will have a 2-centimeter-square deformable mirror with 4,000 actuators. Etched silicon microelectromechanical systems will adjust the mirror's shape to correct for atmospheric distortions 2,500 times per second with an accuracy of better than 1 nanometer. When the imager is operational in 2010, astronomers will be able to detect planets 30 to 150 light years from our solar system.

Imaging Biological Molecules at the Nanoscale

Laboratory scientists and collaborators for the first time have validated the idea of using an extremely short and intense x-ray pulse to capture an image of a biological object before absorbed energy from the pulse destroys the sample. At the same time, the team established a speed record of 25 femtoseconds (25 millionths of a nanosecond) for flash imaging. The research results were featured on the cover of the December 2006 issue of *Nature Physics*.

The experiment was performed at the free-electron laser at Deutsches Elektronen-Synchrotron (DESY) in Hamburg, Germany. The pulse illuminated a nanostructured object, and the team recorded the pattern of diffracted x rays. A Livermore-developed computer algorithm then recreated an image of the object based on the recorded diffraction pattern. The flash images resolved features 50 nanometers in size, about 10 times smaller than what is achievable with an optical microscope.

The diffraction pattern of a short, intense x-ray pulse directed at a protein formed the basis for this image, which was featured on the cover of *Nature Physics*. Flash diffraction imaging is a new method for gaining atomic-scale information about complex biological molecules.

The new method, called flash diffractive imaging, will be applicable to atomic-resolution imaging of complex biomolecules when even more powerful x-ray lasers, currently under construction, are available. The technique will allow scientists to gain insight into the fields of materials science, plasma physics, biology, and medicine.

Experiments under Pressure

In experiments conducted at Livermore, an international team of researchers demonstrated a new kind of "creep," or flow, in a form of ice with the pressure, temperature, stress, and grain size of those in the deep interiors of large icy moons. The new research revealed a creep mechanism that is affected by the grain size of "ice II." Ice II is thought to exist in a 100-kilometer-thick layer in the interior of moons such as Saturn's Titan. The experimental results, presented in the March 3, 2006, issue of *Science*, imply that the ice II layer is significantly weaker than previously thought. The discovery will change scientists' thinking about the thermal evolution and internal dynamics of the medium- and large-size moons of outer planets, and about what was happening in the early solar system.

The same issue of *Science* reported the results of another international collaboration involving Laboratory scientists. They synthesized a novel class of nitrides made from noble metals under extreme conditions. Noble metals do not easily form compounds with other elements. With a diamond anvil cell creating high pressures and a laser creating high temperatures, the researchers made the first bulk nitride of the noble metal iridium. By combining experimental results with first-principles theoretical modeling, the scientists determined the structure of the known nitride of platinum. The semiconductor industry currently uses titanium nitrides because of their strength and durability. These new nitrides may prove to be even more durable than titanium.

At the European Synchrotron Radiation Facility, Laboratory scientists in an international team conducted x-ray scattering experiments to study the lattice dynamics of molybdenum samples. Experimental results combined with simulations enabled scientists to better understand a high-pressure anomaly in molybdenum. The simulations won the Gordon Bell Prize for 2006 (see p. 9).

Biological Discovery

Research has shown that many of the complex biochemical networks needed for the existence of advanced organisms could not have evolved without oxygen. Laboratory scientists used a Monte Carlo computer simulation and a large bioinformatics data base (the Kyoto Encyclopedia of Genes and Genomes, or KEGG) to study the effect of oxygen on metabolic networks—the biochemical systems that enable organisms to convert food and nutrients into life-sustaining energy. Starting with randomly selected seed conditions (a set of reactants), the simulations generated about 100,000 different reaction networks. Analysis showed that the largest and most complex networks require the presence of molecular oxygen, which offers organisms opportunities for respiration and the biosynthesis of entirely new classes of molecules. The results appeared in *Science* on March 24, 2006.

In another computational study, a Livermore chemist revealed the characteristics of the pigment in curcumin that give it the ability to prevent and even treat Alzheimer's disease. Experimental work on mice performed at the University of California (UC), Los Angeles, indicated that curcumin, the yellow pigment in the east Indian root plant turmeric, can penetrate the blood–brain barrier, the natural mechanism that protects the brain. It also can bind to and reduce amyloid plaque in brain cells, which is a cause of Alzheimer's disease. The Livermore study shed light on the hydrophobic and hydrophilic properties of curcumin that make possible both penetration and binding. The simulations further revealed the three-dimensional structure of the most stable form of curcumin, which may allow other drugs to be discovered through molecular similarity.

Laboratory scientists and collaborators took a small but valuable step toward understanding how cells function and how viruses interact with cells. They developed a method that can directly test for the existence of lipid rafts in cellular membranes. Lipids in the cell membrane are believed to form compositionally distinct domains, called lipid rafts, that serve a critical role in the organization of the cell membrane. The research team formed model cell membranes on a silicon chip, induced the formation of lipid-raft-like gel domains, and freeze-dried the membranes. Then, with NanoSIMS, the Laboratory's high-resolution secondary ion mass spectrometer, the scientists were able to detect gel domains and measure their size. Their work was reported in the September 29, 2006, issue of *Science*.

Accelerating Biomedical Research

At Livermore's Center for Accelerator Mass Spectrometry (CAMS), home to the most versatile and productive AMS facility in the world, a team of scientists developed an AMS technique for early detection of bone cancer, which could help physicians design methods to prolong a patient's life or even arrest the disease. Using calcium-41 as an isotopic tracer, AMS can measure small changes in the rate of continually occurring skeletal bone turnover in humans. A small dose of calcium-41 administered to a patient is enough to track skeletal calcium loss over a person's lifetime. Medical researchers know that skeletal disease correlates with bone turnover rate, and the amount of calcium-41 in urine samples can be carefully monitored with AMS. In experiments with mice, the technique has been shown to diagnose changes in bone turnover with high precision. Clinical trials will soon begin.

AMS also shows great potential as a diagnostic tool for determining how

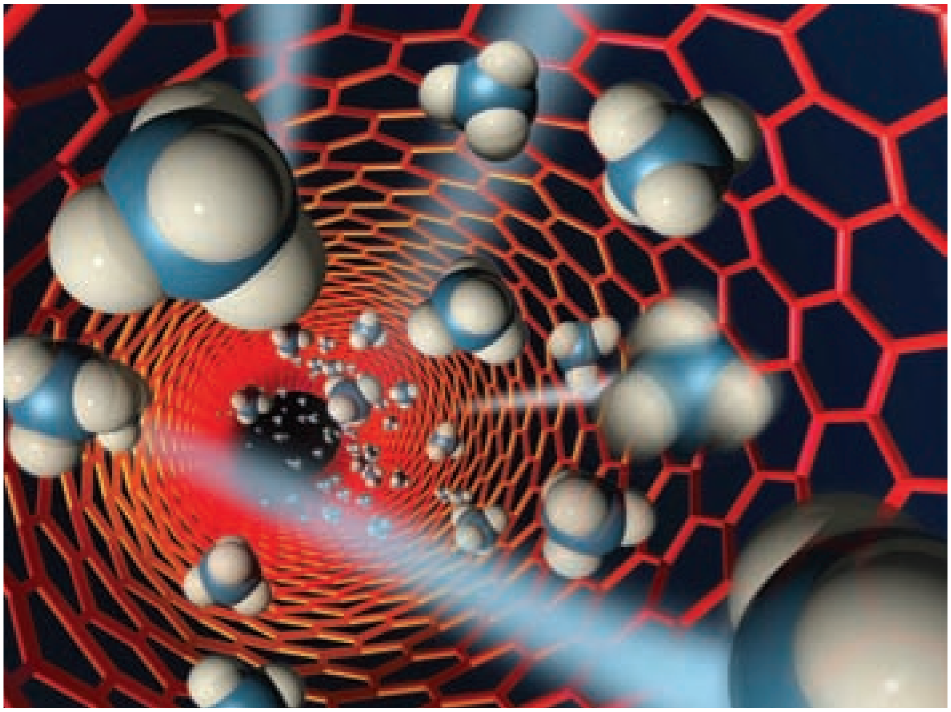
CAMS director John Knezovich explains the AMS process to Vince Stewart (left), director of Federal Government Relations at UC Davis and John Hamilton (center), deputy director of Federal Government Relations at UC's Office of the President. The CAMS accelerator is in the background.

people, especially the elderly, are able to absorb vitamin B12. An estimated 1 million Americans over the age of 65 have a condition known as pernicious anemia, which interferes with their ability to properly absorb the vitamin and puts them at risk for developing debilitating fatigue and neurological problems. Scientists at the Laboratory and UC Davis are developing a diagnostic procedure wherein a patient would take a small tablet of B12 labeled with carbon-14. Blood samples taken by pin prick would then be subjected to AMS analysis.

Uses of Carbon Nanotubes

Laboratory researchers have created a membrane with carbon-nanotube pores that may offer a less expensive way to remove salt from water, just one among many possible nanotube applications. In research that appeared on the cover of the May 19, 2006, issue of *Science*, the team reported that gas and water flows through the membrane are as much as 8,500 times faster than what classical models predict. Hollow carbon nanotubes are about 50,000 times thinner than a human hair— six water molecules can fit across their diameter. Larger molecules, such as contaminants in water, are blocked by the tubes' small size. The team measured the flow of gases and liquids through the membrane, composed of billions of nanotubes, and found the amazing results, which are consistent with quantum simulations of water flow through nanotubes.

Another surprising feature of carbon nanotubes was reported by a different team of Laboratory researchers and collaborators in the January 19, 2006, issue of *Nature*. They found that a single-walled carbon nanotube heated to more than 3,600 degrees Fahrenheit can be elongated by nearly 280 percent, compared to a theoretical maximum of 20 percent under normal conditions. Its diameter shrank by 15 times. This discovery of superplastic deformation could prove useful in helping to strengthen and toughen ceramics and other nanocomposites at high temperatures.



Artist's rendering of methane molecules flowing through a carbon nanotube less than 2 nanometers in diameter.

Fusion Advances

On November 21, 2006, seven parties, including DOE Undersecretary Raymond Orbach representing the United States, met in Paris to sign the agreement to establish the international organization that will implement the ITER fusion energy project. ITER, a large tokamak designed to produce 500 megawatts of fusion power, will be constructed at Cadarache, France. The Laboratory has been participating in the ITER project since its inception. Livermore scientists working at the DIII-D Tokamak at General Atomics in San Diego have led the effort to develop new methods for reducing the heat load on the walls of ITER, and they are developing advanced plasma diagnostics.

In September, the Laboratory was awarded contracts to work on two scoping studies for ITER diagnostic systems. One study will explore the use of infrared cameras to measure temperatures on a plasma wall where tremendous heat fluxes born from the fusion reactions will be deposited. The other study will deal with the design for an optical system that measures the plasma current density. The two diagnostic system designs will be patterned in part after systems deployed by the Laboratory on the DIII-D Tokamak.

A worker inside the DIII-D tokamak at General Atomics in San Diego, California. Diagnostic tools for the new ITER tokamak are based on ones Livermore developed for the DIII-D.

A New Addition to the Periodic Table

A team of researchers from Livermore and Russia's Joint Institute for Nuclear Research (JINR) discovered the newest superheavy element, element 118. They used the JINR U400 cyclotron in Dubna, Russia, to slam an intense beam of calcium-48 nuclei into californium-249 targets. In the gas-filled separator beyond the cyclotron, three atoms of element 118 were created and lived for about a thousandth of a second. Three similar decay chains were observed consisting of two or three consecutive alpha decays terminated by a spontaneous fission event. The Livermore–Dubna team previously discovered elements 113, 114, 115, and 116. Their findings were published in the October 2006 edition of *Physical Review C*.

The Livermore element 118 discovery team includes (from left) Jackie Kenneally, Jerry Landrum, Nancy Stoyer, and Ken Moody. Moody studied under Glenn T. Seabourg, who discovered plutonium and many other elements.

Hydrogen for Future Transportation

Hydrogen as a fuel can help replace imported oil and does not contribute to greenhouse emissions. As part of DOE's National Hydrogen Storage Project, a group of Laboratory researchers is taking an innovative approach to hydrogen storage for vehicles. Livermore's vessel is designed for high-pressure storage of hydrogen as a compressed room-temperature gas, a cryogenic gas, or as a liquid. Most other DOE researchers are concentrating on low-pressure options. The tank was tested on a Toyota Prius hybrid vehicle converted to run on hydrogen by Quantum Fuel Systems Technologies Worldwide of Irvine, California. The goal was to exceed DOE's target driving range of more than 480 kilometers. The team achieved a range of 1,050 kilometers.

The Livermore tank consists of a pressure vessel custom fabricated by Structural Composites Industries, of Pomona, California. Its many layers of insulation are enclosed within a vacuum vessel. Because the tank can hold hydrogen in different forms, the driver can choose a form that meets immediate priorities. The design builds on the success of Livermore's first-generation cryogen-capable vessel, which was tested in 2004 on a Ford Ranger. This successful technology demonstration could help pave the way for hydrogen-powered vehicles.

Vern Switzer and Tim Ross (top) work on a new hydrogen fuel tank for a Toyota Prius, shown below with (from left) Gene Berry, Francisco Espinosa-Loza, and Salvador Aceves.

Genome Sequencing and Biofuels

In May, DOE's Joint Genome Institute (JGI) celebrated the completion of its 100th microbial genome sequence. Scientists use information about the genomes of microbes and other organisms to study how microbes efficiently destroy toxic substances for environmental cleanup and break down plant materials to produce useful sources of energy. Sequencing has focused on microbes that are efficient at ethanol conversion and on a rapidly growing poplar tree, the black cottonwood (*Populus trichocarpa*), which could serve as feedstock for biofuel. The work was featured on the cover of the September 15, 2006, edition of *Science*. Among the JGI's major discoveries is the identification of more than 45,000 protein-coding genes, more than any other organism sequenced to date. The research team identified 93 genes associated with the production of cellulose, hemicellulose, and lignin, the building blocks of plant cell walls.

The JGI unites the expertise of five national laboratories, including Lawrence Livermore, along with the Stanford Human Genome Center. As a national user facility, the JGI has sequenced or is in the process of sequencing more than 380 organisms, more than any other institution in the world.

It was cover news for *Science* when the JGI sequenced the genetic code of plants that could serve as sources of energy.