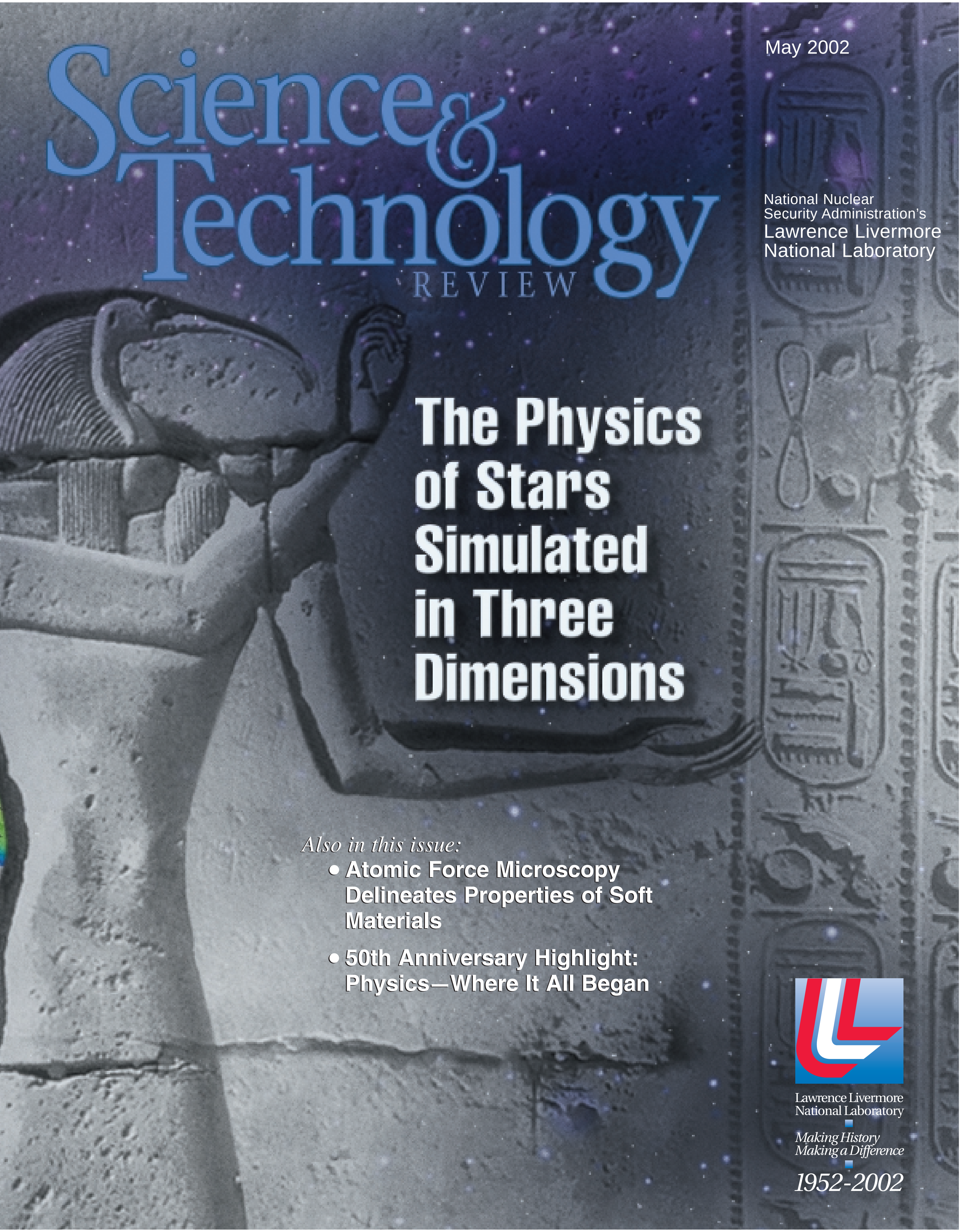


May 2002

Science & Technology REVIEW

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

The Physics of Stars Simulated in Three Dimensions

Also in this issue:

- Atomic Force Microscopy Delineates Properties of Soft Materials
- 50th Anniversary Highlight: Physics—Where It All Began

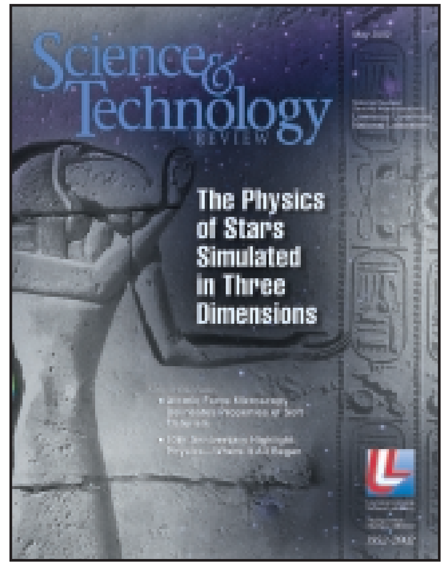
Lawrence Livermore
National Laboratory

Making History
Making a Difference

1952-2002

About the Cover

The Egyptian god Djehuty was a powerful figure ruling heaven, earth, and the netherworld. His name was taken for the astrophysical code that is used to perform three-dimensional simulations of stars. The Djehuty code is described in the article beginning on p. 4. The advent of extremely powerful parallel computers has made it possible for Djehuty to incorporate detailed physics in the multimillion-zone meshes of computer models. The code could be a virtual telescope used to discover the structure of stars and track their evolution.



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About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on 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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Science & Technology Review

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Lawrence
Livermore
National
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Studying the mysteries of black holes

Black holes have fascinated astronomers and the general public alike. Now, with detailed simulations made on massively parallel supercomputers and advances in x-ray astronomy, knowledge about black holes is growing.

At the January meeting of the American Astronomical Society, two Laboratory researchers—Chris Fragile and James Wilson—together with Grant Mathews of the University of Notre Dame, presented findings of what happens when gas flows into rapidly rotating black holes. The findings centered on computer simulations and relied on previous research indicating that gas falling into a black hole orbits the black hole in a disklike pattern. The simulations are a first attempt to model the complicated disk dynamics. Said Fragile, "Simulations such as ours are critical since these environments are too complicated to study by any other means."

The research is of interest to organizations such as the National Aeronautics and Space Administration (NASA) because it may help explain unusual periodic timing properties seen in x rays being emitted near many suspected black holes. "Much of what the NASA Observers [satellites] look for are x rays, and the black holes produce a lot of that," said Fragile. "We're hoping to simulate a system similar to what a NASA Observer might see when it looks at a black hole."

The researchers' work is based on how rapidly rotating black holes would drag space–time around them, acting like tornado funnel clouds. This is a phenomenon called frame-dragging and is predicted by Einstein's theory of general relativity.

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Outer space yields building blocks of life

Geochemist Jennifer Blank and a group of scientists from around the world are shedding light on how life might have begun. In two independent laboratory experiments, published in the March 28, 2002, issue of *Nature*, the researchers suggest that amino acids—key building blocks for organic life—could have come from extraterrestrial sources. Performing experiments at low temperatures and pressures, they produced amino acids in environments that simulated the icy conditions of interstellar space. The results suggest that amino acids could have formed in space and hitched rides on comets and asteroids to planets throughout the universe.

To further support this theory, the researchers had to see if amino acids borne on a comet could survive the heat and pressure of an impact with Earth. Other theories about life's origin hold that amino acids form in water found on Earth rather than in extraterrestrial ice. Blank's work is helping to support the extraterrestrial source theory.

Saying, "I'm thrilled about this work," Blank has been simulating a high-speed comet collision into Earth. She used a 6-meter-long gas gun to blast canisters of amino acids. The gun's impact generates temperatures and pressures comparable to those of a comet collision. Her results indicate that amino acids can survive the impact.

Blank says that showing that chemical reactions in interstellar clouds can form amino acids "is a first big step" in explaining where they can originate and how they might arrive on Earth.

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New kind of cool in a radiation detector

One more tool is coming along to counter terrorism. It's a radiation detector developed by scientists at the Livermore and Berkeley laboratories. Handheld, mobile, and able to distinguish between different forms of radiation, Cryo3, as the new device is called, has clear applications for homeland security. It can be taken into the field—for example, at border crossings, into airports—to do its work unobtrusively and reach into areas that big detectors cannot get to.

The Cryo3 is a germanium radiation spectrometer. The use of germanium crystals allows Cryo3 to detect and measure various types of radiation and distinguish between, for example, plutonium in nuclear weapons and barium in medical diagnostics. To work, germanium spectrometers must be kept very cold and are usually chilled using liquid nitrogen. That need typically confines their work to the laboratory. Cryo3's developers eliminated the need for liquid nitrogen by refining an off-the-shelf cooling engine that is as small as a fist, which they then inserted in the detector and powered with a pair of rechargeable lithium ion batteries.

Their result: a shoe-box-size device weighing just 4.5 kilograms that can operate up to 8 hours on its batteries. Says Livermore physicist John Becker, one of the developers, "Cryo3 couples the high-energy resolution and efficiency of a laboratory-size germanium detector with a low-power, lightweight, long-lived microcooler for the first time, enabling a mobile, handheld package."

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A Project with Multidimensional Purposes

FOR many years, Livermore researchers have played a major role in advancing astrophysical knowledge through their expertise in high-energy-density physics and advanced computer modeling. The astrophysics community has benefited from Livermore contributions in the search for dark matter in the universe, laser guide star optics that sharpen astronomical views made from Earth, advanced instruments for U.S. and European spacecraft, and laboratory-created hot plasmas similar to those existing in distant stars.

Livermore researchers are again breaking new ground by developing, for the first time, a three-dimensional (3D) modeling program that simulates the evolution and structure of stars. The complex code is called Djehuty, after the Egyptian god who is said to have invented writing, the measurement of time, music, magic, art, medicine, mathematics, and astronomy. The physical processes of stars have long been of interest to Livermore researchers because understanding the prime stellar energy mechanism, thermonuclear fusion, is part of the Laboratory's national security mission. In that respect, Djehuty is well aligned with Livermore's programmatic interests that focus on understanding high-temperature physics and performing accurate numerical simulations of complex physical reactions.

As detailed in the article beginning on p. 4, developing the first 3D code to realistically model the evolution of stars was a formidable challenge. The Djehuty development effort is succeeding in large part by leveraging Livermore's experience with massively parallel supercomputers (machines with thousands of processors) and their codes. The Djehuty team took advantage of the expertise developed in the National Nuclear Security Administration's Advanced Simulation and Computing program, an important component of Stockpile Stewardship. Djehuty's development also benefited from our scientific expertise in astrophysics and high-energy-density phenomena.

Djehuty is a good example of our long-standing success in putting together teams of researchers from different disciplines. In this case, specialists from the Defense and Nuclear Technologies Directorate, the Physics and Advanced Technologies Directorate, and the Computation Directorate's Center for Applied Scientific Computing collaborated on the project.

Djehuty resides at the Livermore branch of the University of California's Institute for Geophysics and Planetary Physics (IGPP). The Astrophysics Center at IGPP is the focus of astrophysics and planetary physics activities at Livermore. The center collaborates with all University of California campuses, more than 30 U.S. universities, and more than 20 international universities. One of its goals is to foster collaboration among visiting scientists on projects that are important to astrophysics and that require the unique simulation capabilities of Djehuty.

An important aspect of Djehuty is its funding as a three-year Strategic Initiative (SI) under the Laboratory Directed Research and Development (LDRD) program. LDRD was authorized by Congress to provide a means for directors of the Department of Energy national laboratories to fund innovative, high-risk research and development projects in support of Laboratory and DOE missions.

Strategic Initiatives within LDRD are usually large and technically challenging. An SI project must be aligned with the strategic research and development priorities of at least one of the Laboratory's four strategic councils: the Council on Energy and Environmental Systems, the Council on National Security, the Council on Biosciences and Biotechnology, and the Council on Strategic Science and Technology. Although many deserving SI proposals are considered, less than one-third can be funded; the competition is keen, and only the best ideas can be supported.

The Livermore effort to revolutionize the modeling of stellar evolution and structure is being well received by the international scientific community. I am confident that Djehuty will help advance the astrophysics discipline, strengthen our capabilities in complex modeling, and enable many scientific collaborations with the academic community.

■ Jeff Wadsworth is deputy director for Science and Technology.

Building a Virtual Telescope

A new three-dimensional code simulates for the first time the structure and evolution of stars.

The Egyptian god Djehuty was the guide to heaven, earth, and the netherworld; lord of calculation, wisdom, and judgment; and protector of knowledge, mathematics, and science. His image is seen in many hieroglyphic tablets.

IN the Egyptian pantheon, Djehuty was the guide to heaven, earth, and the netherworld; lord of calculation, wisdom, and judgment; and protector of knowledge, mathematics, and science. It seemed appropriate, then, for Lawrence Livermore astrophysicists David Dearborn and Peter Eggleton to take his name for their breakthrough three-dimensional code that simulates the evolution and structure of stars.

The physical processes of stars have long been of interest to Livermore researchers because understanding the prime mechanism of stellar energy—thermonuclear fusion—is part of the Laboratory's national security mission. "Stars are high-energy-density ovens," says Dearborn. "Several Laboratory programs are interested in the properties of stars, and many Livermore physicists have backgrounds in astrophysics."

Dearborn points out that stars provide the standards of reference for measuring the size, age, chemical composition, and evolution of the universe. Stars have also been used as physics laboratories that strengthen our understanding of complex physical processes. For example, they have been used to better understand the properties of hot plasmas as well as fundamental particles such as neutrinos. Stars have also been used to suggest the properties of exotic particles such as axions, which have been proposed to explain why the universe contains more matter than antimatter.

Eggleton notes that scientific knowledge of stars may appear to be mature, but in fact, much of what we know about stars—especially the way they generate energy and how they evolve from a dust cloud to a supernova or red giant—may well be significantly incomplete. “We need to improve our knowledge about stars,” he says.

The reason for the imperfect understanding is that many stellar processes are complex, three-dimensional phenomena that have been modeled only in coarse approximation using one-dimensional computer codes. For example, the transport of energy through a star by convection from its superhot core is a three-dimensional process, which limits the value of one-dimensional calculations, even for perfectly spherical stars. (See the box on pp. 6–7.) Although a one-dimensional convection simulation could be inaccurate by only 10 percent at any moment in time, such “small” errors can easily accumulate over time. The result might be a final discrepancy of 100 to 200 percent in some properties calculated for such stellar objects as Cepheids, which are large, pulsating stars often used to calculate the distance scale of the local universe.

Need for 3D Codes

Convection is only one of many stellar phenomena that require a three-dimensional simulation code for accurate modeling. Other complex phenomena that astrophysicists have long desired to simulate include the evolution of elements created in a star, the preexplosion structure of supernovas, and the physics of binary stars, which comprise nearly half of the visible mass of the universe.

Dearborn says that developing a three-dimensional code to realistically model stars is challenging for even the most accomplished teams of computer scientists and astrophysicists. Before Djehuty, three-dimensional stellar models were limited to about 1 million zones. (Computer simulations divide an object into numerous small cells, or zones, whose behavior is governed by sets of physics equations. The totality of the zones, or cells, is called a mesh.) The million zones represent only modest segments of a star. Moreover, the simplified models did not incorporate all the physics pertinent to a star’s core where nuclear energy is produced, and they did not simulate gravity in a realistic manner. “While the earlier codes are important starts toward improving our understanding, it is clear that the solutions to some problems necessitate whole-star modeling,” Eggleton says.

The advent of massively parallel computing, wherein computers have hundreds and even thousands of processors, and Livermore’s participation in the National Nuclear Security Administration’s Stockpile Stewardship Program—to assure the safety and reliability of the nation’s nuclear stockpile—led Livermore scientists to gain expertise in supercomputers and parallel codes. Along with astrophysicist Kem Cook, Dearborn and Eggleton saw that Livermore was becoming a uniquely qualified institution to move the calculation of stellar properties to a higher level of understanding. In particular, they saw that one element of stockpile stewardship, which uses massively parallel computing techniques to simulate the performance of nuclear warheads and bombs in a program called Advanced Simulation and Computing (ASCI), would be pertinent to their quest for a whole-star, three-dimensional model.

Dearborn and Eggleton’s vision was to take advantage of Livermore’s expertise in ASCI computations, code and algorithm development for massively parallel computers, astrophysics, high-energy-density physical data and processes, and experience in interdisciplinary coordination to attack the fundamental questions of stellar structure and evolution.

A Laboratory-Wide Team

In 1999, Dearborn and Eggleton assembled a team to develop Djehuty as a three-year Strategic Initiative under Laboratory Directed Research and Development funding. The collaboration has included John Castor, Steven Murray, and Grant Bazan from the Defense and Nuclear Technologies Directorate; Kem Cook from the Physics and Advanced Technologies Directorate; Don Dossa and Peter Eltgroth from the Computation Directorate’s Center for Applied Scientific Computing; and several other contributors. “Collaboration from throughout the Laboratory has been essential in this project,” says Dearborn.

The team designed Djehuty to operate on massively parallel machines with the best available physical data about stars and with algorithms tailored specifically for the massively parallel environment. Notes Dearborn, “There’s been tremendous work at the Laboratory in developing parallel codes and learning how to do calculations in a manner that won’t bog down the machines.” The code development process involved assembling and reconfiguring a number of Livermore codes that already existed, many of them parts of unclassified software belonging to the ASCI program, and optimizing them for astrophysical simulations.

Djehuty also takes advantage of the Laboratory's significant knowledge about opacity (a measure of the distance photons at a particular frequency travel through a particular material) and equations of state (the relationship between a material's pressure, temperature, and volume). Opacity and equation of state are two key pieces of data that are used in stockpile stewardship work for studying matter under extreme conditions. In that respect, says Dearborn, developing Djehuty is well aligned with Livermore's programmatic interests that focus on understanding high-temperature physics and performing numerical simulations of complex physical reactions.

The code currently features accurate representations of different elements' equations of state, opacities, radiative diffusion transport (how photons are absorbed and reemitted when they interact with atoms and electrons in a star's interior), and nuclear reaction network (fusion reaction rates and abundance of species formed). Finally, Djehuty features a gravity package for spherical stars, a provision that is being improved significantly so it will be

Probing the Interiors of Stars

Stars, unlike planets, produce their own energy and do so by thermonuclear fusion. Much of the complexity underlying the computer code Djehuty, Livermore's three-dimensional code for star structure and evolution, is its realistic simulation of fusion, which converts hydrogen nuclei into helium ions. The process is often called hydrogen burning and is responsible for a star's luminosity.

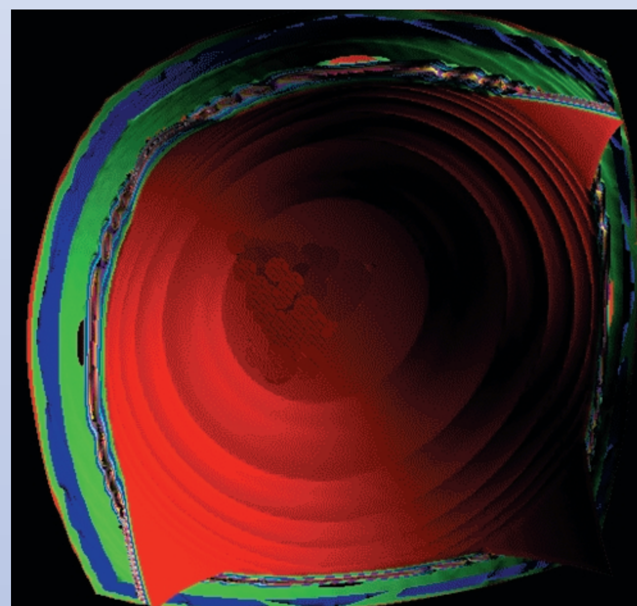
Fusion reactions occur in the core, the innermost part of the star. In a star about the size of our Sun, the hydrogen fuel is eventually consumed after billions of years. The core slowly starts to collapse to become a white dwarf while the envelope expands to become a red giant. Our Sun will reach this stage in about 5 billion years.

In contrast, the core of a star larger than the Sun is driven by a complex carbon–nitrogen–oxygen cycle that converts hydrogen to helium. In these massive stars' cores, hot gases rise toward the surface, and cool gases fall back in a circulatory pattern known as convection. After depleting its hydrogen—and subsequently its helium, carbon, and oxygen—the contracting core of a massive star becomes unstable and implodes while the other layers explode as a supernova. The imploding core may first become a neutron star and, later, a pulsar or black hole.

The cores of stars are turbulent in a manner analogous to a boiling kettle, says Livermore astrophysicist Peter Eggleton. Driven by enormous heat, the material in a core takes about a month to completely circulate (our Sun accomplishes it in about two weeks). "One-dimensional simulations give you an average of what's going on in the kettle instead of telling you what's happening on a second-to-second basis, so we are forced to make some bold assumptions." Eggleton also says that one-dimensional codes cannot model time-dependent convection in such events as helium flashes, which occur in the late stages of a red giant star.

One of the long-standing issues of astrophysics has been determining the correct convective core size of stars. Astronomical observations have suggested that the convection region is larger than has been assumed since the 19th century. Astronomers call the situation convective-core overshoot, meaning that the core probably extends beyond the long-accepted boundary.

Determining the exact size of the convective core is of more than passing interest. If the core is indeed larger than has been assumed, then stars could be much older than has been believed, which has profound implications for how the universe evolved and its real age. "The modeling of convection is one of the weakest points in our

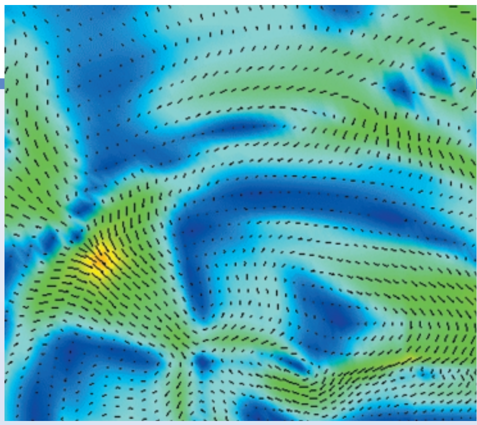


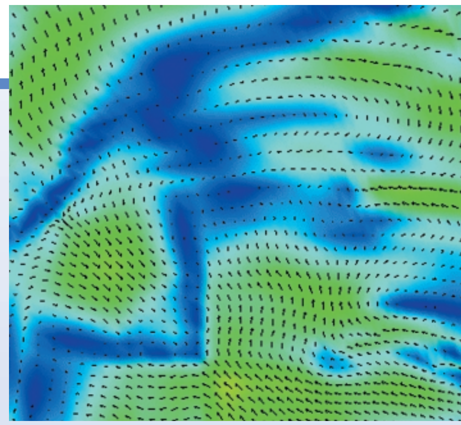
When low-mass stars such as our Sun become red giants, they grow a helium core. Eventually the helium core ignites and begins burning to carbon and oxygen. The ignition begins in a shell that initially expands and drives a weak shock into and out of the star. The image shows the velocity contours of the expanding shell in a cutaway segment of a star in which ignition is beginning. The red areas represent the highest velocity, corresponding to the rapidly expanding shell both in front and in back (barely visible).

possible to simulate a host of aspherical stellar objects.

The First Simulation

The team's early strategy was to test the code's accuracy and achieve some optimization of it. In September 2000, using the 680-gigaops (billion calculations per second) TeraCluster 2000 (TC2K) parallel supercomputer at Livermore, the team successfully executed a three-dimensional simulation of a star. This was the first three-dimensional simulation of an entire star, but it ran on just one of TC2K's 512 processors, using only some of the code's physics on a modest mesh containing approximately 400,000 cubic zones. "Our first models were too small to accurately represent a star's structure, but they were sufficient to study different zone mesh structures and to optimize the physics equations we were using," says Dearborn.





Two simulations taken about 8 minutes apart show the changes inside the core of a star four times the mass of our Sun. Colors represent relative velocity (increasing from blue to yellow), and the arrows show the direction of convective currents.

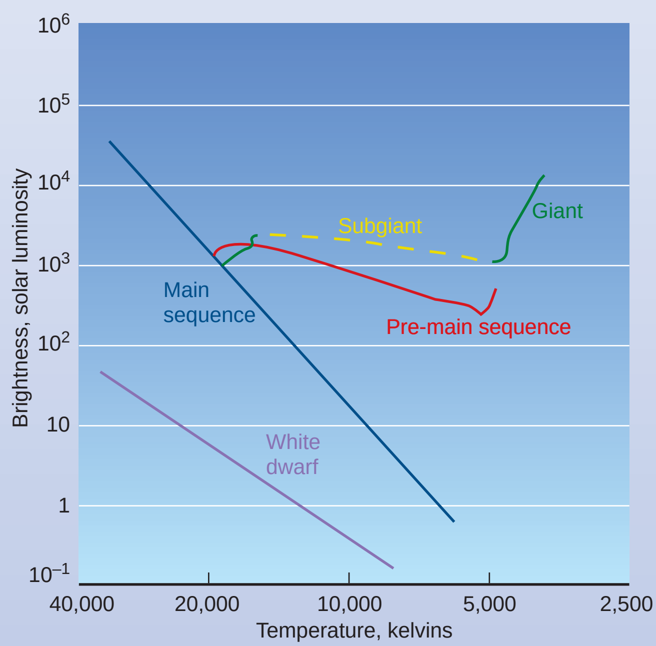
understanding of stellar structure and evolution," says Livermore astrophysicist David Dearborn.

The issue over the size of the convection region is serving as a way to verify and validate the accuracy of Djehuty. The code development team made convective core overshoot a priority in part because the fusion process occurs during the earliest and simplest phase of stellar evolution—during what is called the main sequence. The main sequence is shown on a Hertzsprung–Russell diagram, which plots stars' temperatures versus their brightness, thereby showing their evolution.

"Observations assure us that our best one-dimensional approximations of convection are flawed," says Eggleton. "With Djehuty, we have a three-dimensional code with accurate physics to determine what exactly happens in the core. There are big rivers flowing in stars' cores, and we want to follow them."

One simulation modeled a star early in its evolution, prior to its joining the main sequence. As expected, it did not show any convection motions from thermonuclear fusion. Another simulation studied a massive star that had just reached the main sequence and so witnessed the onset of convective motion from fusion. A third simulation looked at a red giant, a very old star that possesses a large core of helium. The helium eventually ignites in what is called a helium flash.

The simulations suggested that a star's convective core indeed exceeds its classical boundary. Additional computationally intense simulations, each requiring a month of supercomputer time, will be done this year to model a star's convective core at key stages in its lifetime.



The Hertzsprung–Russell diagram plots the temperatures of stars versus their brightness and is useful for plotting their evolution. This diagram follows a star with six times the mass of our Sun. The star spends most of its lifetime in the main sequence, characterized by producing fusion in its inner core. Djehuty simulations are modeling stars in every phase of their evolution.

Satisfied with the early simulations on one processor, the team then modified the code to run in a massively parallel computing environment. “It’s a big transition going from one to many processors because we need at least 10 million zones to model an entire star,” says Dearborn. Fortunately, he says, Livermore has invested significant resources to figure out how to break up a complex physics problem, such as following fusion reactions in time, for efficient processing by hundreds and even thousands of processors.

Generating and monitoring large three-dimensional meshes containing millions of zones is a huge task. To aid computing, the Djehuty team constructs a mesh sphere of seven blocks: one in the center and six surrounding it. The outlying six are distorted at their outer edges to make them spherical. Each block contains at least 1 million zones. Each zone represents thousands of kilometers on a side, and several thousand zones are assigned to a processor. All the processors must communicate efficiently with each other simultaneously. The key to Djehuty’s simulation power is its ability to access many processors to efficiently compute the physics in each of the millions of zones. “We’re fortunate to have so many people who can develop a code like this,” says Dearborn.

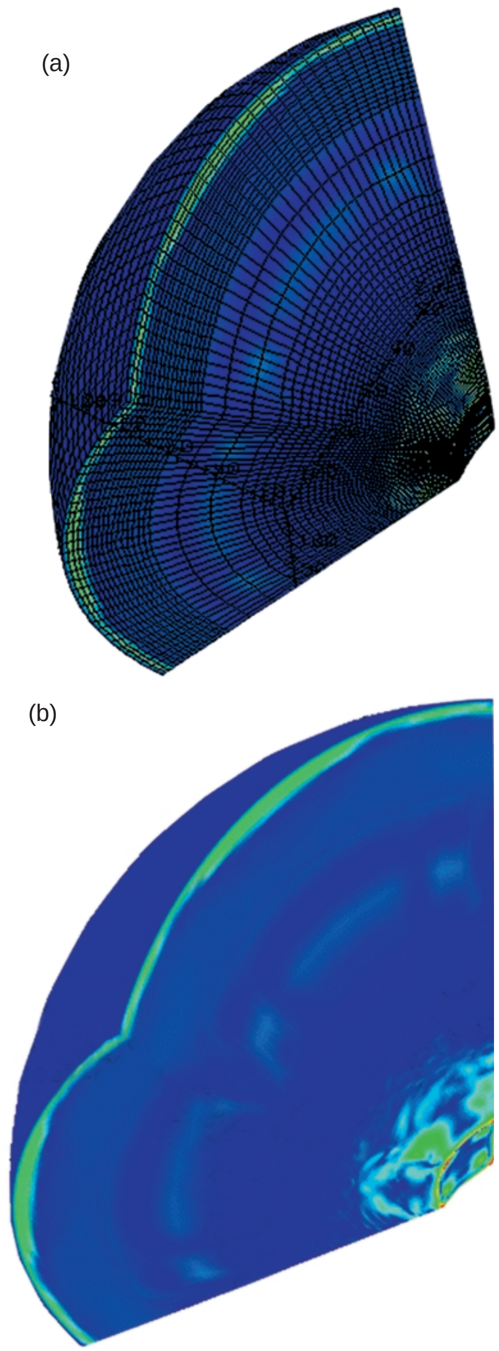
The team has run simulations on increasing numbers of processors on the TC2K. Several simulations, using 128 processors and 56-million-zone meshes, were some of the largest astrophysics calculations ever performed; they generated close to a terabyte (trillion bytes) of data. The team has also begun to perform simulations on Livermore’s ASCI Frost, the unclassified portion of ASCI White, currently the world’s most powerful supercomputer. Simulations on ASCI Frost have used 128 of that machine’s processors to evolve stars with 60-million-zone meshes.

With the code running satisfactorily in a massively parallel environment, Dearborn and Eggleton focused on resolving a long-standing controversy in astrophysics. That controversy surrounds the discrepancy between the results from one-dimensional stellar models and data gained from astronomical observations concerning the size of the convection region inside a star. (See the box on pp. 6–7.) This region is where hot plumes of gas rise and fall. The team has simulated the cores of several stars, ranging from young stars before the onset of fusion reactions to old stars about half the age of the universe. Eggleton says that one-dimensional computer models are especially incomplete in simulating late stellar evolution, which is often characterized by deep mixing of gases and sudden pulses of energy.

Virtual Telescope at Work

Eggleton compares Djehuty to a kind of virtual telescope that can take snapshots during a star’s lifetime of several billion years and examine in detail the star’s structure and the various physical processes at play. “There is no comparable three-dimensional code, although there have been heroic efforts to develop one,” he says. As a result of the early simulations, the Livermore team anticipates being able to accurately model in three dimensions, for the first time, a host of important stellar objects. For example, Djehuty will be vital to understanding supernovas, the brightest objects in the universe, and about which much is unknown, as well as Cepheids.

Dearborn predicts that Djehuty will provide an important link between theory and observation that will further our knowledge of stellar structure and evolution. Livermore’s Stefan Keller is conducting a number of observational studies to verify the Dhejuty simulations. One study uses a certain population of Cepheids to observationally determine the relationship between mass and luminosity that is dependent on the original amount of mixing in the star’s convective core. Preliminary results indicate that these Cepheids are considerably more luminous than predicted by standard one-dimensional models, a result suggesting a larger

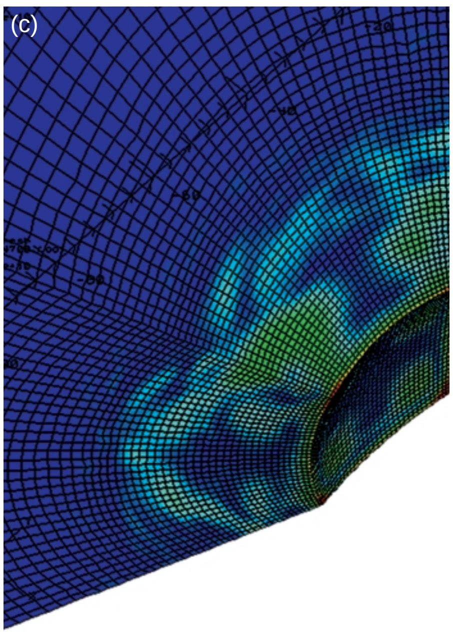


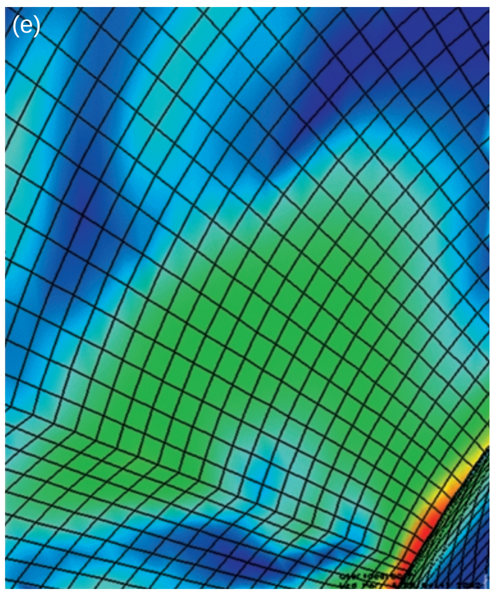
degree of mixing than was previously thought. Djehuty simulations appear to confirm the observations.

In another study, astrophysicist Rob Cavallo is observing variations in the surface abundances of some elements in evolved red giant stars. The variations are caused by some form of nonconvective mixing process, which can only be determined with the use of a fully three-dimentional code such as Djehuty.

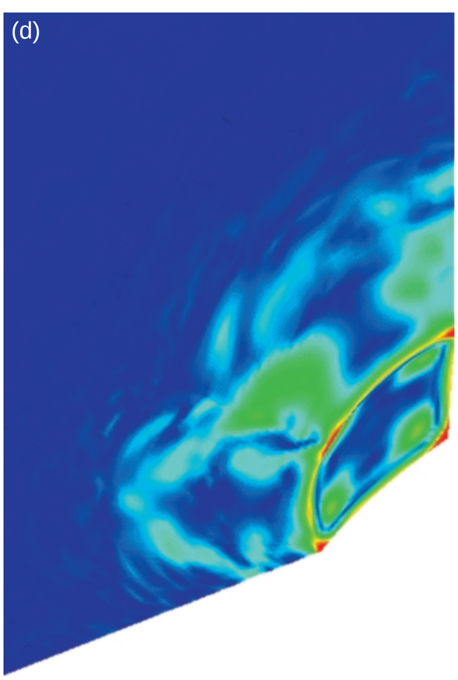
The team is also working to improve the code and better interpret its output. One goal is improving the accuracy of opacities. “There are a range of problems where a star’s behavior depends on the opacity of material whose composition is rapidly changing,” says Dearborn. The team plans to attack those problems by permitting the code to generate opacity levels using OPAL, a database of stellar opacity that was developed at Livermore several years ago. (See *S&TR*, April 1999, pp. 10–17.)

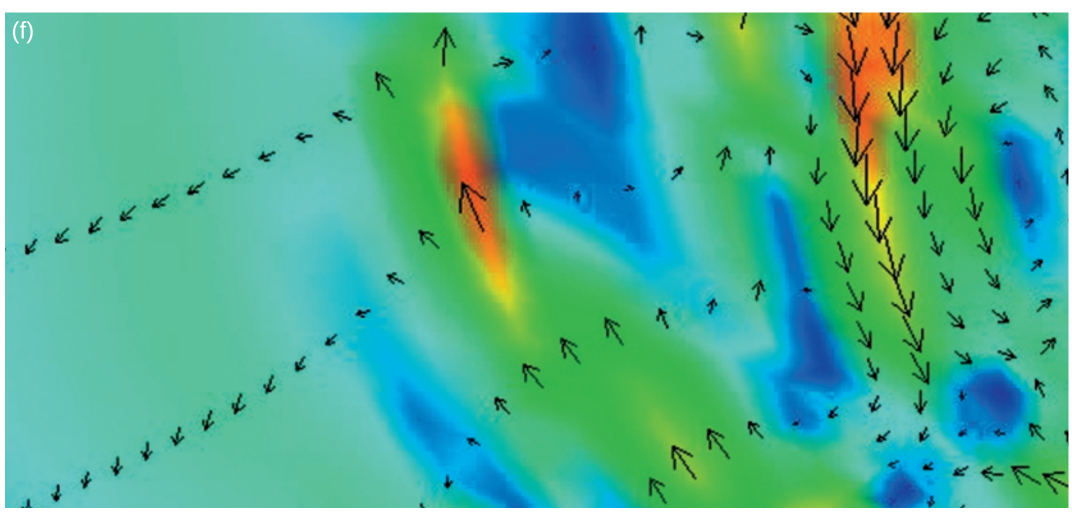
Another task is improving the techniques to better visualize and thereby understand the vast amounts of data generated by Djehuty. Analysis and visualization are the key for turning huge numerical simulations into scientific understanding, says Dearborn, and at present, “We must improve our ability to analyze three-dimensional structures. With longer, larger, and





Increasingly magnified sections of a star with four times the mass of the Sun can be seen in these Djehuty simulations. Here, (a) and (c) are the same as (b) and (d), respectively, but show the location of mesh zones. A closeup of the star’s convective core is shown in (e). Colors represent relative velocity (increasing from blue to yellow). The bulk of motion lies in the core, where convection currents driven by carbon–nitrogen–oxygen burning occur. The areas of convection appear to extend beyond what one-dimensional models depict, but Djehuty’s models are consistent with recent astronomical observations. (f) A two-dimensional slice of a Djehuty three-dimensional simulation depicting convection currents deep inside the core. The arrows signify the directions of the currents.





more realistic simulations, we must develop better tools to analyze our simulations to extract the greatest amount of information. We can't eyeball 10 million zones in three dimensions. We must have ways for a computer to look for irregularities and flag them."

Recently, the team began using MeshTV, a program that was designed at Livermore to visualize data for three-dimensional meshes. MeshTV can display an animation of data changing over time and permit a user to rotate, zoom, or pan an object while a movie assembled from the data is playing. (See *S&TR*, October 2000, pp. 4–12.)

A Continual Code Development

Djehuty development will never be finished, although it will eventually become much less a development code and more a production code ready for use. The team continues to enhance Djehuty's physics and refine its algorithms. Development is also under way to permit simulation of rapidly rotating stars and, in particular, binaries. Binary stars revolve around a common center of gravity and sometimes exchange some of their mass or even merge into one star. Often, one binary is distorted by the gravitational pull of the other, and the result is seen in varying brightness.

"Simulating binaries has become our main physics priority," says Dearborn. "We want to see how mass comes off one star and is absorbed by the other." One-dimensional codes don't work for binaries because when two stars interact, the problem is three-dimensional.

Binary simulations require a more accurate means to simulate gravity, one that automatically changes to reflect a star's size, shape, and internal physics. Once this enhanced gravity treatment is incorporated into Djehuty, the code will be able to represent binaries as well as stellar objects that are not perfectly spherical. "Once work on binaries begins," says Dearborn, "we will enter completely new territory because calculations so far have been very crude."

The Livermore effort to revolutionize stellar evolution and modeling calculations has been well received at two international conferences. The enthusiasm generated by this work has led to two proposals to the National Aeronautics and Space Administration from U.S. academic researchers interested in collaborating with the Djehuty team on binary star evolution. Other researchers have proposed using the code to study white dwarfs, the phase of stellar evolution that occurs late in stars' lifetimes, depending upon their starting masses. Dearborn and Eggleton have also received inquiries about the possibility of modifying the code to run simulations of large planets and brown dwarfs.

Several postdoctoral scientists and university students have joined the Djehuty development team. With a user manual recently completed, the team is seeking university collaborators, both graduate students and visiting scientists, who would visit for several months at a time and join in astrophysical research that can be done nowhere else.

Dearborn and Eggleton hope to see a user facility established at the Livermore branch of the University of California's Institute of Geophysics and Planetary Physics (IGPP). The Livermore IGPP currently collaborates with all UC campuses, more than thirty U.S. universities, and more than twenty international universities. "Djehuty is a unique institutional asset for attracting astronomers and physicists interested in stars and what can be learned from them," says Eggleton.

—Arnie Heller

Key Words: Advanced Simulation and Computing (ASCI), ASCI Frost, ASCI White, binary stars, brown dwarfs, Cepheids, convective core, Djehuty, helium flash, Hertzsprung–Russell diagram, Institute of Geophysics and Planetary Physics (IGPP), Mesh TV, stellar evolution, supernovas, TeraCluster 2000 (TC2K), white dwarfs.

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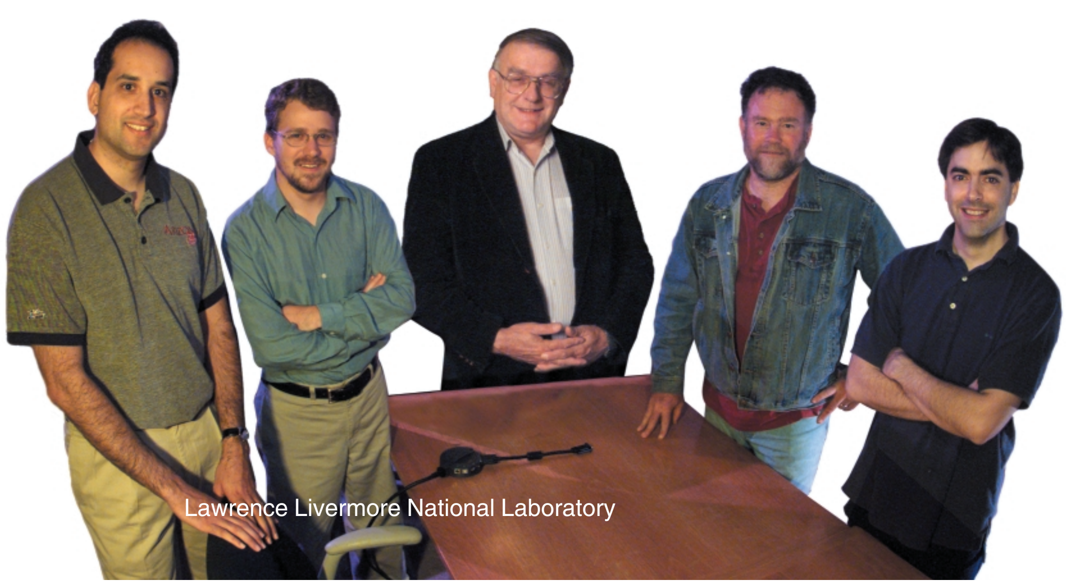


Some postdoctoral scientists and the project leaders on the Djehuty development team. From left, Rob Cavallo, Stefan Keller, team leaders Peter Eggleton and David Dearborn, and Sylvain Turcotte.

A New Understanding of Soft Materials

The hardness and stiffness of soft materials—certain biological tissues, soils, and polymers—can be measured for the first time with a Livermore invention.

RESEARCH in nuclear physics at Lawrence Livermore is performed to serve the Laboratory's national security mission. But along the way, the research has spun off technologies beneficial to human health. One example is PEREGRINE, a tool for calculating the dose that patients receive during radiation therapy for cancer. PEREGRINE combines Livermore's storehouse of data on radiation transport with Monte Carlo statistical techniques. Modeling of radiation transport also came into play in developing optical coherence tomography, a technique that uses infrared light to image through highly scattering media such as blood and the walls of arteries.

Now, in the Chemistry and Materials Science Directorate, physicist Mehdi Balooch is using a new technique he pioneered for examining uranium and other materials inside aging nuclear weapons and applying it to soft materials in the human body. Working with researchers at the University of California at San Francisco (UCSF), he is using this method to learn more about the strength of human teeth. He has also used it to study both healthy and damaged human arteries.

Balooch's new applications make use of a modified atomic force microscope (AFM). Atomic force microscopy has been in use since the 1990s to produce topographic maps of nanostructures. In atomic force microscopy, an extremely sharp tip mounted to a cantilever arm senses the atomic shape of a sample while a computer records the path of the tip and slowly builds up a three-dimensional image.

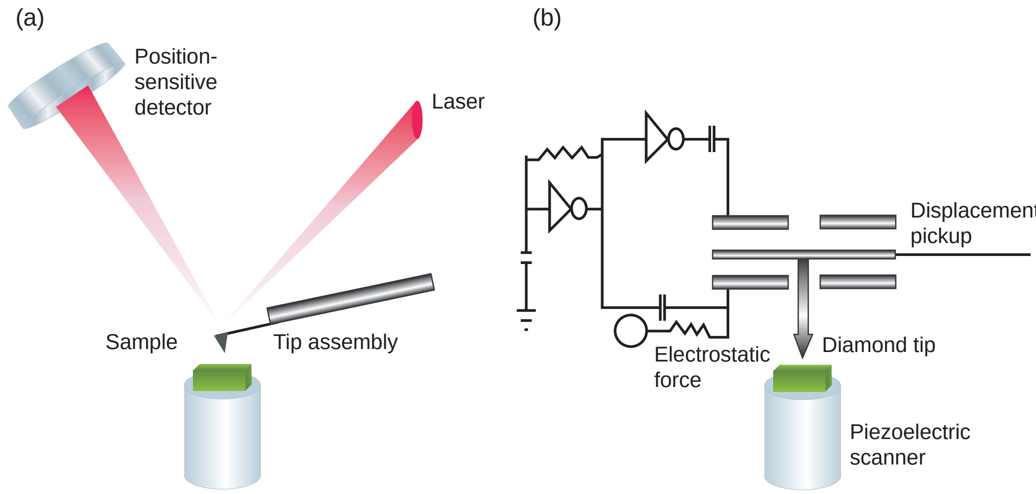
Balooch's modified AFM makes indentations just 20 trillionths of a meter deep on the surface of a sample material. Even such a tiny hole—100,000 times shallower than the width of a human hair—provides extraordinarily useful measurements about the sample. When force and displacement data are combined in various algorithms, the resulting calculations reveal information on mechanical properties—hardness, stiffness, or any other reaction to an applied force.

The modified AFM is unique in its ability to measure the mechanical properties of both hard and soft materials. Hard materials are usually easy to study, but measuring the mechanical properties of soft materials has been more difficult. Part solid and part fluid, soft materials include many biological tissues, polymers, and hydrated clays, an important component of soils. Traditionally, mechanical properties have been obtained using dried samples. But the modified AFM's ability to take measurements in liquid allows accurate measurements of the mechanical properties of soft materials for the first time.

Examining a hard material in liquid has been equally difficult. Teeth, for example, present a challenge because their normal environment is in saliva. The modified AFM allows for measurements of fully hydrated teeth. Two years ago, Balooch's team took some of the first nanoscale measurements of hardness and elasticity at the junction between tooth enamel, a hard mineral material, and the dentin just beneath it. Dentin is a soft material—part mineral, part protein, and part fluid.

Balooch has been working with dental researchers Bill and Sally Marshall at UCSF for 11 years, operating under a grant from the National Institutes of Health. A 5-year extension of the grant for continued research on the hardness and stiffness of dental material begins this month.

The modified AFM is also finding applications beyond weapons and health. Balooch recently began collaborating with colleagues in the Energy and Environment Directorate to study the effect of water on the mechanical properties of clay materials, which cannot be determined by conventional testing methods. The researchers are making first-ever measurements of the mechanical properties of single crystals of clay with water intercalated in the crystal



(a) A traditional atomic force microscope (AFM) traces the atomic shape of a sample with a tip on a cantilevered arm. The path of the tip is recorded on a computer and used to build a three-dimensional image. (b) The modified AFM incorporates the features of a nanoindenter to make tiny holes on the surface of a sample material. Instead of a cantilevered tip assempty, this AFM has a transducer-driven head and tip that can measure the mechanical properties of a fully hydrated sample.

structure. Here, as in teeth, a hard mineral material coexists with liquid matter. Until now, it has been impossible to understand how hard mineral and liquid matter work together on this very small scale.

Problems and a Solution

In Balooch's early work with UCSF on teeth, he used a commercially available nanoindenter, which made indentations 100 to 200 nanometers deep on the surface of samples. It was useful but not quite what was needed. For one thing, it could not operate under water or on hydrated samples. The nanoindenter also could not position an indentation within less than a few micrometers, which was not precise enough. Nor was the nanoindenter an imaging device, so it was impossible to know with certainty where indentations were being made.

To solve these problems, Balooch, in collaboration with a startup company named Hysitron, modified an atomic force microscope to incorporate the features of a nanoindenter. To obtain not only a topographic image but also mechanical-property measurements, the team replaced the AFM tip with a transducer-driven head and tip that can operate on a fully hydrated sample.

This modified AFM can operate in either an imaging mode or an indentation mode. In the imaging mode, the force applied to the cantilever is about 1 micronewton, a force so small that it does not dislodge a single atom in the sample. When used in the indentation mode, the force on the arm is up to 30,000 times as much, though it is still extremely small.

The modified AFM permits positioning the indentation with an accuracy of a few tens of nanometers for site-specific studies, which is a thousand times more accurate than that of a standard nanoindenter with an optical microscope attachment. It allows measurement of hardness values with indentation depths of less than 20 nanometers.

"Now," says Balooch, "with a coat-on-coat dynamic testing capability, we can get pixel-by-pixel information on stiffness or elasticity. Plus, we get topography so we know where we've been."

Getting a Grip on Teeth

Dentin is about 50 percent mineral, 30 percent organic material (mostly collagen), and about 20 percent fluid. Microscopic tubes, called tubules, run through dentin, from the pulp beneath to the junction with the enamel above. Dentin's structure is not precisely the same everywhere in a tooth, and both age and disease affect structure.

Collagen, a major component of dentin, is the most abundant animal protein in mammals, accounting for about 30 percent of all proteins. It is responsible for the tissues that hold us together, such as bone, cartilage, tendons, and skin.

For the UCSF researchers, knowing how hard, soft, brittle, or elastic dentin is will help improve restorative dentistry. Fillings, bridges, crowns, and other dental repairs must bond to the dentin, or they will fail.

Balooch is assisting the project by finding or creating the best tools to supply necessary measurements. His modified AFM may well be the best tool thus far for determining the mechanical properties of dentin. Because of the problems inherent in studying soft materials, especially very small samples of soft materials, there have been large discrepancies among measurements of the hardness and stiffness of dentin. This wide variation has made it impossible to establish the baseline mechanical behavior of dentin or to explore the effects of age, gender, or disease on tooth strength. The accuracy of the modified AFM allows evaluations of nanomechanical properties on a highly site-specific level, for the first time.

With the modified AFM, the team was the first to reveal major differences in the hardness of dentin in and around the tubes that traverse it. Hardness is evaluated using the pressure exerted by the indenter on the contact area. Using a different tip on the modified AFM, they measured fracture toughness by inducing cracks, a standard practice in examining the effects of stress on a material.

At the dentin–enamel junction, hard, brittle tooth enamel overlays soft, ductile dentin. Macroscopic tensile, compression, or shear tests are difficult at the junction, an area that represents a small percentage of the already small human tooth.

“Here, things got very interesting,” says Balooch. As shown in the bottom figure on p. 14, the modified AFM exposed in detail the stiffness and hardness differences between dentin and enamel. The team’s results agreed well with earlier macro- and microscale experiments by others. The smooth transition across the junction suggests that mineral content there must gradually change because the mineral component of calcified tissue is closely related to its mechanical properties.

While creating cracks in enamel is relatively easy, Balooch’s team found that inducing cracks in the dentin–enamel junction is much more difficult. The strength of the junction suggests that this area is critical for preserving the physical integrity of the tooth. Because of these characteristics, the dentin–enamel junction may serve as a model for the linkage of other pairs of highly dissimilar materials, such as those in artificial hip replacements.

Estimates of the precise width of the dentin–enamel junction have ranged from 12 to 200 micrometers using various micro- and nanoscale methods. Balooch, ever the tinkerer, tackled this measurement problem by again modifying an atomic force microscope. He changed it to create nanoscratches across the junction while simultaneously measuring lateral force. By measuring changes in friction, his team estimated a width for the junction of from 1 to 3 micrometers, about 10 times smaller than the smallest width previously estimated.

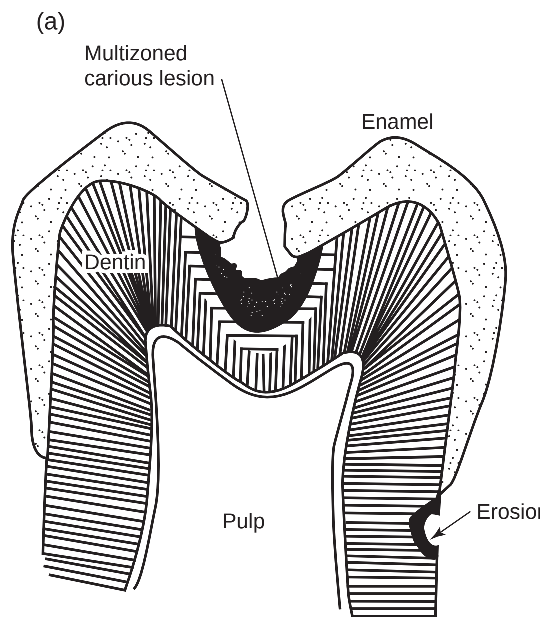
Fighting Vascular Disease

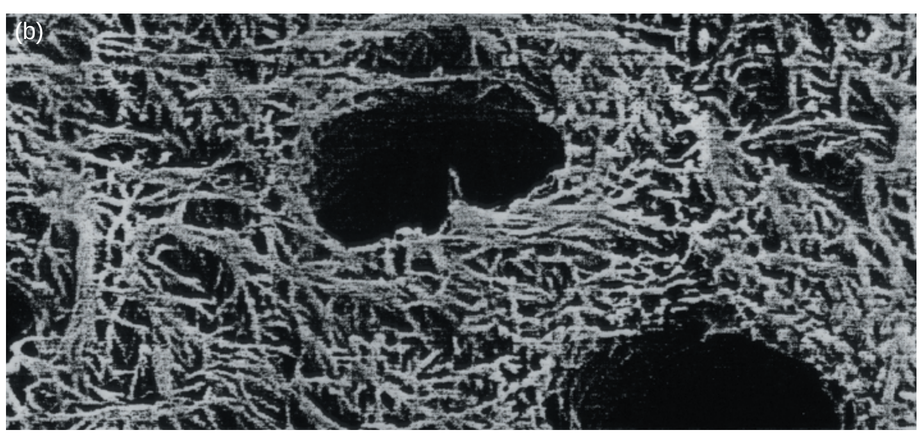
To investigate healthy and diseased human arteries, Balooch joined forces with Livermore physicist John Kinney, whose specialty is x-ray tomography.

Heart disease is the leading cause of death in the U.S. and is most commonly treated by catheter-based balloon angioplasty to dilate obstructed coronary arteries. While this procedure results in a 95-percent immediate success rate, 40 percent of all treated sites renarrow within 6 months. This lack of long-term success has led to considerable interest in how normal and diseased arteries become deformed. In particular, research focused on how the artery wall changes from stretching or from changes to fatty plaque deposits (calcifications).

Using his modified AFM, Balooch first measured local, in vitro mechanical properties of femoral artery tissue in saline solution. Then he moved to diseased calcified arteries. For this work, ultrasound images of arteries were recorded, and the healthy and calcified regions were marked. The healthy regions were extracted, and solid calcified deposits were dissected from the artery wall. More than 40 samples of both types of tissue were then mechanically tested with the modified AFM. Calcified deposits were found to be many orders of magnitude stiffer than the healthy artery wall, even as deposits varied from sample to sample and in their position on the wall.

Kinney took x-ray tomographs of dissected femoral arteries to make dynamic measurements of the deformation of plaque and vessel walls during graded stages of balloon





(a) Schematic diagram of a human tooth, showing enamel, dentin, and pulp. (b) A scanning electron microscope image of dentin showing the collagen fibers and tubules that run through dentin.

inflation and deflation. He found that fatty plaque deposits were less elastic than commonly assumed, which could affect the long-term success of balloon angioplasty.

Solving Seismic Problems

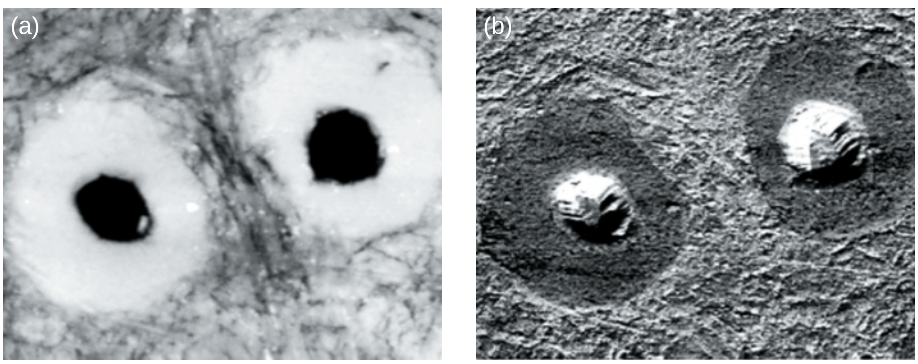
Geophysicists Brian Bonner and Dan Farber and geochemist Brian Viani are using the modified AFM to address seismological issues. Most of us equate seismology with earthquakes. But seismology in its broadest sense is simply the study of Earth's dynamic response to any mechanical stimuli. Seismic research thus encounters not just earthquakes but also problems related to slope stability, mitigating earthquake hazards, tracking the movement of pollutants underground, and exploring for oil, gas, and other hydrocarbons. With its Ground-Based Nuclear Explosion Monitoring program, Livermore also focuses on forensic seismology, which is the detection of clandestine explosions.

The project using the modified AFM addresses a fundamental problem in remote seismic sensing: the role fluids play in the transmission, modulation, and dissipation of seismic energy. "The importance of water, even at very low concentrations, was made clear during analysis of seismic events on our Moon," says Bonner.

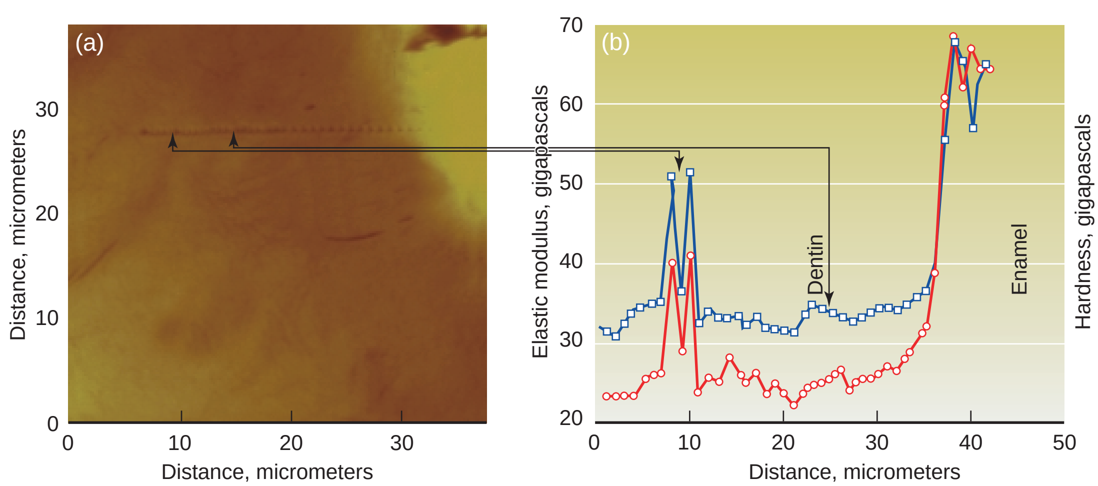
When the Apollo astronauts blasted off, they took along instruments, including seismometers, to study the Moon's properties. The seismograms from the Moon proved to be totally different from seismograms here on Earth. "They showed that the Moon rang like a bell," says Bonner.

But later, when rock samples were brought back by the Apollo astronauts, their seismic response became Earth-like. Conversely, scientists found that when Earth rocks were baked in high-temperature vacuum ovens, they took on Moon-like attenuation characteristics. The scientists assumed that the change in the Moon rocks must have been caused by tiny amounts of water acquired in Earth-bound laboratories. Even a small amount of water made a big difference. Now, after more than 30 years, Balooch's apparatus finally is providing the means to study this effect directly.

Bonner, Farber, and Viani's experiments are similar to the Moon-rock scenario in that they are studying the effects of an extremely small amount of water in a mineral. They use a type of clay, montmorillonite, which can confine very thin layers of water (0.25 nanometer per layer) between the sheets of silicate that make up the clay.



(a) A standard atomic force microscope (AFM) topographical image of a polished dentin specimen. The dark areas are the tubules that run through dentin. (b) An image with the modified AFM measures the stiffness of the same site. The peritubular dentin, the area immediately around the tubules, is stiffer than the rest of the surface.



(a) An atomic force microscope (AFM) image of indentations across the dentin–enamel junction. (b) Curves show the corresponding hardness and stiffness (elastic modulus) determined from indentations with the modified AFM. The smooth increase in stiffness across the junction suggests that mineral content must gradually change there because the mineral component of calcified tissue is closely related to its mechanical properties.

An image of the experimental sample is shown in the figure at bottom right. Samples were tested using the modified AFM in dry nitrogen and in air with about 30-percent relative humidity. Stiffness decreased dramatically when the sample was hydrated, as indicated by force modulation tests. Attenuation—the dissipation of mechanical energy—increases greatly in the hydrated sample. The measurements show the samples behaving like a classical viscoelastic material, that is, a viscous material that has some elastic properties. "Now we can say with confidence that a viscoelastic model is an appropriate one for seismic response in clay-dominated geologies, even for seismic displacements," says Bonner.

These results make perfect sense on an intuitive level because we know what water does to soil. But the experiments make this observation quantitative for the first time. Collecting data on the nanoscale removes the effect of other interfering phenomena, such as rock porosity. Nanoscale effects—which had never before been observed—reveal the important mechanisms of seismic deformation and are consistent with observations on a large scale.

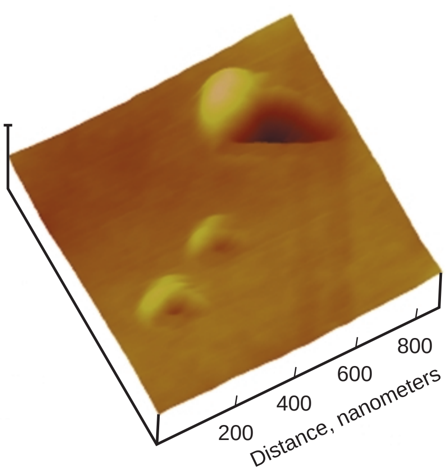
The team is now studying other sheet silicates to observe the effects of additional layers of water. They are also beginning to use molecular dynamics and effective-medium modeling to make predictions on a scale that is useful in the field.

"These measurements of mechanical properties of clay are important for several other energy and environmental uses," says geophysicist Pat Berge, acting division leader for Geophysics and Global Security, who applies these results to field-scale issues. " With them, we can model larger-scale behavior of clay-bearing soils and rocks."

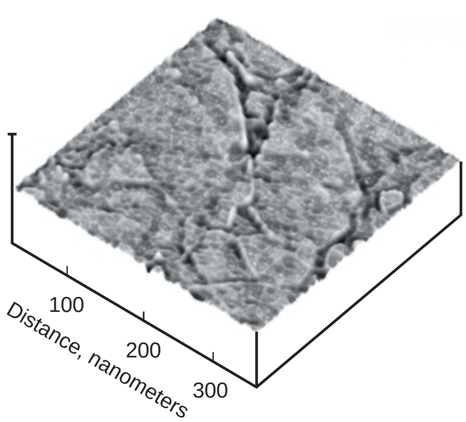
Geophysicists estimate the unknown composition of rock and soil underground by making seismic measurements at environmental cleanup sites, oil fields, or other regions of interest. Then they use rock-physics theories to interpret the seismic data and figure out how much fluid and what types and amounts of minerals are present. The success of these calculations depends on having good estimates of the seismic velocities of the pure fluids and minerals that make up the fluid-bearing soil or rock. Properties of water, quartz, calcite, and other minerals found in sandstones and sandy soils are readily available. Until Balooch's new technique came along, geophysicists did not have good estimates of the properties of clay, particularly at the smallest scales of individual clay platelets. This made modeling silty sands and shales difficult, leading to problems in underground imaging for oil reservoirs and environmental sites. Livermore researchers such as Berge suspected that the seismic velocity estimates commonly used for clay were too large by a factor of at least two and possibly a factor of five. But without laboratory corroboration, it was not possible to change the minds of the geophysical community. The new measurements by Farber, Bonner, and Viani show that clay is indeed a very soft material.

Most recently, Balooch has been working with chemist Wigbert Siekhaus to modify the AFM further so that stiffness can be imaged directly. This process, presently being patented, only adds to Livermore's unique ability for nanoscale examination of soft materials, an intermediate regime that until now has eluded researchers.

—*Katie Walter*



Nanoindentation on a calcified artery. The deposits can be mechanically tested with the modified atomic force microscope to determine their stiffness and thus reveal how the artery wall has been changed by calcification.



A prepared sample of a clay before it is measured with the modified atomic force microscope. The clay is montmorillonite, which can confine very thin water layers (0.25 nanometer per layer) between the sheets of silicate.

Key Words: atomic force microscope (AFM), dentin, mechanical properties, nanoindenter, plaque, seismic response, vascular disease.

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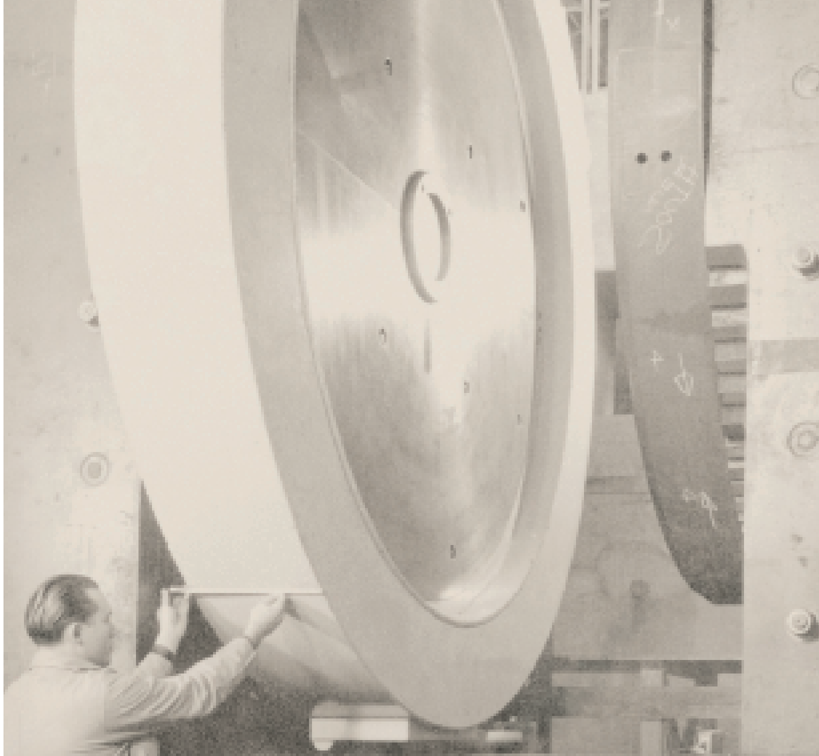
At Livermore, Audacious Physics Has Thrived for 50 Years



The 90-inch cyclotron, a leading particle accelerator of its time, started operation in 1954. For 16 years, it was a faithful, if sometimes cranky, workhorse, producing neutrons for a variety of experiments. Most of the data obtained on neutron cross sections during this time came from this machine. It was the first vertical cyclotron built, and, according to physicist John Anderson, was the last cyclotron that E. O. Lawrence had a personal hand in designing.

WHEN E. O. Lawrence selected Herbert York, a young physicist from Lawrence's Radiation Laboratory at Berkeley, to head the laboratory at Livermore, York had to come up with a starting point for possible programs, organization, and personnel at Livermore. The plan York developed called for four activities: thermonuclear weapons design, design and development of diagnostics for weapons experiments for both Los Alamos and Livermore, work on controlled thermonuclear reactions (in other words, fusion) for potential power sources, and basic physics research. All of these activities are, at heart, issues of physics. To understand the inner forces that govern a nuclear weapon, a fusion power source, or, indeed, the interior of a star requires knowing how the thermonuclear process works.

From the Laboratory's earliest days, physicists have explored some of the most difficult issues in the highly specialized fields of nuclear, condensed-matter, plasma, atomic, and molecular physics. As a result, the physics organization has always been a testing ground for new concepts and an integral contributor to major Laboratory programs, many of which it

> *"Every great advance in science has issued from a new audacity of imagination."*
>
> *John Dewey, philosopher*

The Laboratory has always been interested in astrophysics puzzles. In the 1960s, Laboratory physicists authored key papers on gravitational collapse and supernova explosions. In 1976, Livermore physicists John Browne (left), now director of Los Alamos National Laboratory, and Barry Berman used the Livermore's linear accelerator to gather key data to revise estimates of the age of the universe.

helped create. From their initial focus on the thermonuclear process, the Laboratory's physicists have advanced theoretical understanding and spearheaded breakthrough after breakthrough in applied physics—from the inner workings of the atom to the farthest reaches of the universe.

Exploring the Heart of a Weapon

Understanding a weapon's performance requires a thorough understanding of the properties of matter at extreme conditions—up to stellar temperatures and pressures—and of the interaction of matter with intense radiation. From the first days at Livermore, physicists made it their goal to better measure and validate material properties such as equations of state, opacities, and nuclear cross sections for these unique environments. Their tools included accelerators, gas guns, nuclear reactors, lasers, and nuclear tests on the one hand and advances in theory, powerful computers, and physics simulation codes on the other.

The nuclear cross section is particularly important for understanding how well a nuclear weapon performs; it has been of interest to the Laboratory from the start. The cross section is a measure of how likely it is that a particular reaction will occur between a nucleus of a particular material and an impinging particle. For nuclear weapons research, the particle of interest is usually a neutron, and the material is uranium, plutonium, steel—any of the materials that go into a nuclear device. Physicist John Anderson, who came to the Laboratory in 1956 and was associate director for Physics from 1978 to 1983, remembers, "In the 1950s, neutron physics was a hot topic. Many places were researching cross sections, but Los Alamos and Livermore were the only ones generating information applicable to weapons." Early Livermore physicists used two machines for gathering cross-section measurements: a Cockroft–Walton accelerator and the 90-inch cyclotron. These were replaced by the 100-megaelectronvolt linac, a linear accelerator still active today. The cross-section measurements obtained with these machines were used to continually improve weapons computer codes used to calculate a weapon's yield.

Cross-section measurements are also needed in the nation's present-day Stockpile Stewardship Program. Bill Goldstein, associate director for Physics and Advanced Technologies (PAT), explains, "One of the directorate's primary stockpile stewardship responsibilities is to support the Physical Data Research Program by providing validated data on material properties that are basic to weapons research." Just as in the past, physicists combine theory with computer simulations and laboratory measurements to provide the validated data needed for nuclear weapons simulations. With today's sophisticated tools, researchers can revisit some of the more difficult problems, reevaluating and refining measurements. One such example is a cross section in which a neutron smashes into a plutonium-239 atom, resulting in one plutonium-238 atom and two neutrons. Getting a good value for this cross section is particularly important because the production of plutonium-238 by neutrons is a major diagnostic for interpreting the results of past underground nuclear tests. For more than 40 years, large uncertainties in this cross section's value have limited the usefulness of plutonium-238 production as a nuclear test diagnostic.

In 2001, a five-year collaboration between Livermore and Los Alamos produced new measurements of this crucial reaction. The Livermore team, led by physicist John Becker, developed an innovative measurement approach using gamma-ray spectroscopy. Resolving the cross section from the experiments required a combined, intensive effort by experimentalists, nuclear theorists, and modelers. The new

measurements promise a better understanding of the data collected from past nuclear tests, aiding current stockpile stewardship efforts.

The Laboratory's tradition in developing and using state-of-the-art accelerators has continued unabated since the early days. Livermore partnered with the Stanford Linear Accelerator Center and Lawrence Berkeley National Laboratory in the 1990s to build the 2.2-kilometer-circumference B Factory, which is elucidating the origin of the matter–antimatter asymmetry in the universe. (See *S&TR*, January/February 1997, pp. 4–13.) The team is now helping design the 25-kilometer-long teraelecronvolt Next Linear Collider to better analyze physics beyond the Standard Model. (See *S&TR*, April 2000, pp.12–16.)

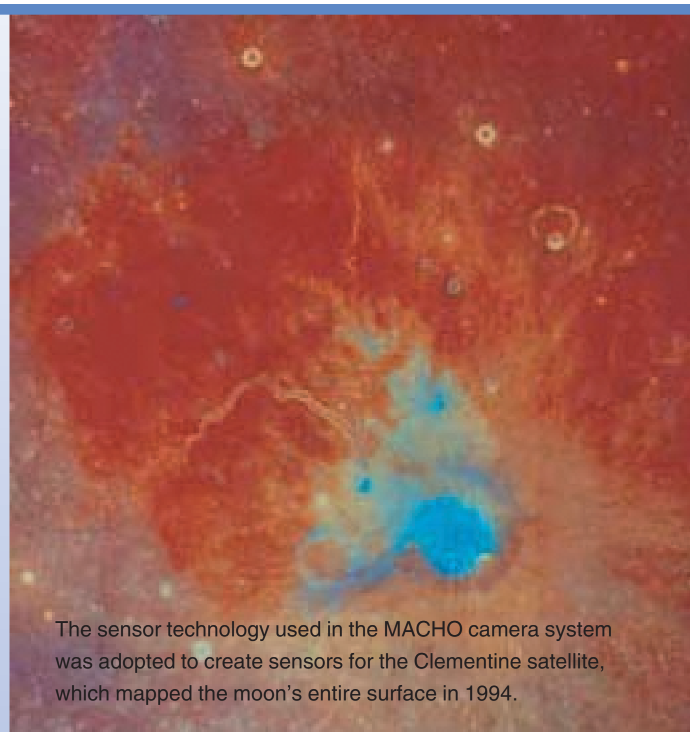
Divining the Heart of a Star

The same thermonuclear processes that drive a nuclear weapon drive the heart of a star. So, it's no surprise that astrophysics research at Livermore draws on the Laboratory's expertise in high-energy-density physics and complements the Laboratory's important stockpile stewardship responsibilities. In *Memoirs*, Edward Teller, who founded Livermore Laboratory along with E.O. Lawrence, notes, "From the beginning, and throughout the years to this date, Livermore has emphasized astrophysics and other branches of pure science in the recognition that great progress in applications cannot be made if science itself is neglected." In particular, Teller noted a paper by Stirling Colgate and Montgomery Johnson in 1960 that correctly described the mechanism and effects of an exploding star—a supernova. "The novelty in Montgomery and Stirling's work," explains Teller, "was their recognition that a shock wave, taking its origin in the center of the star and accelerating as it spread into the less dense regions of the star, was the first step in producing cosmic rays. That work is still cited as one of the more important papers in our current understanding of the universe." Research into astrophysics and general relativity continues, both at the Livermore branch of the University of California's Institute of Geophysics and Planetary Physics (see the box below) and within the PAT Directorate.

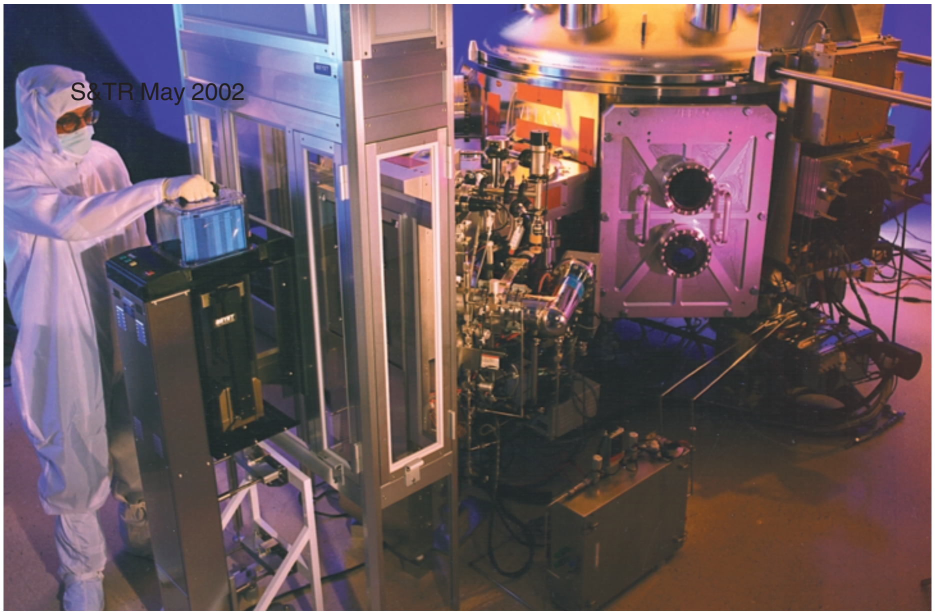
One example of current research applicable to astrophysics and stockpile stewardship is work on radiative opacity—that is, the study of how opaque a material is to the transport of photons. (See *S&TR*, April 1999, pp. 10–17.) Stellar opacity is concerned primarily with lighter elements, while opacity of nuclear weapon plasmas focuses on heavier elements; yet, the physics is similar for both. Researchers generally use detailed computer models to calculate opacities because it is extremely

Searching the Universe

One ongoing project of the Livermore branch of the University of California's Institute of Geophysics and Planetary Physics (IGPP) involves an attempt to identify the dark, invisible matter thought to comprise most of the universe's mass. (See *S&TR*, April 1996, pp. 6–11.) In the late 1980s, Livermore astrophysicist Charles Alcock, applying an innovative imaging technology invented for the Strategic Defense Initiative, searched for occasional amplifications of starlight from outside the galaxy caused by the gravitational effects of large objects known as MACHOs (massive compact halo objects). In 2000, Alcock, now a professor at the University of Pennsylvania, won the American Astronomical Society's Beatrice Tinsley Prize for his research. The data, which were collected by early 2000, are now being analyzed. They are also being used in another IGPP project to study the Milky Way's structure and composition. The IGPP is also home to the Djehuty project to develop a next-generation, fully three-dimensional, stellar structure and evolution code that will run on massively parallel computers. (See article beginning on p. 4.)



The sensor technology used in the MACHO camera system was adopted to create sensors for the Clementine satellite, which mapped the moon's entire surface in 1994.



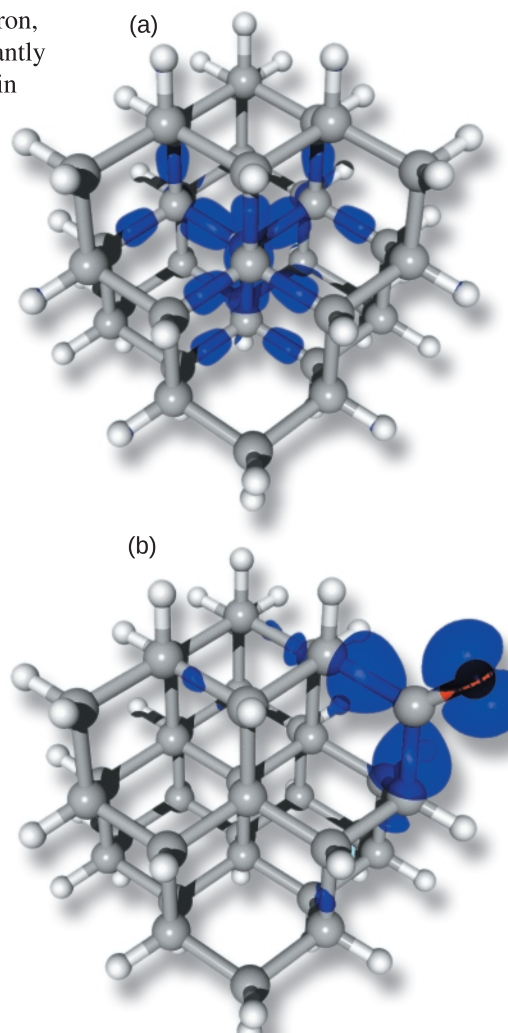
Livermore's early work on x-ray lasers and optics established technologies that led to its collaboration with industry and other national laboratories to develop extreme ultraviolet lithography for manufacturing the next generation of computer chips. Resulting microprocessors will be 100 times more powerful, and memory chips will be able to store 1,000 times more information than they do today. Livermore is the lead laboratory for optical design and fabrication, metrology, multilayer coating development, and mask fabrication for this project.

difficult to directly measure the opacity of materials hot enough to be in plasma form. In the early 1990s, physicists Forrest Rogers, Carlos Iglesias, and Brian Wilson built OPAL, a new model of stellar opacity that avoids many of the approximations and simplifying assumptions of earlier codes. In particular, OPAL accurately treats the myriad energy transitions in iron, which were previously overlooked in blocking radiation. OPAL calculations showed that iron, the most abundant heavy element in a star, can significantly impede radiation flow and therefore plays a major role in stellar properties. Throughout the 1990s, OPAL was refined through experiments on Livermore's Nova laser and on the Saturn pulsed-power machine at Sandia National Laboratories in Albuquerque. Data from these experiments and the codes they validate are being used to deepen astrophysicists' understanding of stars, strengthen fundamental knowledge of atomic processes in extreme environments, and provide greater confidence in the computational tools needed to maintain America's nuclear forces.

Creating Fusion in the Laboratory

It's little wonder that Herb York's original plan for the Laboratory included a group to research controlled thermonuclear reactions (CTR), or fusion energy. Not only are the physics processes of fusion similar to those of a nuclear weapon, but also interest in using fusion for power production was gaining ground in the early 1950s. The prospect was for a virtually inexhaustible, low-cost, safe, and environmentally attractive energy source.

The Laboratory initially concentrated on the magnetic confinement concept for producing fusion power, in which a magnetic force field traps a plasma long enough to achieve fusion. Livermore's approach was to use reflecting magnetic fields—or magnetic mirrors—to confine the fusion fuel. The first CTR group leader, physicist Dick Post, remembers, "In 1952, hardly anyone understood even the simplest aspects of the confinement of plasma by mirrors. There just wasn't any prior work to go on." Livermore physicists started with the basics, studying fundamental plasma processes; developing



Recent Livermore quantum molecular simulations examined the effects of contaminants such as oxygen on silicon quantum dots. A single oxygen atom can make a big difference on a quantum dot because of the dot's large ratio of surface area to volume. (a) In a simulation of a nanometer-size (71-atom) silicon quantum dot, the white hydrogen atoms bond to the surface, making the dot less reactive. The purple region, or "cloud," shows where light-absorbing electrons are most likely to be located inside the dot. (b) When two hydrogen atoms are replaced by an even more reactive oxygen atom, the electron charge cloud is drawn toward the oxygen atom, dramatically changing the optical properties of the silicon dot.

Sensors for Personal Health and the Health of the Nation

Innovative sensor and detector development for medical, national security, and defense-related applications is another focus of Livermore's physicists. In the Medical Technology Program, physicists, bioresearchers, and others are developing tools to provide cost-effective treatment for acute stroke, cancer detection and therapy, diabetes treatment and diagnostics, and therapy for other prevalent diseases of national importance.

For example, a microbead immunoassay dipstick system under development could be used by personnel such as firefighters and paramedics to run sophisticated diagnostics at the emergency site using a simple, one-step measurement. It could also be used as a portable clinical laboratory for military operations and for detection of biowarfare agents. Another tool, the Smart Probe, promises to provide early and accurate detection of breast cancer. The probe's sensors measure optical, electrical, and chemical properties that differ between healthy and cancerous tissues. Sensors play an important role in a program to develop an advanced interceptor for missile defense programs. The Advanced Technology Kill Vehicle uses lightweight integrated sensing systems to guide and control it while intercepting a missile. Cryogenic detectors, such as the one developed by physicist Simon Labov and his team, can distinguish between background radiation and nuclear materials and show promise in helping guard against the proliferation of nuclear weapons. (See *S&TR*, April 1998, pp. 16–18.)

methods to measure the temperature, density, and diffusion rates in a hot plasma; and exploring ways to contain the plasma.

Weapons and fission energy research also benefited fusion energy efforts, particularly in the search for reactor materials. John Anderson explains, "Fusion reactions produce large quantities of neutrons that can 'activate' the materials they hit, making the materials radioactive. You need to know how much radioactivity is generated, and you need accurate neutron transport models, topics of interest to weapons researchers as well." Beginning with the Table Top Reactor in 1954, Livermore created a series of machines to study the concept of plasma confinement using magnetic fields. More recently, Livermore fusion energy scientists are revisiting the spheromak concept of magnetic fusion. (See *S&TR*, December 1999, pp. 18–20.)

The tantalizing possibility of fusion energy took another turn with the invention of the laser in 1960. Some Livermore researchers, including physicist John Nuckolls (who later became a Laboratory director), wondered whether laser light might be able to trigger fusion reactions. Nuckolls and fellow physicists Ray Kidder and Stirling Colgate used Livermore-developed codes to study the possibility of compressing and igniting a small amount of deuterium–tritium fuel with powerful, short-duration laser pulses. These calculations revealed that to achieve energy gain—that is, to get more energy out than is put in—the laser would have to compress the fuel to about 1,000 times its liquid density.

In 1962, a small laser fusion project started in the Physics Department to explore this possibility. In the early 1970s, new computer calculations showed that interesting laser fusion experiments could be done with lasers as small as 10 kilojoules and that energy gains could be achieved with a megajoule-size laser. By this time, interest in laser fusion was widespread, and in 1972, the Inertial Confinement Fusion (ICF) Program was formed at the Laboratory. From this program sprung a series of increasingly powerful lasers, beginning in 1975 with Janus, a two-beam system with under 50 kilograms of laser glass, and leading to the National Ignition Facility, which will have 192 beams and over 180,000 kilograms of optics and is now under construction.

The x-ray laser also owes its existence to Livermore's early research into the physics of lasers. In the 1970s, physicists realized that laser beams could be generated by ions with high-lying energy states. In the 1980s, Livermore generated the first-ever x-ray laser beams in an underground test and demonstrated the first x-ray laser in a laboratory setting. In the 1990s, a Livermore team developed a small tabletop x-ray laser ideal for probing and imaging high-density plasmas. (See *S&TR*, September 1998, pp. 21–23.) These small x-ray lasers are used to fine-tune equations of state for a variety of materials, including those of interest to stockpile stewardship. Development of the x-ray laser also established the technical skills that helped lead to short-wavelength projection lithography for mass production of integrated circuits—a technology of significant importance to the nation's semiconductor industry. (See *S&TR*, November 1999, pp. 4–9.)

Understanding the World, Atom by Atom

"The preeminent goal of physics in the 20th century was to understand the workings of the world at the most fundamental level," says Goldstein. In the earlier part of the century, as physicists began studying atoms and their constituents, they learned that Newton's laws of motion did not apply on the small scale. The powerful mathematical tools of quantum mechanics were developed, and when computers arrived mid-century, with their geometric growth in computing power, physicists were in a better position to address the complexities of many particles interacting to produce the bulk properties of material systems.

At Livermore today, physicists such as Giulia Galli use the supercomputers of the Advanced Simulation and Computing (ASCI) program to simulate matter at a more fundamental level than was previously feasible. (See *S&TR*, April 2002, pp. 4–10.) Computer codes have been developed that allow researchers to simulate the interactions of 10 to 1,000 atoms and see in detail the dynamic activity of nanoparticles of individual atoms and molecules. For the silicon nanoparticles known as quantum dots, quantum simulations reveal unique optical properties that vary with size and surface characteristics. Lasers made of silicon are now possible, as are silicon dots that could be used as fluorescent markers in biological research and as biological sensors.

Growing Leaders and Programs

Throughout Livermore Laboratory's history, the physics organization has been the birthplace of new scientific concepts. It has grown programs that then split off to become their own considerable forces, provided inspiration and support for a recent Nobel Prize winner whose work was carried out at the Laboratory, and developed many of the Laboratory's top leaders. All but one of the Laboratory's directors were physicists, and many—including Edward Teller, John Nuckolls, and Bruce Tarter—at one time or another headed the physics organization. "From early on, Physics has provided top leaders to the Laboratory, and we've also played a role in providing new programmatic directions for the Lab," says Goldstein. "I see both roles continuing into the future in our work to keep the Laboratory at the scientific cutting edge."

—Ann Parker

Key Words: astrophysics, dark matter, fusion energy, nuclear cross section, opacity, quantum mechanics, sensors, stockpile stewardship, tabletop laser, thermonuclear processes, weapons research, x-ray laser.

For further information about the Physics and Advanced Technologies Directorate, see:

www-pat.llnl.gov/

For further information about the Laboratory's 50th anniversary celebrations, see:

www.llnl.gov/50th_anniv/

In December 1998, Robert B. Laughlin, a longtime Livermore employee and a professor of physics at Stanford University, received the 1998 Nobel Prize for physics for work he did in the Laboratory's condensed-matter division in 1983. The prize—shared with Horst Stormer of Columbia University and Daniel Tsui of Princeton University—was awarded for the discovery that electrons acting together in strong magnetic fields can form new types of particles with charges that are fractions of electron charges. (See *S&TR*, January/February 1999, pp. 15–18.)

Photo: AP/Jonas Ekstromer

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

Chirped Pulse Inverse Free-Electron Laser Vacuum Accelerator

Frederic V. Hartemann, Hector A. Baldis, Eric C. Landahl
U.S. Patent 6,345,058 B1
February 5, 2002
A chirped-pulse inverse free-electron laser (IFEL) vacuum accelerator for high-gradient laser acceleration in vacuum. By using an ultrashort (femtosecond), ultrahigh-intensity chirped laser pulse, both the IFEL interaction bandwidth and accelerating gradient are increased, thus yielding large gains in a compact system. In addition, the IFEL resonance condition can be maintained throughout the interaction region by using a chirped-drive laser wave. Also, diffraction can be alleviated by taking advantage of the laser optical bandwidth with negative dispersion focusing optics to produce a chromatic line focus. The combination of these features results in a compact, efficient laser vacuum accelerator with many applications, including high-energy physics, medical imaging and therapy, material science, and basic physics.

NO_x Reduction by Electron Beam-Produced Nitrogen Atom Injection

Bernardino M. Penetrante
U.S. Patent 6,345,497 B1
February 12, 2002
Deactivated atomic nitrogen generated by an electron beam from a gas stream containing more than 99 percent nitrogen is injected at low temperatures into an engine exhaust to reduce NO_x emissions. High NO_x reduction efficiency is achieved with compact electron beam devices without the use of a catalyst.

Alternating-Polarity Operation for Complete Regeneration of Electrochemical Deionization System

Tri D. Tran, David J. Lenz
U.S. Patent 6,346,187 B1
February 12, 2002
An electrically regeneratable battery of electrochemical cells for capacitive deionization (including electrochemical purification) and regeneration of electrodes is operated at alternate polarities during consecutive cycles. By polarizing the cells, ions are removed from the electrolyte and are held in the electric double layers formed at the carbon aerogel surfaces of the electrodes. As the electrodes of each cell of the battery are saturated with the removed ions, the battery is regenerated electrically at a reversed polarity from that during the deionization step of the cycle, thus significantly minimizing secondary wastes.

Thermally Robust Semiconductor Optical Amplifiers and Laser Diodes

Sol P. Dijaili, Frank G. Patterson, Jeffrey D. Walker, Robert J. Deri, Holly Petersen, William Goward
U.S. Patent 6,347,106 B1
February 12, 2002
A highly heat-conductive layer is combined with or placed in the vicinity of the optical waveguide region of active semiconductor components. The thermally conductive layer enhances the conduction of heat away from the active region, which is where the heat is generated in active semiconductor components. This layer is placed so close to the optical region that it must also function as a waveguide and causes the active region to be nearly the same temperature as the ambient temperature or heat sink. However, the semiconductor material itself should be as temperature-insensitive as possible, and therefore, the invention combines a highly thermally conductive dielectric layer with improved semiconductor materials to achieve an overall package that offers improved thermal performance. The highly thermally conductive layer serves two basic functions. First, it provides a lower index material than the semiconductor device so that certain kinds of optical waveguides may be formed, for example, a ridge waveguide. Second and most important, this layer provides a significantly higher thermal conductivity than the semiconductor material, which is the principal material in the fabrication of various optoelectronic devices.

High Average Power Scaleable Thin-Disk Laser

Raymond J. Beach, Eric C. Honea, Camille Bibeau, Stephen A. Payne, Howard Powell, William F. Krupke, Steven B. Sutton
U.S. Patent 6,347,109 B1
February 12, 2002
Using a thin-disk laser gain element with an undoped cap layer enables the scaling of lasers to extremely high-average output-power values. Ordinarily, the power scaling of such thin disk lasers is limited by the deleterious effects of amplified spontaneous emission. By using an undoped cap layer diffusion bonded to the thin disk, the onset of amplified spontaneous emission does not occur as readily as it would if no cap layer is used, and much larger transverse thin disks can be effectively used as laser gain elements. This invention can be used as a high-average-power laser for material processing applications as well as for weapon and air defense applications.

Low Cost Impulse Compatible Wideband Antenna

Erwin T. Rosenbury, Gerald K. Burke, Scott D. Nelson, Robert D. Stever, George K. Gorverno, Donald J. Mullenhoff
U.S. Patent 6,348,898 B1
February 19, 2002
An antenna apparatus and method for building the antenna. Impulse signals travel through a feed point of the antenna with respect to a ground plane. A geometric fin structure is connected to the feed point and through a termination resistance to the ground plane. A geometric ridge structure connected to the ground is positioned with respect to the fin to receive and radiate electromagnetic energy from the impulse signal at a predetermined impedance and over a predetermined set of frequencies. The fin and ridge can be either a wire or a planar surface. The fin and ridge may be disposed within a radiation cavity such as a horn. The radiation cavity is constructed of stamped and etched metal sheets bent and then soldered together. The fin and ridge are also formed from metal sheets or wires. The fin is attached to the feed point and then to the cavity through a termination resistance. The ridge is attached to the cavity and disposed with respect to the fin to achieve a particular set of antenna characteristics.

Self Adjusting Inclinometer

Steven L. Hunter
U.S. Patent 6,349,477 B1
February 26, 2002
An inclinometer using synchronous demodulation for high-resolution and electronic offset adjustment provides a wide dynamic range without any moving components. A device encompassing a tiltmeter and accompanying electronic circuitry provides quasilevel tilt sensors that detect highly resolved tilt change without signal saturation.

Junction-Based Field Emission Structure for Field Emission Display

Long N. Dinh, Mehdi Balooch, William McLean II, Marcus A. Schildbach
U.S. Patent 6,351,254 B2
February 26, 2002
A junction-based field emission display, wherein the junctions are formed by depositing a semiconducting or dielectric, low-work-function, negative electron affinity (NEA) silicon-based compound film (SBCF) onto a metal or *n*-type semiconductor substrate. The SBCF can be doped to become a *p*-type semiconductor. A small forward bias voltage is applied across the junction so that electron transport is from the substrate into the SBCF region. When the voltage enters this NEA region, many electrons are released into the vacuum level above the SBCF surface and accelerated toward a positively biased phosphor screen anode, hence lighting up the phosphor screen for display. To turn off the screen, the user can simply switch off the applied potential across the SBCF/substrate. The invention may be used for field emission flat-panel displays.

Combined Dispersive/Interference Spectroscopy for Producing a Vector Spectrum

David J. Erskine
U.S. Patent 6,351,307 B1
February 26, 2002
A method of measuring the spectral properties of broadband waves that combines interferometry with a wavelength disperser having many spectral channels to produce a fringing spectrum. Spectral mapping, Doppler shifts, metrology of angles, distances, and secondary effects such as temperature, pressure, and acceleration that change an interferometer cavity length can be measured accurately by a compact instrument using broadband illumination. Broadband illumination avoids the fringe skip ambiguities of monochromatic waves. The interferometer provides arbitrarily high spectral resolution, simple instrument response, compactness, low cost, high field of view, and high efficiency. The inclusion of a disperser increases fringe visibility and signal-to-noise ratio over an interferometer used alone for broadband waves. The fringing spectrum is represented as a wavelength-dependent two-dimensional vector, which describes the fringe amplitude and phase. Vector mathematics such as generalized dot products rapidly computes average broadband phase shifts to high accuracy. A moiré effect between the interferometer's sinusoidal transmission and the illumination heterodyne's high- to low-resolution spectral detail allows the use of a low-resolution disperser. Multiple parallel interferometer cavities of fixed delay allow the instantaneous mapping of a spectrum, using an instrument more compact for the same spectral resolution than a conventional dispersive spectrometer, and do not require a scanning delay.

Portable Gas Chromatograph Mass Spectrometer for On-Site Chemical Analyses

Jeffrey S. Haas, John F. Bushman, Douglas E. Howard, James L. Wong, Joel D. Eckels
U.S. Patent 6,351,983 B1
March 5, 2002
A portable, lightweight (approximately 25 kilograms) gas chromatograph–mass spectrometer (GC–MS), including the entire vacuum system, can perform qualitative and quantitative analyses of all sample types in the field. The GC–MS has a conveniently configured layout of components for ease of serviceability and maintenance. The GC–MS system can be transported under operating or near operating conditions (that is, under vacuum and at elevated temperature) to reduce the downtime before samples can be analyzed on site.

Coatings on Reflective Mask Substrates
William Man-Wai Tong, John S. Taylor, Scott D. Hector, Pawitter J. S. Mangat, Alan R. Stivers, Patrick G. Kofron, Matthew A. Thompson
U.S. Patent 6,352,803 B1
March 5, 2002
A process for creating a mask substrate involving depositing (1) a coating on one or both sides of a low-thermal expansion material, extreme-ultraviolet-light mask substrate to improve defect inspection, surface finishing, and defect levels; and (2) a high-dielectric coating on the backside to facilitate electrostatic chucking and correct for any bowing caused by the stress imbalance imparted either by other deposited coatings or the multilayer coating of the mask substrate. A film, such as tantalum silicon, may be deposited on the front or back of the low-thermal-expansion material, before the material coating, to balance the stress. The low-thermal-expansion material with a silicon overlayer and a silicon and other conductive underlayer enables improved defect inspection and stress balancing.

Microfluidic DNA Sample Preparation Method and Device
Peter A. Krulevitch, Robin R. Miles, Xiao-Bo Wang, Raymond P. Mariella, Peter R. C. Gascoyne, Joseph W. Balch
U.S. Patent 6,352,838 B1
March 5, 2002
Manipulation of DNA molecules in solution has become an essential aspect of genetic analyses used for biomedical assays, identifying hazardous bacterial agents, and decoding the human genome. Currently, most of the steps involved in preparing a DNA sample for analysis are performed manually and are time-, labor-, and equipment-intensive. These steps include extraction of the DNA from spores or cells, separation of the DNA from other particles and molecules in the solution (for example, dust, smoke, cell/spore debris, and proteins), and separation of the DNA itself into strands of specific lengths. Dielectrophoresis, a phenomenon whereby polarizable particles move in response to a gradient in electric field, can be used to manipulate and separate DNA in an automated fashion, considerably reducing the time and expense involved in DNA analyses as well as allowing for the miniaturizaiton of DNA analysis instruments. These applications include direct transport of DNA, trapping of DNA to allow for its separation from other particles or molecules in the solution, and the separation of DNA into strands of varying lengths.

Awards

Physicist **Charles Carrigan** was recently named a **Fulbright Distinguished Scholar**. Fulbrights are grants made for a variety of educational activities. Carrigan is one of typically 11 recipients selected to perform research and teaching in the United Kingdom. He has been invited by the Department of Earth Sciences at Cambridge University to pursue research there for a year. Carrigan also has been selected as visiting fellow of St. Edmund’s College, one of the colleges of Cambridge University.

Carrigan received his Ph.D. from the University of California at Los Angeles. At the Laboratory, he is a group leader of the subsurface flow and transport group in the Energy and Environment Directorate.

Building a Virtual Telescope

Lawrence Livermore astrophysicists have developed a three-dimensional code that simulates the evolution and structure of stars. The code is named after Djehuty, the Egyptian god of calculation, wisdom, and judgment. The Djehuty code was developed because the complex processes found in stars have been imperfectly modeled with one-dimensional codes. These simplified codes do not incorporate all the physics pertinent to a star's core, where nuclear energy is produced, and do not simulate gravity in a realistic manner. Djehuty was designed to be used with massively parallel supercomputers (machines with thousands of processors working together). The code development work has taken advantage of Livermore's expertise in computations for the National Nuclear Security Administration's Advanced Simulation and Computing program, massively parallel computer code and algorithm development, astrophysics, high-energy-density physical data and processes, and experience in interdisciplinary coordination. The code is being applied to resolve a long-standing issue in astrophysics concerning the size of a star's convection region, where hot plumes of gas rise and fall.

Contact:
David S. Dearborn (925) 422-7219 (dearborn2@llnl.gov).

A New Understanding of Soft Materials

A device that combines an atomic force microscope and a nanoindenter can, for the first time, measure the mechanical properties of soft materials. These materials include certain biological tissues, polymers, and hydrated clays, an important component of soils, as well as hard materials in fluid. In conjunction with the University of California at San Francisco, Laboratory researchers are studying human teeth, most recently measuring hardness and stiffness across the junction between tooth enamel, a hard material, and dentin, a soft material. Their results indicate that this area may provide a model for the linkage of other pairs of highly dissimilar materials such as those in artificial hip replacements. Healthy and diseased human arteries have also been studied. Other researchers are applying this new apparatus to a nanoscale examination of clay crystals intercalated with water. They found that stiffness properties observed on the nanoscale—which had never before been measured—resolve longstanding questions about the role of water in seismic attenuation measurements made in the field.

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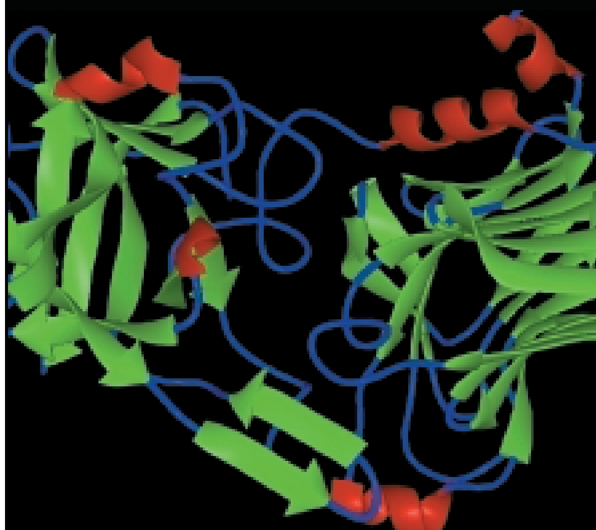
U.S. Government Printing Office: 2002/783-051-70016

Coming Next Month

Molecules That Detect and Disarm Pathogens



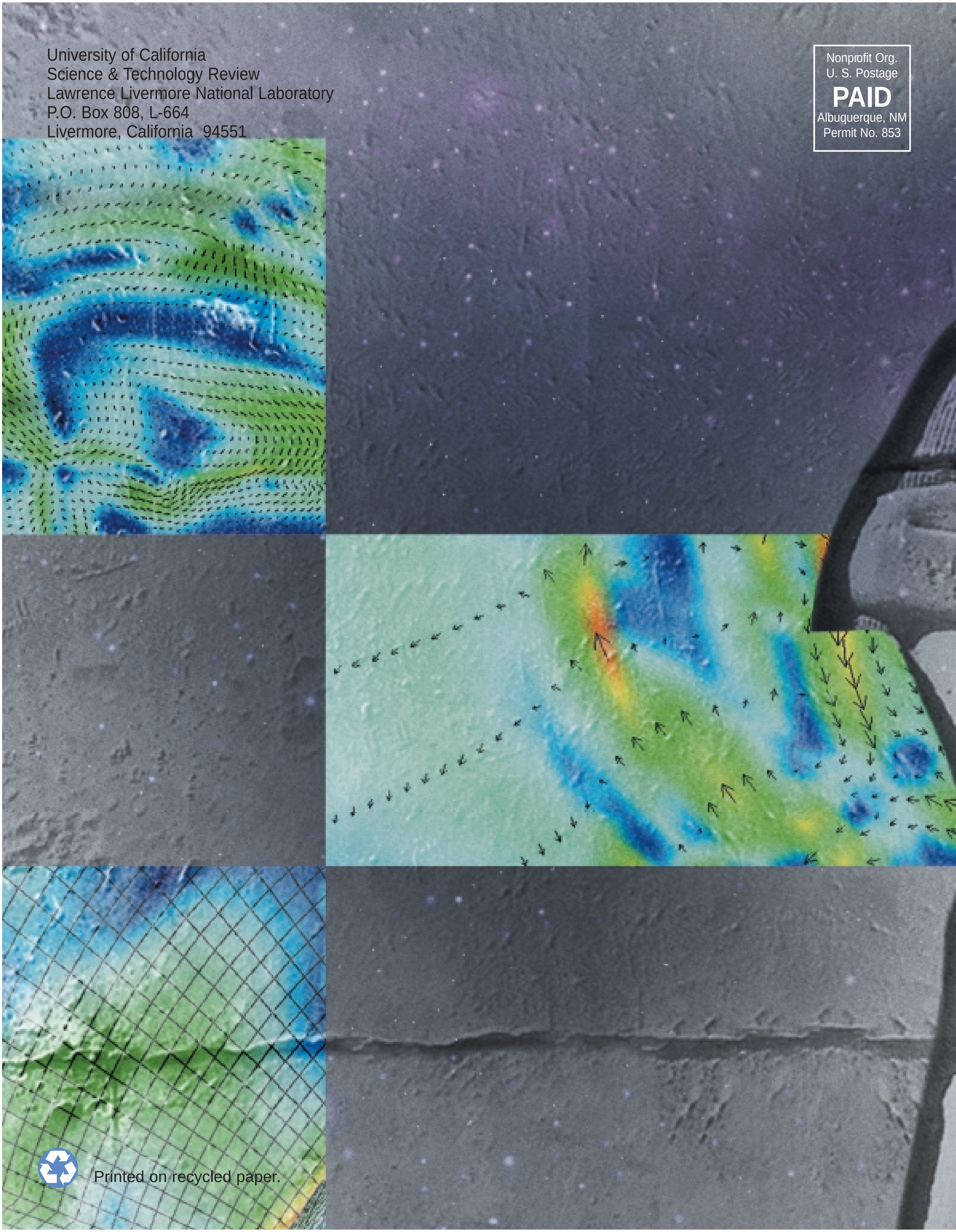
Livermore scientists are designing tiny antibodylike molecules to detect biowarfare agents and fight cancer.

Also in June:

- ***Adaptive optics reveal astronomical detail with excellent resolution.***

- ***Experiments using Livermore's electron beam ion trap and a NASA-designed x-ray spectrometer are deepening understanding of the x rays emitted by comets as they pass the Sun.***

- ***50th Anniversary Highlight—Chemists and materials scientists have supplied the elemental understanding of the chemical processes and developed the innovative materials needed for Livermore's national security mission.***



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