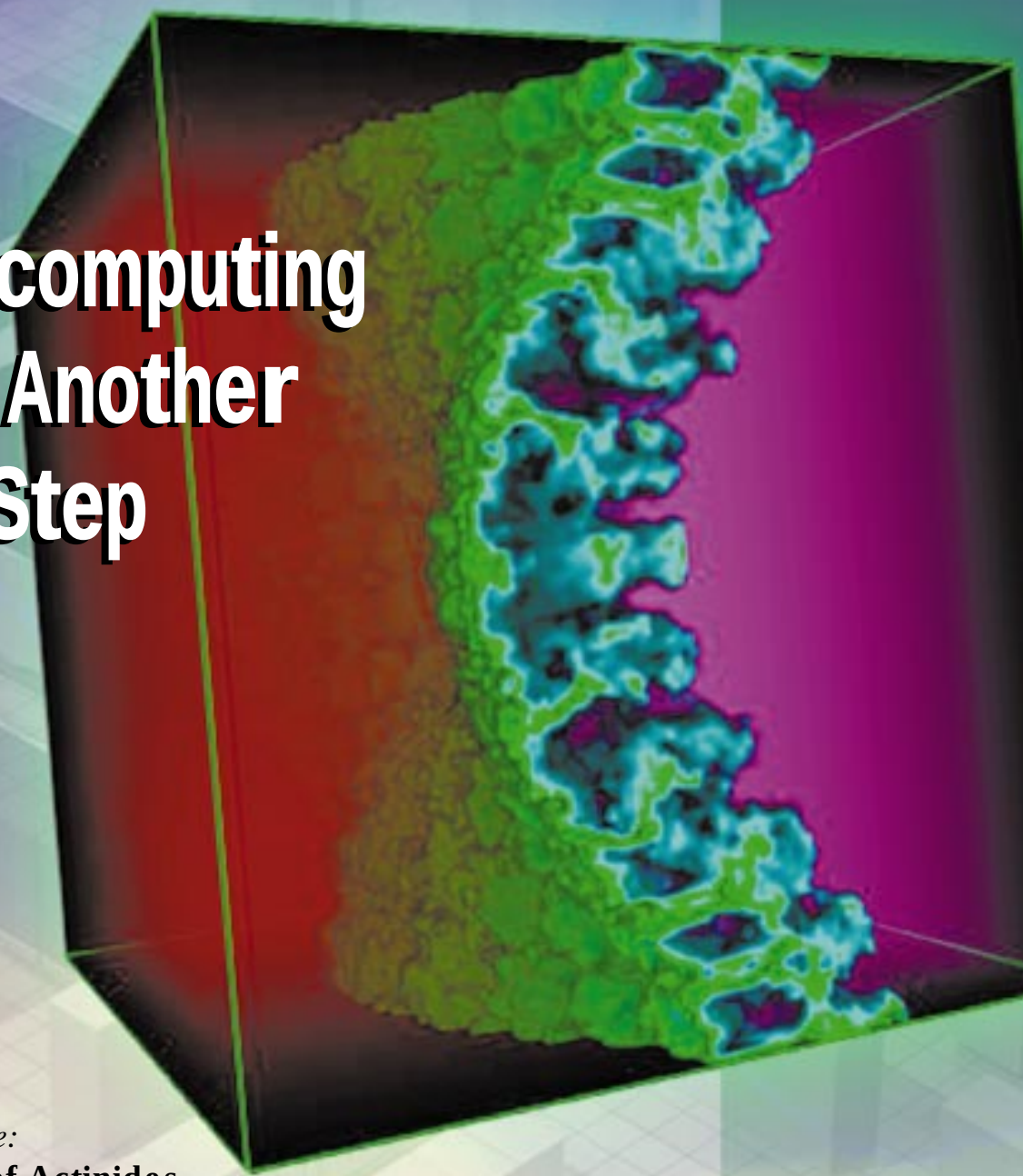
Science & Technology REVIEW

June 2000

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



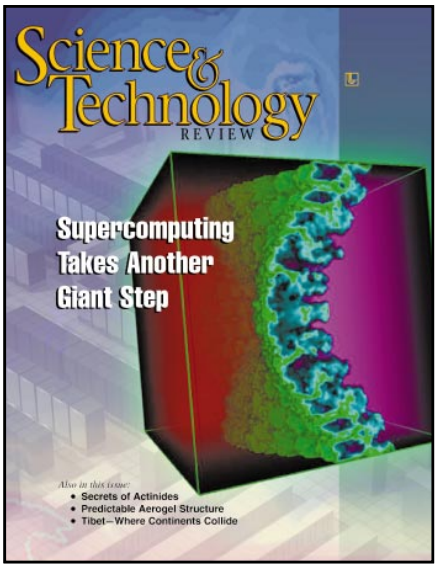
Supercomputing Takes Another Giant Step

Also in this issue:

- **Secrets of Actinides**
- **Predictable Aerogel Structure**
- **Tibet—Where Continents Collide**

About the Cover

When the ASCI White supercomputer comes online at Livermore this summer, it will carry forward the achievements of its predecessor, the Blue Pacific machine, toward the ultimate goal of DOE's Accelerated Strategic Computing Initiative—full-scale simulations of nuclear behavior in support of stockpile stewardship. The article beginning on p. 4 reports both the accomplishments of Blue Pacific in terascale simulations and the promise of ASCI White in helping to fulfill stockpile stewardship's mission. On the cover is the prize-winning Blue Pacific simulation of what happens when a shock wave passes through the interface of two fluids of differing densities. It took 5,832 processors to make this calculation, the largest, most detailed of its kind to date.



About the Review

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

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June 2000

Lawrence Livermore National Laboratory

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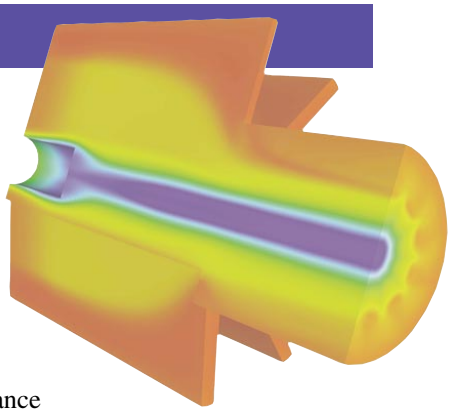

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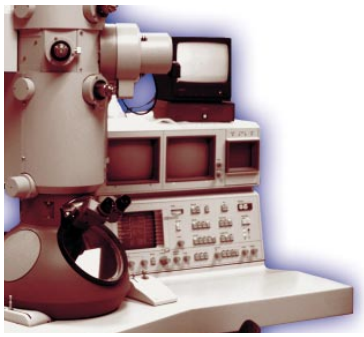

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Lab signs cooperative contracts with Russians

The Laboratory signed two contracts recently in Moscow that will assist Russian weapons experts from the closed city of Snezhinsk in their transition to civilian employment. (A closed city is a formerly secret city where nuclear weapons research was conducted.) The projects include developing oil production technology and improving Russia's fiber-optic cables for the commercial market. Both contracts were signed by representatives of the Laboratory and SPEKTR, a State Unitary Enterprise.

When oil wells are drilled, they are lined with metal casings that support the surrounding geology and prevent gas, oil, and water from mixing in the well. SPEKTR, which already provides explosive charges for perforating the casings to allow oil to flow effectively at selected depths will use the approximately $220,000 in U.S. support over the next year to develop perforation technologies that apply to diverse geologic conditions and casings.

Under the second agreement, SPEKTR will raise to world standards the quality of its multimode optical fiber, demonstrate production capability to satisfy commercial demands, and develop relationships with cable suppliers to commercialize its product.

The two new contracts are part of U.S.–Russian strategic plans for the city of Snezhinsk under the auspices of the Nuclear Cities Initiative (NCI), a Department of Energy effort to help the Russian government provide civilian employment opportunities to weapons scientists in closed Russian nuclear cities. The goal of the NCI is to enable Russian scientists to remain in their homeland and work on sustainable civilian and commercial projects as facilities in Russia's weapons complex are downsized or closed.

The All-Russian Research Institute of Technical Physics also agreed in principle to form an open computer center at Snezhinsk. Lawrence Livermore and the institute will work toward a contract to begin a commercial software and scientific computations effort. Skilled Russian software engineers working at the center will be able to relieve some of the worldwide shortage of programming talent. High-speed Internet lines will connect the center with customers inside and outside Russia, just as they do at other commercial software development centers around the world.

The Laboratory has also signed an agreement to assist the Avangard plant in the closed city of Sarov in converting from nuclear weapons manufacturing to the production of kidney dialysis equipment. A non-Russian firm, which has asked not to be identified for proprietary reasons, will purchase and market three components manufactured by Avangard for use in machines distributed worldwide. The hope is that as a result of this U.S.–Russian agreement, Russian-made parts and eventually systems will make kidney dialysis more available to Russians.

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Breakthrough in laser glass manufacture

A major laser glass milestone has been achieved for the Laboratory's National Ignition Facility (NIF) thanks to extensive research and development spearheaded by the Laboratory and two leading high-technology glass vendors.

Schott Glass Technologies, based in Duryea, Pennsylvania, has successfully demonstrated a process to ensure continuous production of economical, high-optical-quality, neodymium-doped, phosphate laser glass needed for NIF. A second vendor, Hoya Corp. in Fremont, California, began similar glass-melting operations in April.

Schott has produced more than 20 of the glass slabs needed for NIF's demanding optical specifications—at a rate 20 times faster than is possible using existing one-slab-at-a-time batch-melting technology.

More than 3,500 laser glass slabs will be needed for NIF. Each slab is about 80 centimeters long, 45 centimeters wide, and 4 centimeters thick and weighs about 37 kilograms.

The costs for developing the continuous melting process have been shared equally by Livermore and the French Commissariat à L'Energie Atomique (CEA). CEA plans to purchase a similar quantity of slabs for its Laser Megajoule to be constructed later in this decade.

In 1999, Schott and Hoya demonstrated the feasibility of continuous-melt production, but certain glass specifications were not achieved at that time. In particular, the glass contained trace quantities of contamination from small amounts of moisture in the surrounding air and in the initial glass raw materials. And attempts to remove the moisture-derived contamination degraded other glass properties.

Recently, however, Livermore, Schott, and Hoya have carried out cooperative research aimed at reducing moisture contamination. Schott first demonstrated the success of this research and the improved technology, which both vendors will use to manufacture the laser glass for NIF and Laser Megajoule.

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Accelerating on the ASCI Challenge

AS fast as computer technology is advancing, the Department of Energy's Accelerated Strategic Computing Initiative (ASCI) must advance the technology even faster.

The reason for the push lies in the inexorable aging of the country's nuclear stockpile and DOE's responsibility to keep this stockpile viable. On September 25, 1995, President Clinton directed DOE to undertake the necessary activities to ensure continued stockpile performance in an era of no nuclear testing, no new weapon development, a production complex with reduced capacity and capability, and an aging stockpile of fewer weapons and fewer types of weapons.

The Stockpile Stewardship Program—of which ASCI represents one key component—is DOE's response to this challenge. It must provide the tools researchers need to develop a detailed understanding of the science and technology that govern all aspects of nuclear weapons. It must also proceed quickly so that the necessary tools and scientific understanding are in place within about a decade.

In this race against time, three national laboratories—Lawrence Livermore, Los Alamos, and Sandia—have teamed up with the supercomputing industry to accelerate the development of high-performance supercomputers. Just as fighter planes regularly break the speed-of-sound barrier, ASCI supercomputers are breaking speed barriers of a different sort set by Moore's law. That is, they are doubling computing speeds in terms of teraops (trillions of floating-point operations per second) faster than every 18 months.

The current high-end computer at Livermore is the ASCI Blue Pacific machine built by IBM and delivered in the fall of 1998. It was used to perform the first-ever three-dimensional simulation of an exploding nuclear weapon primary. This calculation, completed in November 1999, represented the first successful completion of an ASCI milepost application. In addition, this machine has performed a series of first-principles simulations detailing the molecular interactions of the highly corrosive compound hydrogen fluoride, which occur in some high explosives.

The newest candidate for this innovative lineup is ASCI White, scheduled for delivery to Lawrence Livermore this summer. In terms of pure speed, ASCI White will be at least two and a half times faster than the Blue Pacific machine, which is itself an impressive system. One of the big triumphs of ASCI Blue Pacific—which will become routine with White—is performing detailed three-dimensional simulations of complex physical phenomena. Clocking in at more than 12 teraops, White is the next step in the ASCI plan to produce a 100-teraops system by 2004. One hundred teraops is the entry-level performance needed to perform full-scale simulations of exploding nuclear weapons. The results from these incredibly complex three-dimensional simulations will be combined with existing nuclear test data and new, nonnuclear experiments to ensure the safety, reliability, and performance of U.S. nuclear weapons.

The national weapons laboratories and the U.S. high-performance computer industry are not the only entities engaged in the ASCI challenge. Through DOE's Academic Strategic Alliance Program, the U.S. academic community also draws on the power and speed of these supercomputer systems to advance unclassified science-based modeling and simulation technologies applicable to all of ASCI's research areas.

At Livermore, ASCI efforts engage talents across the Laboratory's organizations, with the Defense and Nuclear Technologies and the Computation directorates providing the focus and the leadership. This issue's feature article, beginning on p. 4, highlights the accomplishments of ASCI Blue Pacific and the promise of ASCI White. The progress in computing inherent in these machines has placed researchers in the DOE community and in academia on the verge of being able to simulate first-principle physics without resorting to oversimplified models. It's an exciting prospect, one that promises breakthroughs not only for stockpile stewardship but also for areas as diverse as biochemistry, materials science, and astrophysics.

n Michael Anastasio is Associate Director, Defense and Nuclear Technologies. David Cooper is Associate Director, Computation, and the Laboratory's Chief Information Officer.

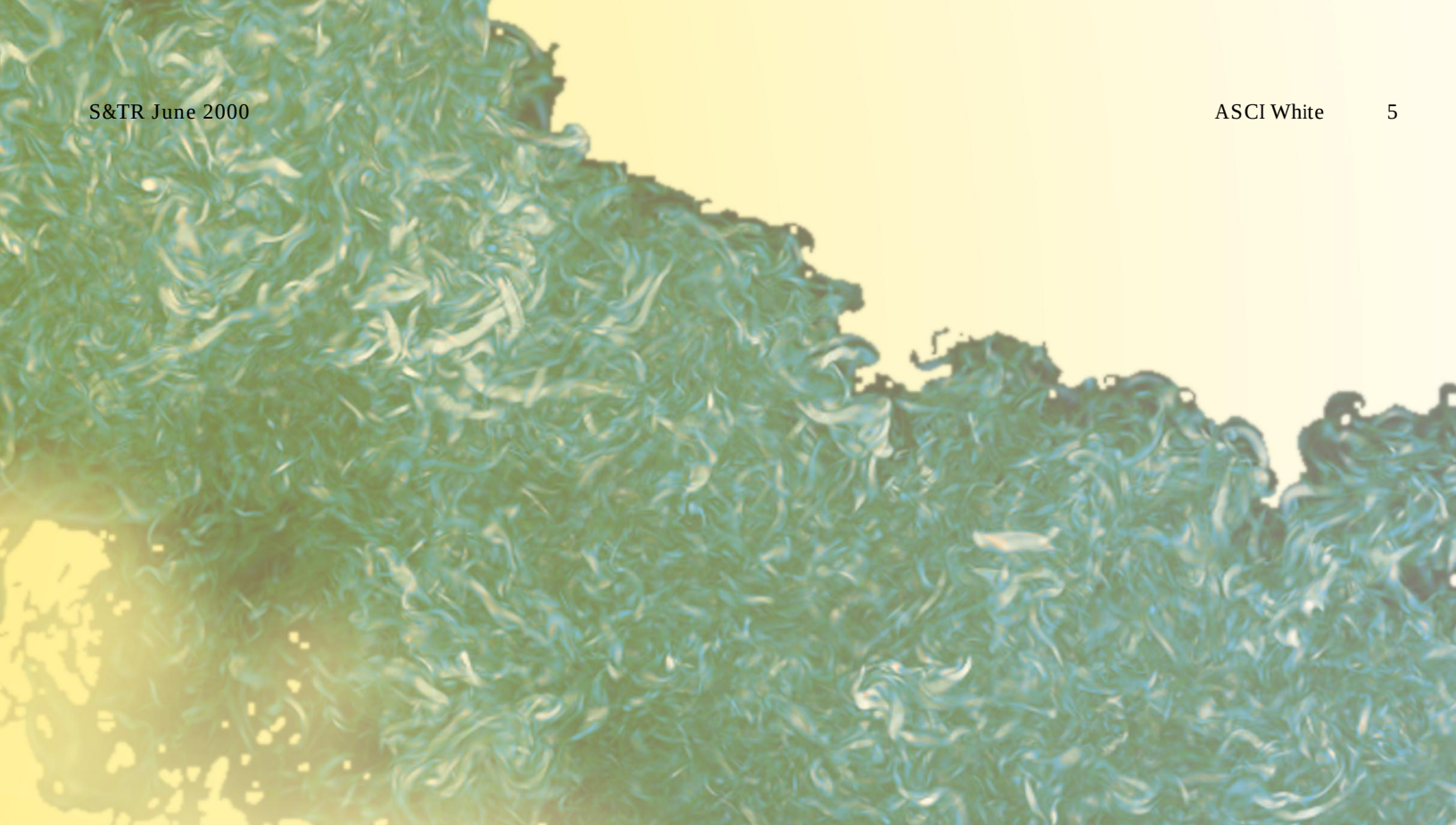
New Day Dawns in Supercomputing

The ASCI White supercomputer will take DOE significantly closer to its stockpile stewardship goal of using full-scale simulations of nuclear behavior to help ensure the safety, reliability, and performance of U.S. nuclear weapons.

AS the beam of a flashlight is to the illumination of a modern sports stadium, so is the power of an average personal computer to the Department of Energy's Blue Pacific supercomputer. And now, the Blue Pacific, located at Lawrence Livermore National Laboratory, is about to be eclipsed by another even higher performance supercomputer. Dubbed White, the monster machine developed by IBM for Lawrence Livermore is the latest computing system in DOE's Accelerated Strategic Computing Initiative (ASCI)—a program whose mission is to produce a system capable of calculating at 100 teraops (trillion floating-point operations per second) by 2004. "On a logarithmic scale," says Mark Seager, Livermore's principal investigator for ASCI platforms, "we're halfway to that goal with the 10-teraops ASCI White."

The Clock Ticks for the Stockpile

The push to produce a 100-teraops machine is tied to the aging of the U.S. nuclear weapons stockpile and the country's commitment to maintaining



and preserving a nuclear deterrent. With the advent of the U.S. nuclear test moratorium in 1992, the rules of the game changed for the nuclear weapons stockpile. No longer can the reliability, safety, and performance of these weapons be confirmed by underground nuclear tests. Originally designed with lifetimes of 20 years or more, these weapons must now be kept ready to serve the country indefinitely.

Doug Post, associate leader for the Laboratory's Computational Physics Division, explains, "In the early days, when the Lab was in the business of developing nuclear weapons, the overriding design question was 'Would it work?' Back then, we had nuclear testing to prove out the designs. It wasn't really necessary to be efficient as long as Mother Nature got to vote." As the number of underground tests shrank from hundreds to tens per year and the simulation codes and computers running them became more capable, the design process for nuclear weapons and supporting computer codes became more efficient. "After the test ban, the question became 'How long?' Aging nuclear weapons had never been an issue, because we'd always replaced old systems with new designs before their retirement dates. And we'd had underground nuclear tests to confirm the viability of the stockpile."

The answer to that question became DOE's Stockpile Stewardship Program. Weapon reliability, safety, surety—all once verified by underground nuclear tests—must now be confirmed using nonnuclear experiments, historical underground nuclear test data, and high-fidelity computer simulations.

A key component of the Stockpile Stewardship Program, ASCI is pushing

One Program—Three Laboratories

The goal of the Accelerated Strategic Computing Initiative (ASCI) is to provide the numerical simulation capability needed to model the safety, reliability, and performance of a complete nuclear weapon—from start to finish. The three national laboratories working on this initiative are Lawrence Livermore, Sandia, and Los Alamos. Project leaders at each laboratory, guided by the DOE's Office of the Deputy Administrator for Defense Programs, work with ASCI's industrial and academic partners. The overriding challenge is to synchronize the various technological developments. For example, sufficient platform power must be delivered in time to run new advanced codes, and networking capabilities must be in place to enable the various parts of the system to behave as one.

ASCI's program elements are Applications Development, Platforms, Pathforward, Problem-Solving Environment, Alliances, Visual Interactive Environment for Weapons Simulation, Verification and Validation, and Distributed and Distance Computing.

computational power far beyond present capabilities so weapon scientists and engineers can, with confidence, simulate the aging of nuclear weapons and predict their performance. If high-performance supercomputing were constrained to continue developing at a normal pace as predicted by Moore's Law (that is, computer speed doubling every 18 months to 2 years), the capability necessary to perform these calculations would still be a long way from reality by the year 2004. The three national laboratories that are part of ASCI—Lawrence Livermore, Los Alamos, and Sandia—have teamed up with the supercomputing industry to accelerate the development of high-performance supercomputing in the marketplace and meet this critical timeline.

The 10-teraops IBM White machine is scheduled to arrive at Lawrence Livermore this summer. With more than two-and-a-half times the horsepower of Blue Pacific, White is an important rung in the ASCI ladder. "One hundred teraops is the entry level we need to do full-scale simulations of exploding nuclear weapons," Seager explains. "These simulations must take into account three-dimensional, multiple-physics, high-resolution, coupled calculations. ASCI White will shed light on those areas of physics we don't yet understand, so that when we have the 100-teraops machine in 2004, we'll have a better handle on the issues."

Beating Moore's Law

To reach its 2004 goal, ASCI is building the world's fastest supercomputers using commercially manufactured parts. "Because we need to move faster than Moore's law allows," explains Seager, "we're building our supercomputers by taking thousands of processors—basically just like the PC on your desk—and linking them together. For ASCI White, we are tying together 8,192 processors to get a corresponding increase in capability and speed."

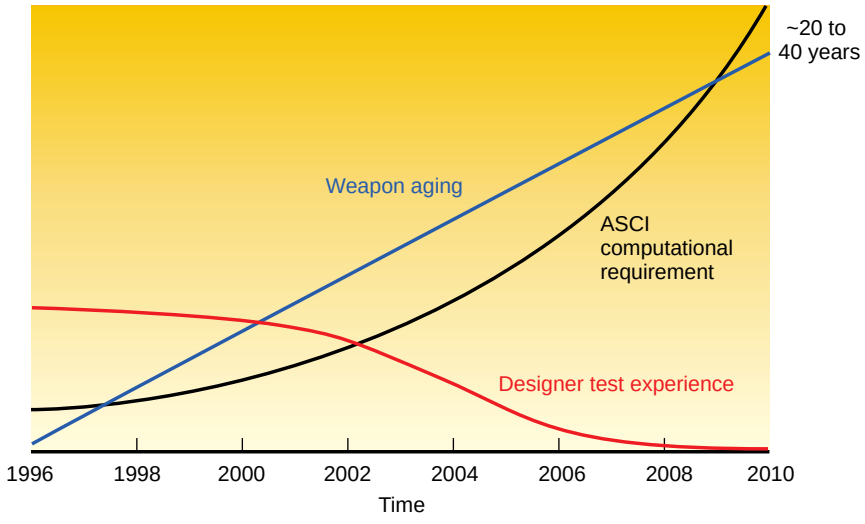
The processors in White are based on IBM's latest chip—the Power 3-II. Sixteen processors are grouped into a symmetric multiprocessor node; 512 nodes form the system. Code developers take advantage of the fact that proximity plays an important role in the speed of communication. Thus, the processors within a node can pass information between themselves quickly, while information between nodes moves a bit slower. Housing and bringing power to this enormous parallel machine are a project in and of themselves. For the machine to replace White, Lawrence Livermore is constructing the Terascale Simulation Facility. (See the box on p. 7.)

As Seager points out, "When we speak of accelerating the technology, we're talking about more than just the computer. Everything around the computer platform must also develop at an increased pace—applications, infrastructure, networks, archives, visualization tools. In fact, for every dollar spent on computer hardware, the initiative spends two on software." (See the box on pp. 10–11.)

Building on Blue's Triumphs

It's not easy to develop applications software for these parallel machines, notes Post. Many of the algorithms used in past weapons-related codes were not designed with parallel computing in mind. Plus, they were written to examine physics in two dimensions, not three, and had to run on machines much less capable than today's workstations. Consequently, simplified assumptions about the physics processes and the geometries involved are part of those codes. To produce the high-fidelity simulations required for stockpile stewardship, ASCI codes must remove

The year 2004 is a critical one for the Stockpile Stewardship Program. By then, almost all of the country's nuclear weapon systems will be at least 20 years old—their typical design lifetime—and most of the weapon scientists and engineers who worked on weapons during the nuclear-test era will have reached retirement age.



these assumptions and replace them with much more accurate methods based, in many cases, on a first-principles approach.

As part of ASCI, the Laboratory's code developers set about writing codes to take advantage of the architecture of this new generation of supercomputers. Simulation codes for ASCI include nuclear performance codes that can predict the details of an exploding nuclear weapon, materials modeling codes that use molecular dynamics to study the long-term degradation of materials under the influence of low-level radiation, and multiphysics codes that simulate what happens within an inertial confinement fusion target during implosion. Many of these codes have run on the ASCI Blue Pacific machine with impressive results.

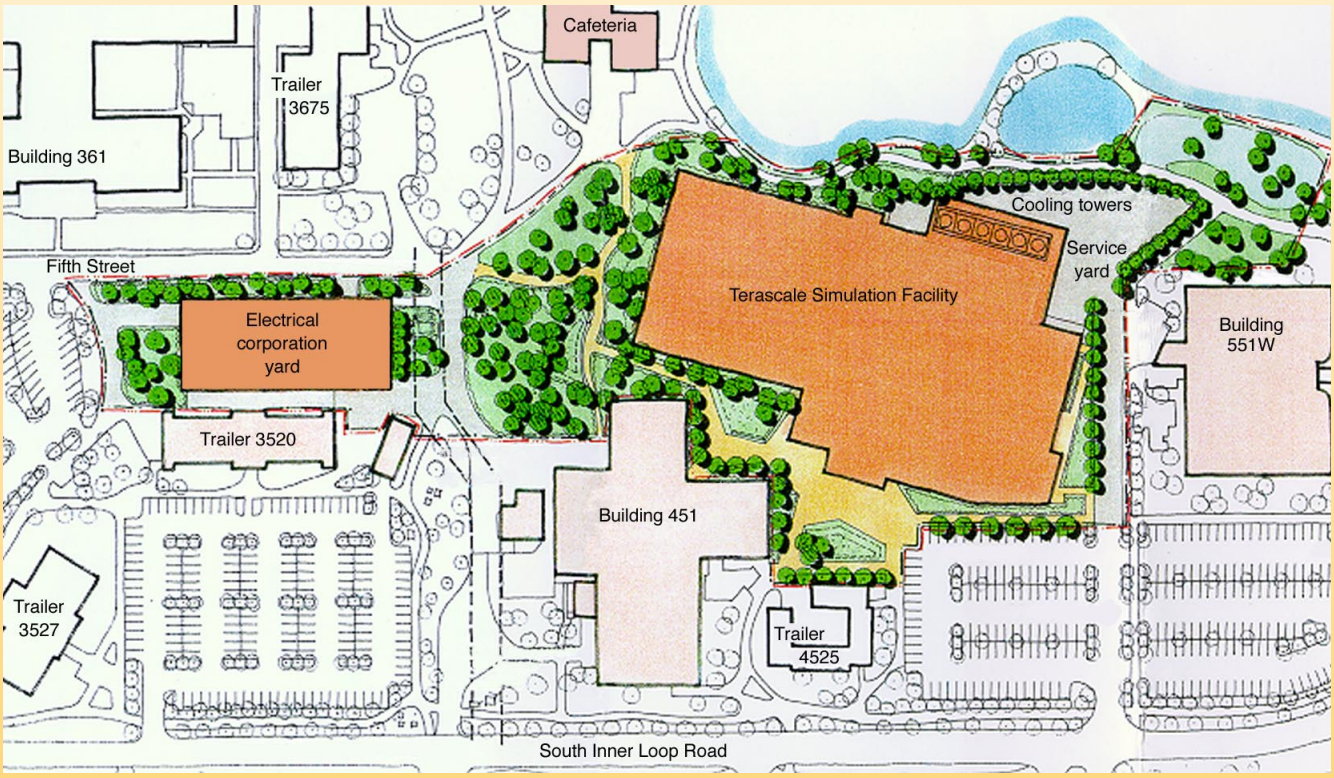
Modeling a Primary

In one notable ASCI Blue Pacific triumph, Lawrence Livermore, with strong support from IBM, completed the first major ASCI scientific milestone in November 1999—the first-ever three-dimensional simulation of an explosion of a nuclear weapon primary. (Nuclear weapons have two main components: the primary or trigger, and the secondary, which produces most of the energy.) Demonstrating the ability to computationally simulate, visualize, and analyze what happens to each of a nuclear weapon's components is a

The Terascale Simulation Facility

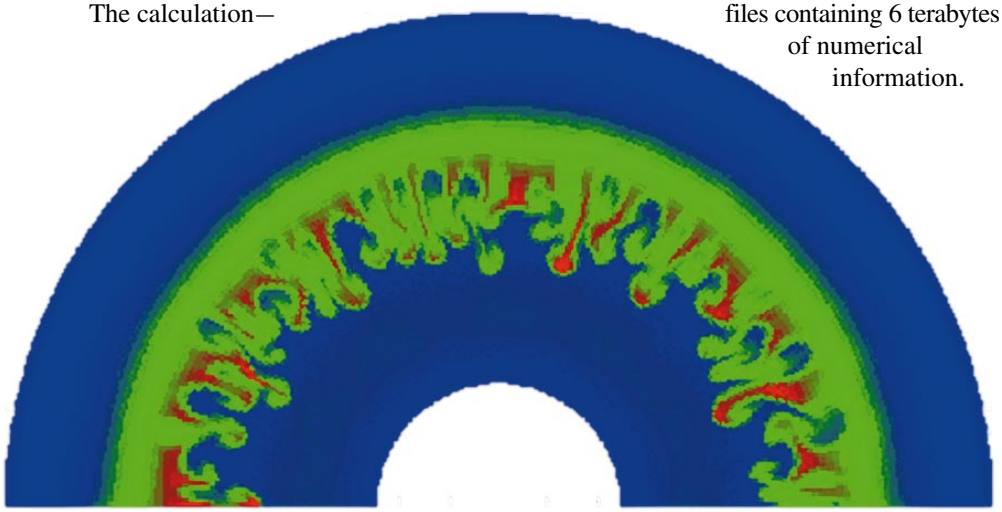
The time scales and demands of ASCI require a facility of extraordinary scope: the Terascale Simulation Facility (TSF). The $89-million facility will house a computer complex and data assessment and networking capability. It will require a significant increase in electrical power, mechanical support, physical space, and networking infrastructure. The TSF will provide an acre of raised computer floor and a power plant equivalent to that servicing a city of 15,000 homes.

ASCI White, with a delivery date of mid-2000, will reside next door to the proposed TSF in Building 451, where power and cooling systems have been tripled to meet the requirements of the 10-teraops supercomputer.

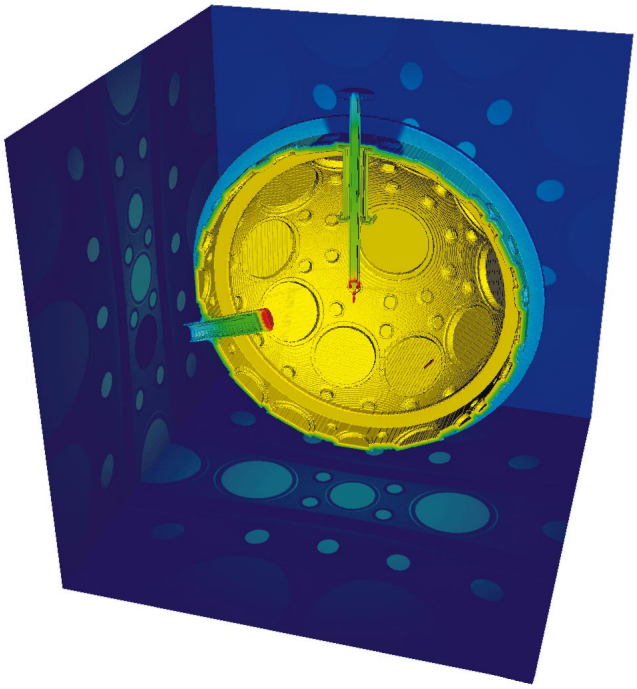


critical step in simulating an entire nuclear weapon's explosion in three dimensions.

The simulation required about 300,000 megabytes of random-access memory (RAM). For comparison, a conventional desktop computer typically comes with only about 100 megabytes of RAM. The calculation—which would have taken 30 years on a desktop—ran for more than 20 days on the Blue Pacific using 1,024 processors. The complex computer model, referred to as the burn code, employed tens of millions of zones—hundreds of times more than a comparable two-dimensional simulation using traditional codes. The calculations produced 50,000 data files containing 6 terabytes of numerical information. Just looking at this much information presents a formidable challenge.



A simulation of the the fluid motion as a function of increasing temperature, pressure, and density (a Richtmyer–Meshkov instability) in an imploding inertial confinement fusion capsule calculated with an arbitrary Lagrange–Eulerian hydrodynamics code on ASCI Blue Pacific.



ASCI Blue Pacific was used to create the largest-ever three-dimensional direct simulation of neutron transport. The colors represent flux values—with red highest and blue lowest—of fusion neutrons coming out of the Nova laser target chamber.

Tom Adams, an associate division leader in Defense and Nuclear Technologies Directorate, explains, "We had so much data that we needed to use the ASCI machine to analyze the results as well." ASCI's visualization software was also put to the test. Results were displayed as movies, in which scientists could look inside the primary to see what was happening at different points in time, and as graphic renditions of temperatures, pressures, and so on.

"This burn code 'milepost' was originally set in 1996 as a target to hit before the year 2000," continues Adams. "It was a daunting objective that some thought we'd never meet. In accomplishing it, we've shown that the ASCI program is on track, that the hardware and software systems are working, and that we can bring in results. The run also tested the teamwork of the people from the physics code teams, the Computation Directorate, and IBM. They all worked hard to solve the problems and make this happen. We see this exercise on Blue Pacific as a model for what we plan to do with White."

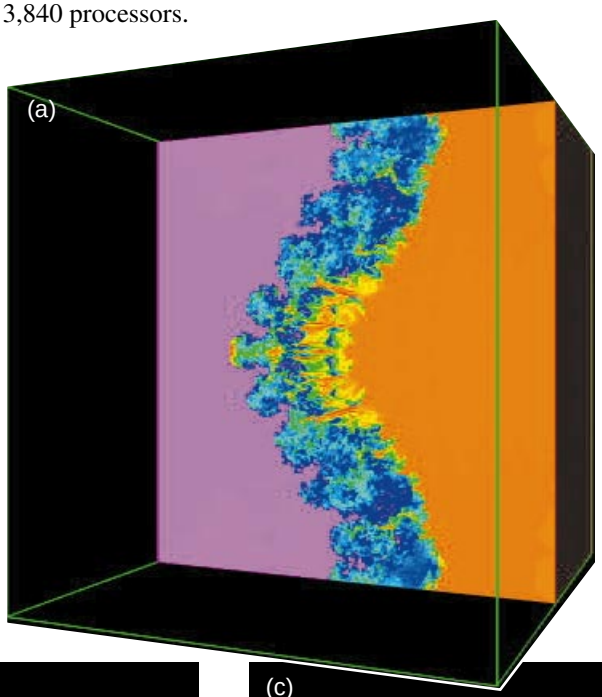
Adams expects that with White, the simulations will get more detailed. "We'll be able to model a larger part of the full weapon system, input more details on the weapon's configuration, and use more complex coupled physical models. All of this will improve the fidelity of our simulations."

The next ASCI scientific milestone is to model the secondary, something that will require White's increased power and speed. "In addition, we're moving from this, our first complete calculation, to something that nuclear weapon scientists and engineers can use for analyzing the stockpile," says Adams. "We're working with these users to apply the codes to current stockpile stewardship issues."

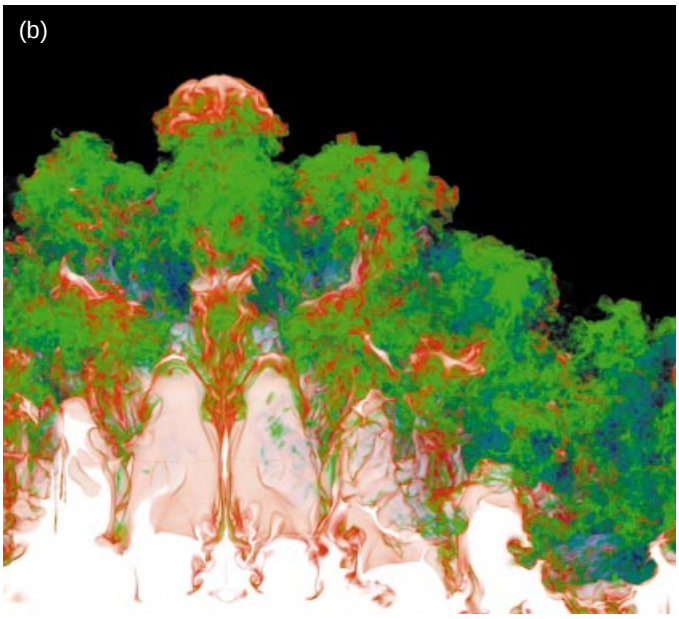
Dissecting ICF

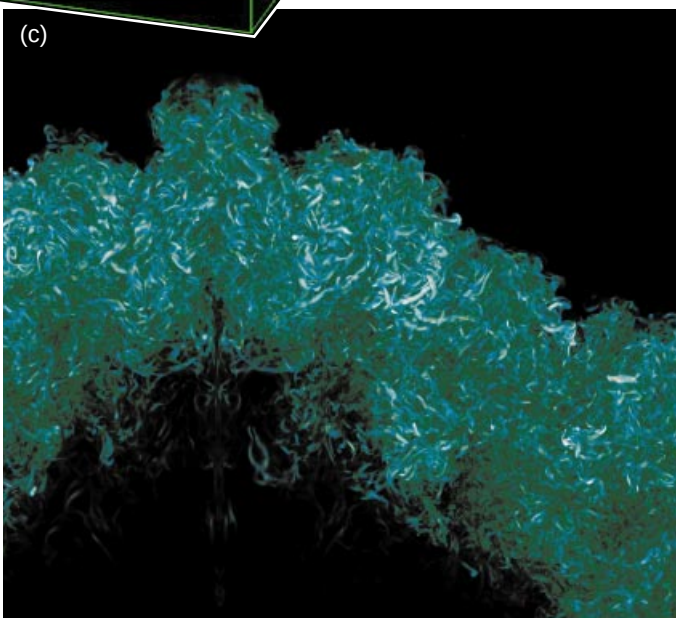
Several of the codes developed for ASCI examine various physics processes related to inertial confinement fusion (ICF). For instance, one three-dimensional code examines what occurs inside an ICF pellet when x rays hit the pellet's surface. The code models the fluid motion within the capsule as temperature, pressure, and density increase. It also models the transport of x rays emitted by the high-temperature material and the energy released from the fusion process. Another effort focuses on methods for modeling radiation transport. Seager notes, "Radiation transport is central to many physics applications, including nuclear weapons, inertial confinement fusion, plasma processing, and combustion. Many production codes in ASCI spend about 80 percent of their time claculating radiation transport. Doing these calculations more efficiently is a big time-saver."

Another parallel code, which ran on the ASCI Blue Pacific in 1999, simulated the flux of fusion neutrons that comes out of the Nova laser target chamber. This high-fidelity simulation had to take into account complex three-dimensional geometries, a wide range of distances (from the 6-meter-diameter test chamber to a target pellet less than 1 millimeter in diameter), and a number of different materials (air, aluminum, gold) with densities varying by a factor of 10^8. This calculation employed more than 160 million zones with over 15 billion unknowns and took 27 hours to solve on 3,840 processors.



(a) A volume rendering of entropy created at the conclusion of the largest calculation ever run of a Richtmyer–Meshkov instability. (b) and (c) The high resolution of the three-dimensional ASCI simulations revealed fine-scale physics of the turbulence never seen before. This 8-billion-zone simulation was completed in just over a week; over 2 terabytes of graphics data were produced in more than 300,000 files. (This and other visuals and movies can be viewed at www.llnl.gov/CASC/asciturb/simulations.html.)





From Shock Waves to Buckyballs

In other first-time-ever Blue Pacific calculations, researchers explored such diverse areas as turbulence, ab initio molecular dynamics, and quantum chemistry.

What happens when a shock wave passes through an interface of two fluids of differing density? A detailed simulation on 5,832 processors aimed at answering this question netted a team from Lawrence Livermore, the University of Minnesota, and IBM the prestigious Gordon Bell Award last November. The simulation, the largest calculation of its type, achieved a greater level of detail than any previous turbulence simulations. The effort has applications in a variety of disciplines, including supersonic propulsion, combustion, and supernova evolution.

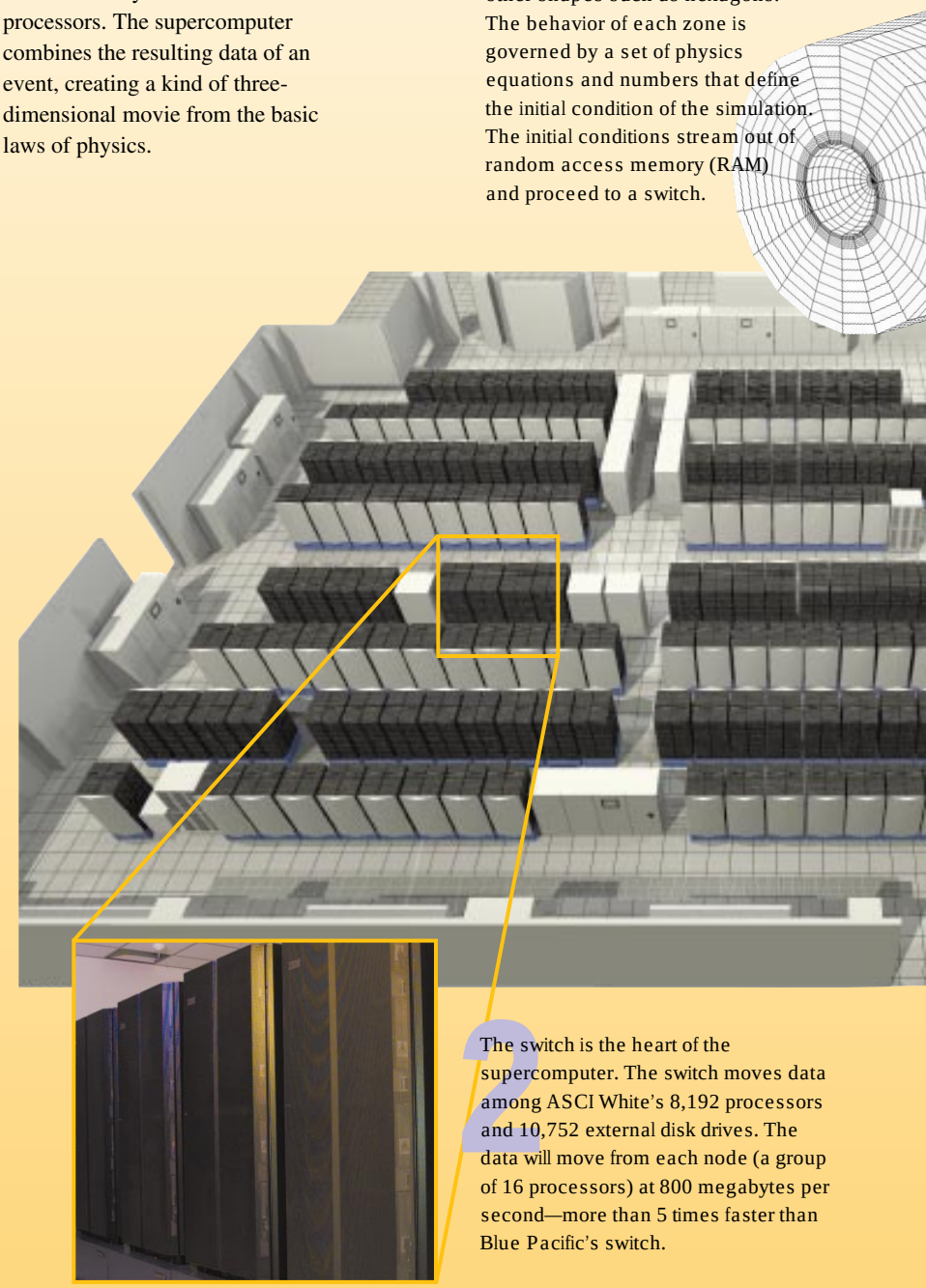
Researchers at the Laboratory used 3,840 processors to simulate from first principles the molecular interactions of hydrogen fluoride, an extremely toxic and corrosive byproduct of insensitive high-explosive detonations. Little experimental data are available on hydrogen fluoride, particularly at high temperatures and pressures. Quantum molecular dynamics simulated the interaction of hydrogen fluoride and water at the microscopic level—the only input being the identities of the atoms and the laws of quantum mechanics. This ASCI simulation involved 600 atoms with 1,920 electrons. The simulations provided crucial insight into the properties of hydrogen fluoride–water mixtures at high pressures and temperatures, adding to the understanding of how insensitive high explosives perform. (See *S&TR* July/August 1999, pp. 4–11, for more information about quantum molecular dynamics and this simulation.)

A research collaboration from Lawrence Livermore, the University of California at Berkeley, and Sandia National Laboratory at Livermore used ASCI Blue Pacific to perform the largest first-principles quantum chemistry calculations ever done. One of the initial

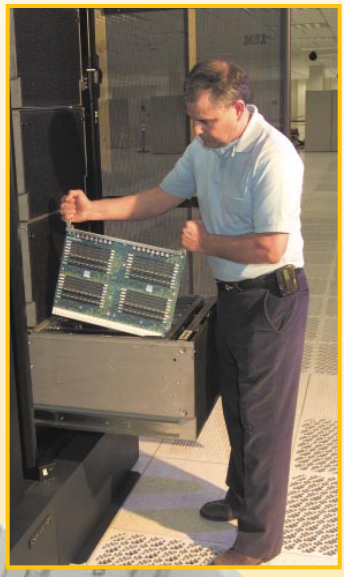
Tomorrow's Supercomputer Today

As with Blue Pacific, ASCI White will perform incredibly complex calculations by dividing up programs so that they will run simultaneously on thousands of processors. The supercomputer combines the resulting data of an event, creating a kind of three-dimensional movie from the basic laws of physics.

1 Whether modeling supernovas or exploding nuclear weapons, the simulation starts with the software taking an object and dividing it into billions of smaller cells or zones. Sometimes, these gridded zones are cubical; sometimes they take other shapes such as hexagons. The behavior of each zone is governed by a set of physics equations and numbers that define the initial condition of the simulation. The initial conditions stream out of random access memory (RAM) and proceed to a switch.

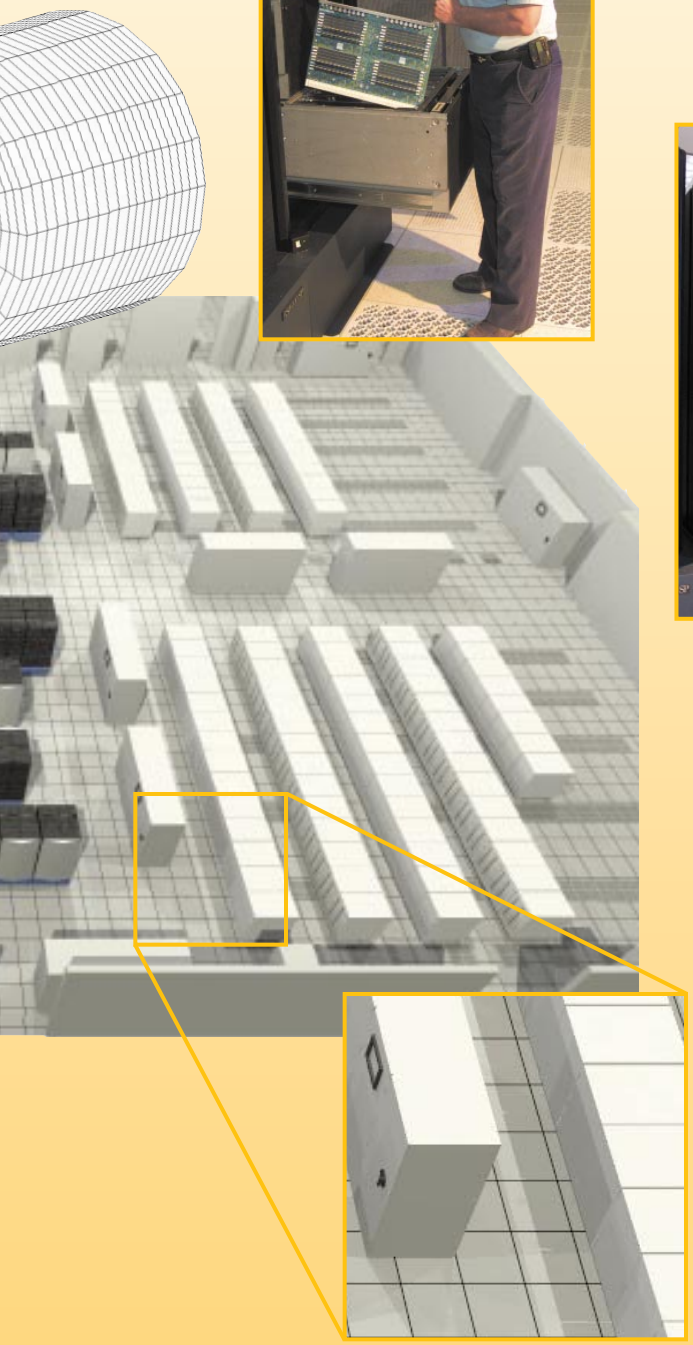


2 The switch is the heart of the supercomputer. The switch moves data among ASCI White's 8,192 processors and 10,752 external disk drives. The data will move from each node (a group of 16 processors) at 800 megabytes per second—more than 5 times faster than Blue Pacific's switch.

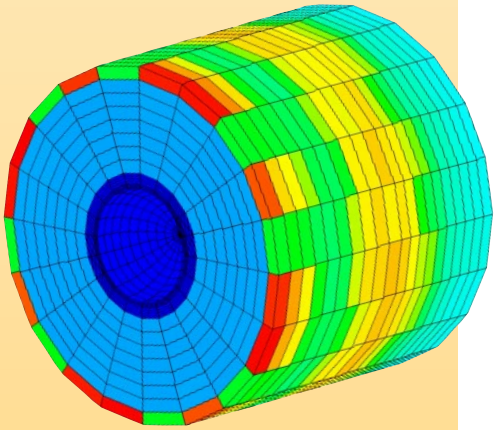


3 In ASCI White, each 375-megahertz Power 3-II processor simultaneously executes four floating-point calculations and contains 8 megabytes of cache RAM. Sixteen processors make up a single node, compared with the IBM Blue Pacific, which had four processors per node. Each White node also contains about 8 gigabytes of local memory and two internal 18-gigabyte hard drives.

4 As zone data enter the nodes, they flow into local memory and are distributed among the processors. The processors perform mathematical calculations and produce results for each zone. The zone results are sent back through the switch and stored in the "disk farm."



5 The massive amounts of data—hundreds of trillions of zones—are stored in 195 terabytes of external disk storage (for comparison, all the printed material in the Library of Congress is about 10 terabytes worth of information).



6 By means of ASCI's special visualization software, the results are displayed in three-dimensional movies, cutaway views, and graphs showing the distribution of density, pressure, temperature, and other quantities needed to understand the calculation and its implications.

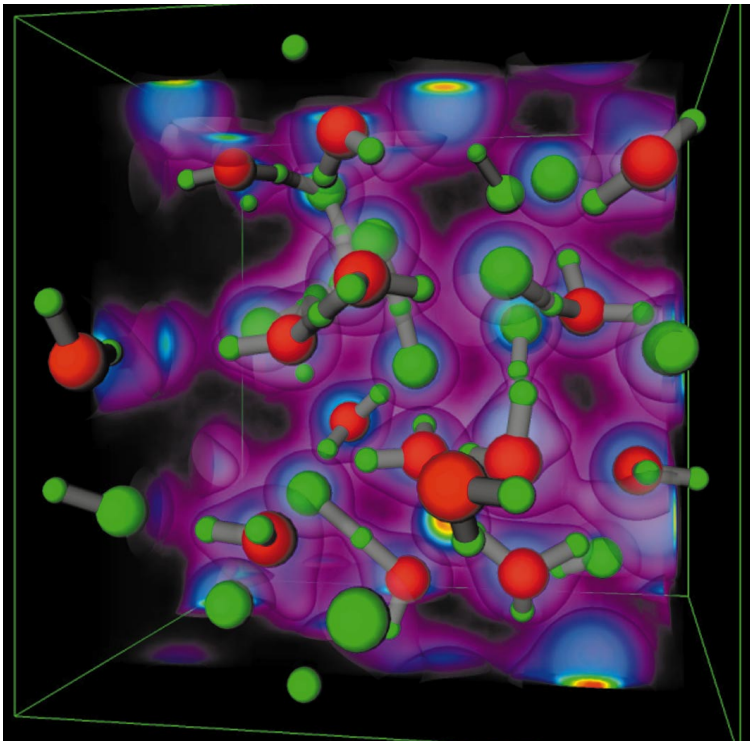
applications was to determine the three-dimensional structure and electronic state of the carbon-36 "buckyball," one of the smallest, most stable members of the buckminsterfullerene family of compounds. Possible applications for these unusual compounds include high-temperature superconductors and precise delivery of medicines to cancer cells. Previous quantum chemical calculations narrowed down the possible structure of carbon-36 to one of two possibilities, shown below right. Experimental data favored the structure in (a), but theoretical results slightly favored the one in (b). The two structures have different chemical properties, so determining which is more stable was critical to understanding this compound. A high-fidelity ASCI calculation provided the definitive—and unexpected—answer. As it turned out, the structure in (a), the one favored by the experimentalists, was the most stable. "This exercise was a reminder of how low-fidelity simulations with their simplifications and interpolations can lead to catastrophic results," notes Seager. "In a weapons calculation, for instance, you don't want to get the wrong answer to the question 'Will it work?'"

Universities Logging On

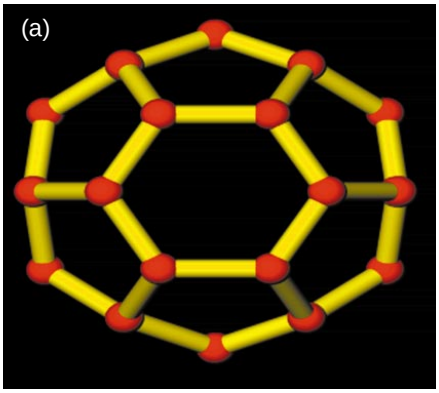
Significant scientific work on ASCI Blue Pacific is proceeding not only at the national laboratories, but also at associated universities through DOE's Academic Strategic Alliance Program. This program aims to engage the U.S. academic community in advancing science-based modeling and simulation technologies. Although the specific computing problems universities are tackling do not directly involve nuclear weapons research, the methodologies and tools being developed can be applied to all of ASCI's areas of research.

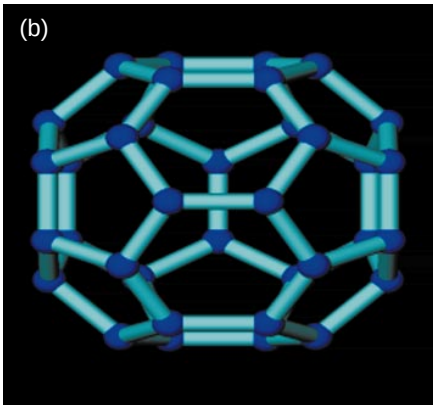
The program funds five major centers of excellence. Each uses multidisciplinary teams working over the long term to provide large-scale, unclassified simulations that represent ASCI-class problems. The centers collectively have access to up to 10 percent of the ASCI computing resources at the three national laboratories. The projects are part of a 10-year program, in which projects come up for renewal after five years.

"The problems being studied in these projects are comparable in their complexity to those involving nuclear weapons," explains Dick Watson, Lawrence Livermore's manager for the program. "We expect that through this program, the laboratories and universities will see revolutionary advances in both the physical and engineering sciences and the mathematical and computer sciences."



This quantum-level simulation of hydrogen fluoride–water mixtures at high temperatures and pressures took 15 days on the ASCI computer. Trillions of operations per second were performed to calculate 1 picosecond's worth of atomic interactions.





Two possible structures for the carbon-36 fullerene. It took a high-fidelity run on ASCI Blue Pacific to determine that the correct structure is (a).

The Center for Simulating Dynamic Response of Materials, based at the California Institute of Technology, is developing simulation codes for its virtual shock physics test facility. Simulations have applications to materials design, oil exploration, earthquake prediction, and environmental analysis.

Stanford University's Center for Integrated Turbulence Simulations focuses on jet-engine simulations. Researchers at this center are developing massively parallel codes for high-fidelity flow and combustion simulation.

The Center for Astrophysical Thermonuclear Flashes at the University of Chicago is studying the physics of supernovas, including the physics of ignition, detonation, and turbulent mixing of complex fluids and materials. Once completed, the integrated code will provide the highest resolution calculation ever done showing how these stellar outbursts begin.

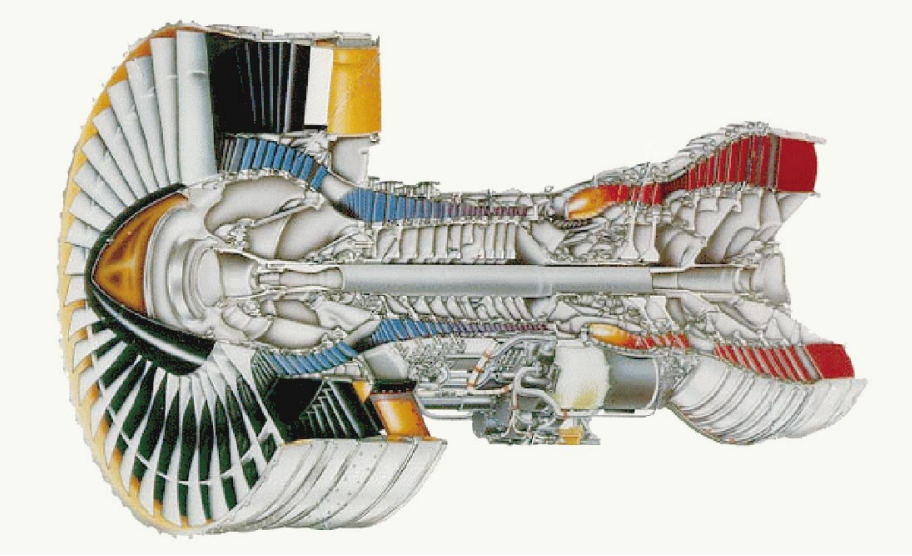
The University of Illinois Urbana–Champaign is home to the Center for Simulation of Advanced Rockets. This center plans to provide a detailed, whole-system simulation of solid propellant rockets. Earlier this year, center staff completed a simplified version of a three-dimensional integrated rocket simulation code. The next-generation code will characterize various burn scenarios, and the fully integrated code will address potential component failures. Research will benefit technologies such as gas generators used for automobile air bags and fire suppression.

Finally, the University of Utah is focusing on the physics of fire at the Center for the Simulation of Accidental Fires and Explosions. These problems draw on fundamental gas- and condensed-phase chemistry, structural mechanics, turbulent flows, convective and radiative heat transfer, and mass transfer.

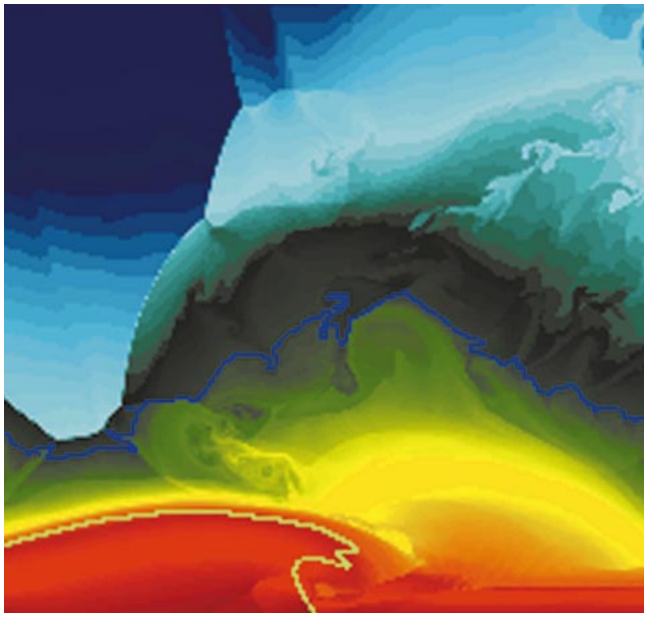
At Lawrence Livermore, all of the alliance work is being conducted on the unclassified sector of ASCI Blue Pacific.

Building a Model for the Future

"One of the key challenges to fielding the fastest supercomputers in the world is that this scale of computing requires a new operational model in order to succeed," says Seager. "In the past, the model has been a large, but fundamentally traditional, scientific computing center. ASCI needs to be run as if it were an experimental research facility. The scientific applications being developed today promise a level of physical and numerical accuracy that is more like that of a scientific experiment than a



A simulation of the flow through a compressor in a jet engine, showing entropy contours. Red is high entropy; blue is low.



A snapshot of a density field simulation for an x-ray burst on the surface of a neutron star. The yellow curve is the detonation front, racing across the stellar surface. The blue curve shows how the initial surface of the accreted atmosphere deforms.

traditional numerical simulation. The effort required to run a full-scale, three-dimensional scientific application is like running a big experimental weapon test. In a way, this operational change parallels the changing role of large-scale experiments in the physics world."

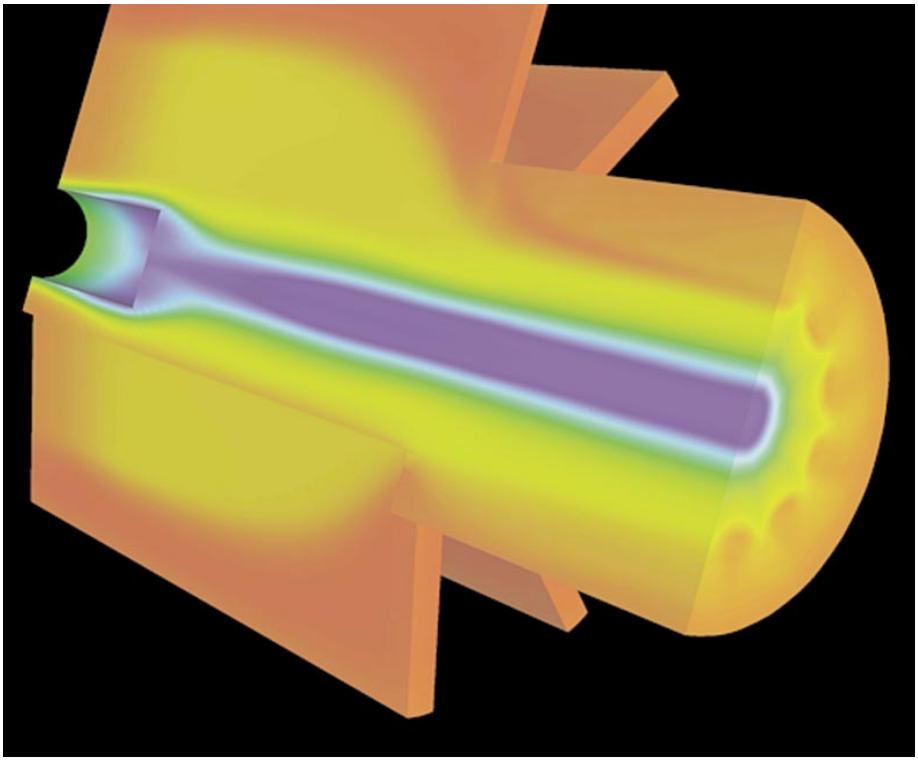
For a long time, the two accepted branches of physics have been theory and experiment. Yet, there are experiments that, for various reasons, are unrealistic—either the conditions can't be created in the laboratory, or it's far too dangerous or expensive to do so. And, in many cases, the theory has been too complex to analyze, even with many simplified assumptions. "All that has changed with the coming of ASCI's supercomputers," says Seager. "Computer simulation is now poised to become the new branch of science, on the same level as experimentation and theory."

—Ann Parker

Key Words: Academic Strategic Alliance Program, Accelerated Strategic Computing Initiative (ASCI), ASCI White, Blue Pacific, Stockpile Stewardship Program, Terascale Simulation Facility (TSF).

For more information contact Mark Seager (925) 423-3141 (seager1@llnl.gov).

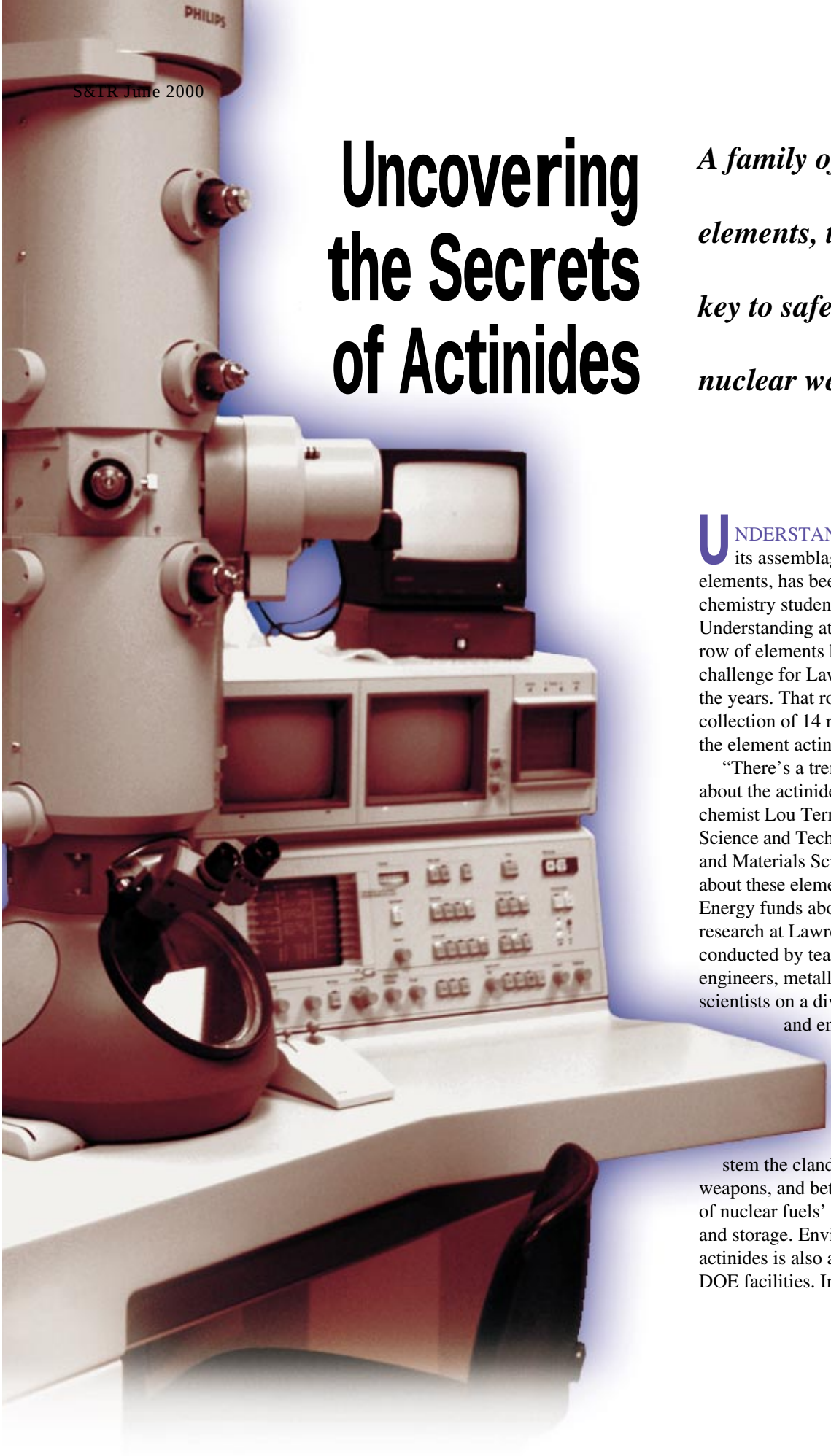
Also see the following Web sites:
- *ASCI at Lawrence Livermore, www.llnl.gov/asci/*
- *ASCI at Los Alamos, www.lanl.gov/asci/*
- *ASCI at Sandia, www.sandia.gov/ASCI/*
- *ASCI's Academic Strategic Alliances Program, www.llnl.gov/asci-alliances/*



A three-dimensional simulation of the gas temperature at about 0.04 seconds after rocket-propellant ignition. Orange represents the hottest region. (Based on simulations of gas flow and pressures induced by the shape of the propellant inside the ignition segment of a Space Shuttle booster.)

About the Scientist

MARK SEAGER is the principal investigator for the Accelerated Strategic Computing Initiative's terascale system at Lawrence Livermore National Laboratory. His interests are currently in large, scalable system architecture, performance, and integration. Seager received his B.S. in mathematics and astrophysics from the University of New Mexico at Albuquerque in 1979 and a Ph.D. in numerical analysis from the University of Texas at Austin in 1984.



Uncovering the Secrets of Actinides

A family of radioactive elements, the actinides, is key to safe stewardship of nuclear weapons.

UNDERSTANDING the periodic table, with its assemblage of columns and rows of elements, has been a perennial challenge for chemistry students. (See the box on p. 17.) Understanding at the atomic level a remarkable row of elements has been a particular research challenge for Lawrence Livermore scientists over the years. That row is called the actinides, a collection of 14 radioactive elements named after the element actinium.

"There's a tremendous amount we don't know about the actinides," says Lawrence Livermore chemist Lou Terminello, who leads the Materials Science and Technology Division of the Chemistry and Materials Science Directorate. To learn more about these elements, he says, the Department of Energy funds about $100 million per year for research at Lawrence Livermore. The research is conducted by teams of chemists, physicists, engineers, metallurgists, and environmental scientists on a diverse set of national security and environmental issues.

Terminello says that a more fundamental understanding of actinides is needed to better assess the nation's nuclear stockpile, help stem the clandestine proliferation of nuclear weapons, and better understand the implications of nuclear fuels' (such as enriched uranium) use and storage. Environmental contamination by actinides is also a major concern at several major DOE facilities. In addition, actinides such as

uranium, neptunium, plutonium, and americium are the major contributors to the long-term radioactivity of nuclear waste currently targeted for the proposed Yucca Mountain repository in Nevada.

Stockpile stewardship, DOE's program for certifying the long-term safety and performance of the enduring stockpile without underground nuclear testing, has heightened the importance of assessing and predicting the long-term behavior of actinides. A major focus is on obtaining a better scientific understanding of the isotopes uranium-235 and, especially, plutonium-239.

Plutonium is the most complex and perplexing element in the periodic table. The element's complexity stems in part from its mercurial nature. Depending on temperature, it assumes one of six different forms or phases, each with a different density and volume. Because of plutonium's enigmatic behavior and the need for stringent safety and environmental procedures when handling the toxic material, much of the extensive characterization work done on other metals has not been performed on plutonium.

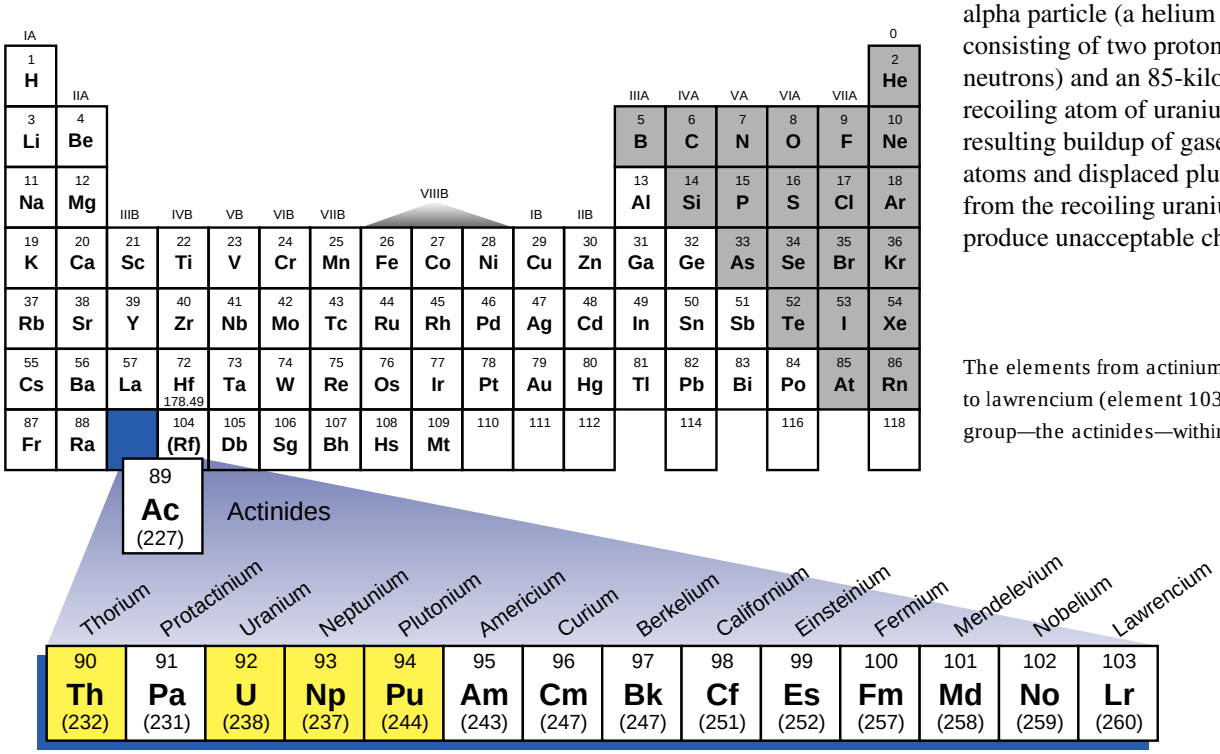
Surrogates Inadequate

Materials scientist Mike Fluss points out that because of plutonium's unpredictability, experimenters prefer not to use surrogate materials. "It's as challenging a material as you can imagine," he says. Even the process of measuring its electrical resistance has proven surprisingly complex because of its unexpected and not fully understood dependency upon temperature.

"We're rebuilding plutonium metals science at Lawrence Livermore," says metallurgist Adam Schwartz. He points to a growing number of experiments measuring the structural, electrical, and chemical properties of plutonium and its alloys and determining how they change over time as a result of the cumulative effects of radioactive decay and consequential damage. These measurements will enable scientists to better model and predict the material's long-term behavior in the nation's aging nuclear stockpile.

Schwartz also cites the recent acquisition of advanced instruments such as a transmission electron microscope capable of nearly perfect resolution at the atomic scale. Additionally, Livermore experts are taking advantage of one-of-a-kind facilities at Lawrence Berkeley and Argonne national laboratories, the Stanford Linear Accelerator Center, and other DOE sites to more completely characterize the electronic and atomic structure of plutonium alloys and compounds.

One line of research is studying the evolution of damage to plutonium metal's crystalline structure on scales as small as a billionth of a meter. This so-called microstructure is always changing because when plutonium-239 decays, it emits a 4-megaelectronvolt alpha particle (a helium nucleus consisting of two protons and two neutrons) and an 85-kiloelectronvolt recoiling atom of uranium-235. The resulting buildup of gaseous helium atoms and displaced plutonium atoms from the recoiling uranium could produce unacceptable changes in the



The elements from actinium (element 89) to lawrencium (element 103) form a distinct group—the actinides—within the periodic table.

plutonium metal. Fluss notes that after 10 years, every plutonium atom has been displaced at least once from its lattice site, but most atoms eventually return there. The plutonium decay itself is slow; in about 24,000 years, only half the plutonium-239 has changed to uranium-235.

The concern, says Fluss, is that atoms of helium and the actinides americium and uranium, also present in the weapon environment, might slowly change the chemistry of the plutonium metal. At the same time, the accumulation of small-scale radiation damage to plutonium alloys over several decades could affect a weapon's safety or its performance. Like other solids, plutonium metal is made of many crystals (or grains) with different orientations. If vacancies or defects coalesce, they may cause changes in properties, with possible unwanted effects to a warhead. By better understanding the nature of the changes, scientists can refine their predictive codes.

100-Year Predictions Needed

"We need to know how plutonium in our stockpile will react over 100 years," says Fluss. "We're asking harder questions today because nuclear weapons must last a lot longer than their designers ever intended." The answer, he says, lies in obtaining fundamental understanding at the atomic level.

Schwartz and colleague Mark Wall are using the transmission electron microscope to document the differences between plutonium from old, disassembled nuclear warheads and newly cast plutonium. By using electrons instead of light waves, the transmission electron microscope can image features at near-atomic resolution. They start with plutonium samples measuring less than 3 millimeters in diameter and 120 micrometers thick. The center of each sample is thinned to create a region only 100 nanometers

Actinides Can Mean Nuclear Chemistry

The group of elements known as the actinides are the elements from actinium (element 89) to lawrencium (element 103). All members of the series can resemble actinium in their chemical and electronic properties, and so they form a separate group within the periodic table. (An element's atomic number is the sum of the protons and neutrons in the nuclei of its atoms.)

All actinides are metals and all are radioactive. As a result, they dominate the study of nuclear chemistry. The elements emit energy in the form of alpha particles, beta particles, or gamma rays. By emitting these particles, the atoms lose protons and therefore become another element with a lower atomic number. If the immediate product of radioactive decay is radioactive, it also decays to form another element. This process continues until a stable element is formed.

Actinides undergo radioactive decay at different rates; that is, they have different half-lives. Elements with higher atomic numbers have short half-lives and rapid radioactive decay. Some actinides with lower atomic numbers, however, have half-lives ranging between thousands to millions of years.

The two actinides of most interest to Livermore scientists are uranium and plutonium. Uranium, a silver and lustrous metal, has four main isotopes. Because uranium-235 is fissionable, it is used to fuel nuclear power plants and as a component in nuclear weapons.

Plutonium is a silver-gray metal that has 16 isotopes. The isotope of chief interest is plutonium-239, which, like uranium-235, is fissionable. Most nuclear weapons are based on plutonium-239, while plutonium-238 is used as a power source in long-mission space probes.

Metallurgists are probing the microstructure of actinides with a transmission electron microscope capable of near-atomic resolution.

(100 billionths of a meter) thick for the electron beam to pass through. The resulting electron micrographs reveal the nature and extent of defects in unprecedented detail.

Researchers are also doing a variety of accelerated aging studies in which plutonium samples are exposed to higher than normal levels of radiation so that the aging process is significantly accelerated. Such experiments provide an important basis for validating computer models. Other aspects of the physics of radiation effects are being studied by ion irradiation using various light and heavy ions to investigate the predictions of the models.

Lawrence Livermore scientists are also benefiting from fundamental work on plutonium performed by their colleagues in Russia. One study, done over the past 25 years and announced last year, claims to have produced plutonium's correct phase diagram, the roadmap between its six different phases or structural forms. The Russian study, says Schwartz, clarifies certain details about how delta-phase plutonium transforms to a less desired alpha state.

Fluss, Schwartz, and others are planning research that will tap the Laboratory's resources to review the Russian work and test its conclusions. The likely outcome, says Schwartz, is a refinement of current computer codes to more realistically simulate the nature of plutonium.

New Look at Old Data

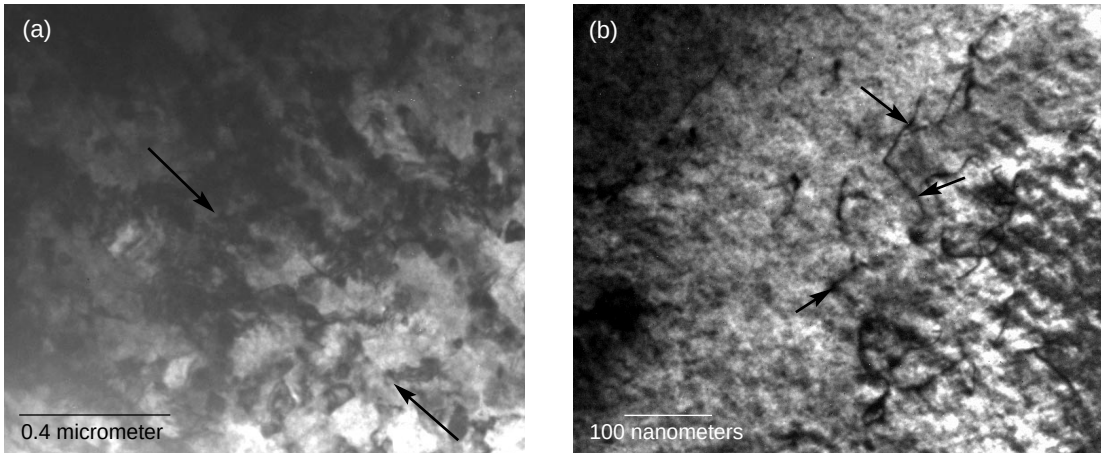
Other Lawrence Livermore researchers are taking a different approach to strengthening the ability of scientists to predict the likely performance and safety of aging weapons. The scientists are looking at results from years of underground nuclear detonations at DOE's Nevada Test Site.

According to nuclear chemist Ken Moody, new measuring techniques and instruments, along with improved understanding of actinide chemistry, warrant revisiting test data that are decades old. Moody is one of a dwindling number of nuclear chemists who did the original chemical separation of actinides from underground tests before they ceased in 1992. He notes that stored actinide samples and even debris from tests could be a treasure-trove of data, despite their reduced radioactivity due to age. The reanalysis could give stockpile stewards a clearer idea of how the nuclear devices performed when they were detonated and how those same designs would perform today.

Livermore researchers are applying their actinide know-how and a suite of sensitive instruments to nuclear forensics work. Chemists like Moody are working with Lawrence Livermore's Forensic Science Center to help America's intelligence agencies stem the proliferation of nuclear materials, especially those from the former Soviet Union. Experts have raised concern about the security of large amounts of weapons-grade nuclear materials in Russia and neighboring states that inherited the materials as a result of the breakup of the Soviet Union. In particular, the dismantlement of thousands of old Soviet nuclear weapons has resulted in large quantities of surplus nuclear materials.

Some actinides, such as uranium-235 (used in nuclear fuel rods) and plutonium-239, have shown up in small quantities in unauthorized hands and on black markets in Western Europe. The concern, of course, is that such materials might make their way to a terrorist group or a nation that supports terrorist activities.

Lawrence Livermore's actinide forensics capabilities are formidable, Moody says. Radiochemical methods can reveal, for example, when a sample of plutonium was manufactured and even the chemical techniques used in its



Images of plutonium metal taken with the transmission electron microscope reveal changes to the plutonium's microstructure. At the 0.4-micrometer scale, diagonal bands in (a) are typical of accumulations of a deformed microstructure. Dark lines in (b) at the 100-nanometer scale are individual dislocations.

Educating Future Actinide Scientists

The Department of Energy national laboratories have long been the stewards of expertise in actinides in the United States. However, many actinide experts are retired or in the process of retiring, and they are not being replaced in adequate numbers.

The situation largely results from a sharp downturn in the number of students graduating with specialties in nuclear chemistry. Across the nation, only a few colleges and universities still provide facilities for actinide research, and professors teaching actinide science have mostly retired. Also, fewer undergraduates are expressing an interest in pursuing careers in nuclear chemistry.

According to Livermore actinide experts, U.S. leadership in heavy-element science will fast erode unless the national laboratories address this issue, which is vital to DOE stockpile stewardship and other missions such as nuclear waste disposition. "One of the most important challenges facing stockpile stewardship is the successful passing of the torch in actinide science," says Lawrence Livermore chemist Lou Terminello.

The University of California's Glenn T. Seaborg Institute for Transactinium Science is attempting to remedy the labor shortage by attracting and training the next generation of actinide scientists. The institute was established in 1991 with facilities at both Lawrence Livermore and Lawrence Berkeley national laboratories. (A third chapter was added in 1997 at Los Alamos National Laboratory.)

The institute is named for the late UC Berkeley professor in recognition of his enormous contributions to the field, including the discovery of 10 elements, among them plutonium. The institute advances fundamental and applied science and technology of transactinium elements (actinides and beyond). Workshops, conferences, lectures, and research projects focus on national security, nuclear energy, environmental protection and remediation, and nuclear waste isolation and disposition.

The institute emphases training at the undergraduate through postgraduate levels. In this way, says Terminello, who serves as institute director, Lawrence Livermore is making a long-term investment in its future. To that end, the institute's Livermore facility operates a summer school for undergraduates who have shown an interest in nuclear chemistry. "We want to capture the imagination of young people by giving them hands-on experience in nuclear science. We want them to go to graduate school and return to Livermore, where they will form our next generation of actinide scientists," Terminello says.

Whatever the expense of improving education, it is an investment in the future we must make. Excellence costs. But in the long run mediocrity costs much more.

—Glenn T. Seaborg

Performing research on actinides for stockpile stewardship often requires training beyond that which is available from universities. As a result, the institute also trains chemists who have recently obtained a Ph.D. For example, young scientists are learning the techniques of x-ray absorption that were refined for actinides by Livermore chemists such as Patrick Allen, deputy director of the institute.

The researchers use the facilities of the Stanford Synchrotron Radiation Laboratory, a part of the Stanford Linear Accelerator Center. The laboratory generates synchrotron radiation, a name given to x rays produced by electrons circulating in a storage ring at nearly the speed of light. The extremely bright x rays excite electrons closest to the nucleus, yielding detailed information about the chemical nature, molecular structure, and electron distribution of actinide-containing materials.

Lawrence Livermore researchers use x-ray absorption to probe samples of uranium and plutonium alloys and compare the results to current computer models. The results are useful in addressing stockpile stewardship issues as well as understanding the behavior of actinides in contaminated soils and potential radioactive waste storage facilities.

Professor Glenn T. Seaborg poses with college students participating in the first summer session (1998) at the Glenn T. Seaborg Institute for Transactinium Science at Lawrence Livermore.

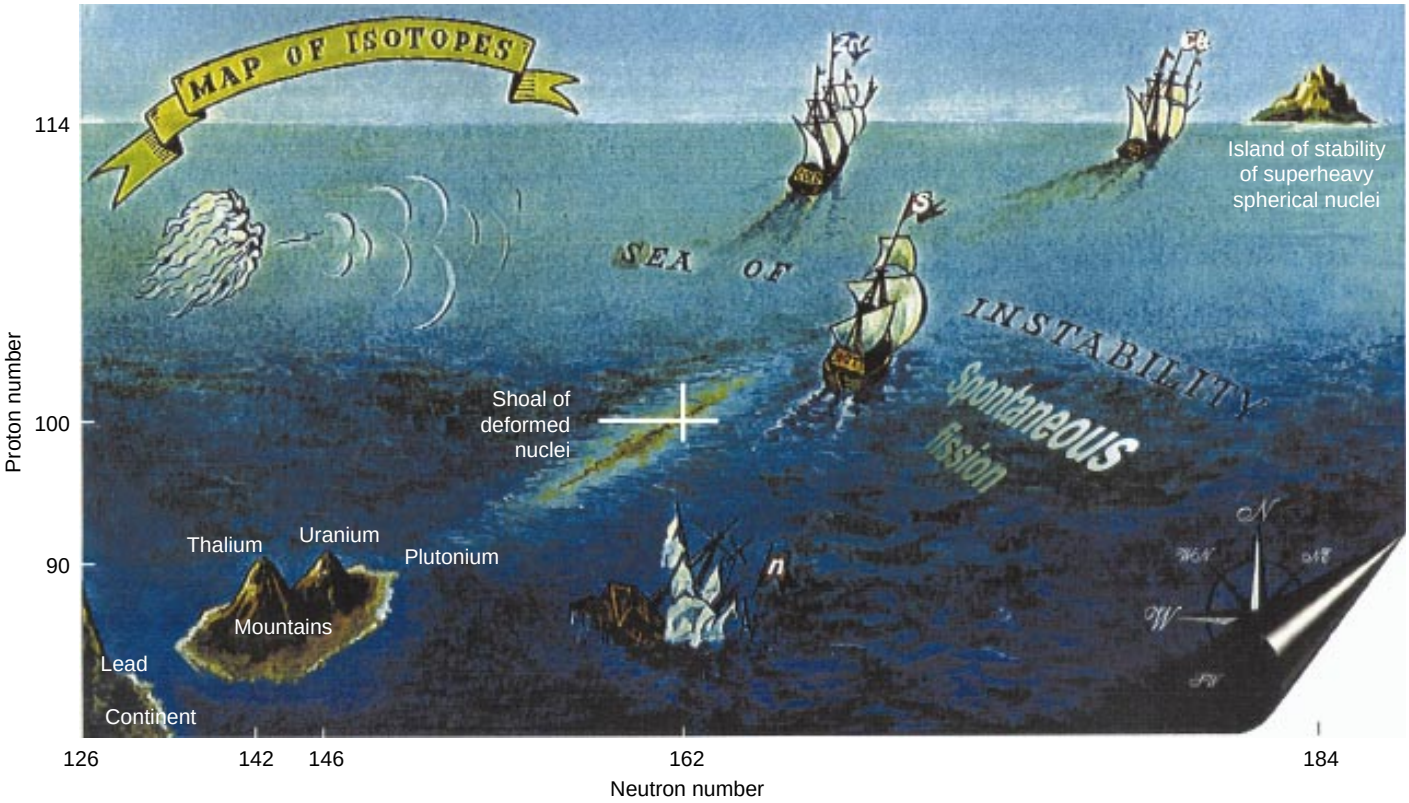
creation. They can also readily show if a suspect material is a hoax rather than a real threat.

Creating Element 114

The accumulated knowledge of actinides' nuclear structure has helped Lawrence Livermore scientists create entirely new elements. In 1989, a Livermore team led by nuclear chemist Ken Hulet (now retired) began a collaboration with scientists at the Joint Institute for Nuclear Research in Dubna, Russia. Over the past decade, the international team discovered isotopes of elements 106, 108, and 110 at the Russian institute.

The researchers' goal in 1998 was far more challenging: to create element 114 and demonstrate a long-postulated region of enhanced nuclear stability against

For more than a decade, Russian and Lawrence Livermore collaborators have used the facilities of the Joint Institute for Nuclear Research in Dubna, Russia.



A Russian artist depicts the modern nuclear theory of the heaviest elements. At the upper far right is the island of stability, which was demonstrated by the production of long-lived element 114 in 1998 by a Russian–Livermore team.

spontaneous fission. This region, considered by some impossible to reach, was theorized to lie amidst a "sea" of extremely short-lived, super-heavy nuclei.

The most recent experiment, led by Moody, involved a team of five Livermore scientists and 17 Russian researchers. The team bombarded ions of the rare isotope calcium-48 onto a target of plutonium-244 (the heaviest long-lived plutonium isotope) supplied by Livermore. It took the team 40 days of irradiation to create one atom of the new super-heavy element 114 in December 1998. The new element lasted 30 seconds, some 100,000 times longer than if there were no enhanced stability in that area of the periodic table.

Moody believes the discovery of element 114 has strengthened interest in heavy-element science. Since the discovery, Lawrence Berkeley researchers have found two new elements—116 and 118. The continuing discoveries are providing important insights into the arrangement of electrons in atoms and chemical bonding.

The Livermore–Russia connection is still going strong. Since the December 1998 discovery, the U.S.–Russian team has found a different isotope of element 114, one with a decay time of one second. The team is currently working on finding another isotope of element 116, this time with a curium isotope target, so they can continue mapping the region of enhanced stability.

Plutonium Moves Differently

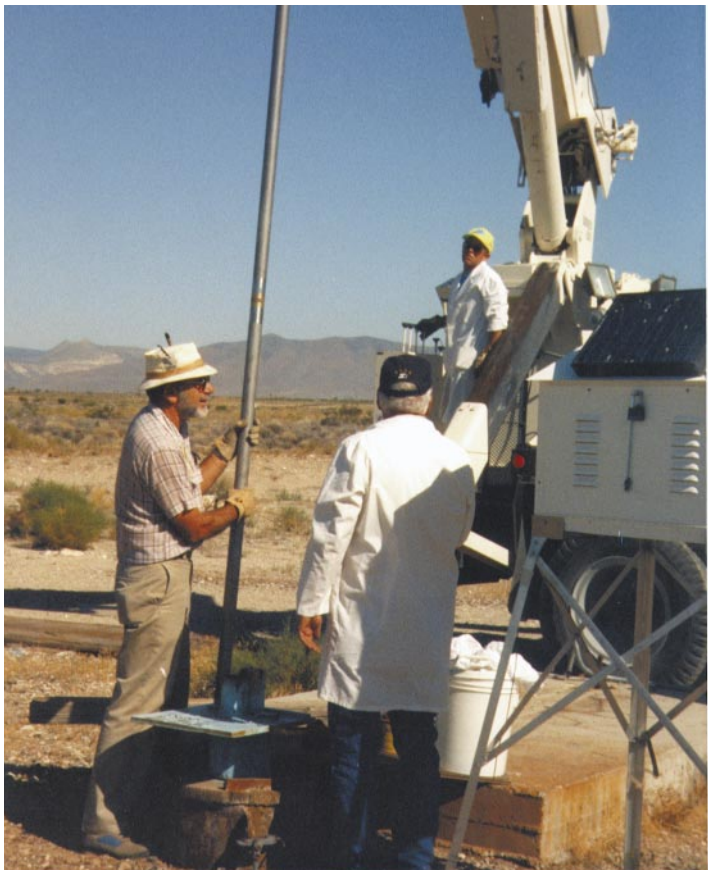
An important aspect of Lawrence Livermore actinide research is studying how these elements behave in the environment, particularly how they migrate underground in solution. The research results have challenged some long-established scientific assumptions.

For example, scientists assumed that plutonium, because of its low solubility in water and its strong tendency to sorb (adhere) to clumps of dirt and rocks, does not travel far in groundwater. A Lawrence Livermore–Los Alamos team led by Livermore geochemist Annie Kersting has shown, however, that plutonium can adhere to colloids, which are naturally occurring particles of rock smaller than a micrometer in diameter. In this way, small amounts of plutonium can be transported considerable distances by groundwater.

The team studied the distances plutonium ions had traveled from the Pahute Mesa region of DOE's Nevada Test Site. The group analyzed some of the groundwater pumped from two deep sampling wells dug near the sites where four underground nuclear tests had been conducted. The researchers discovered that colloids filtered from the water contained more than 99 percent of the small amount of plutonium found in the well-water samples. (In contrast, 99 percent of the tritium was found in solution, and virtually none was found in the filtrates.) The team proposed that small amounts of plutonium had adhered to mineral colloids that were transported by groundwater away from the test location.

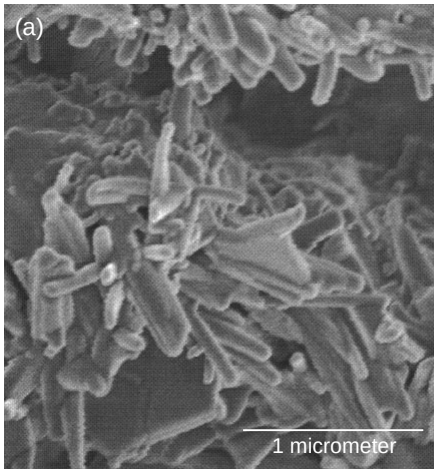
The team ascertained which of the four tests conducted in the area had produced the plutonium by measuring the ratio of the plutonium-240 isotope to the plutonium-239 isotope. (Every nuclear test can produce a unique ratio of the two plutonium isotopes.) The isotopic ratio measured on the groundwater colloids matched that of the 1968 Benham underground test, which was conducted 1.3 kilometers from one of the wells.

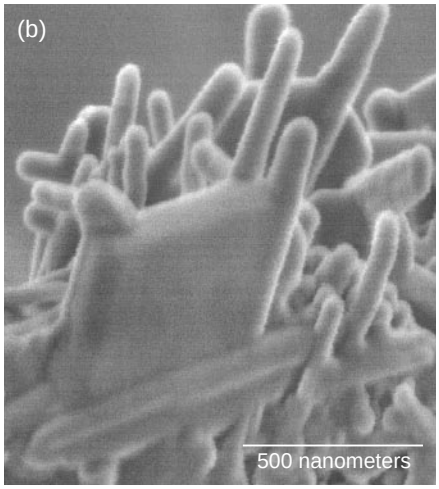
"We were surprised to find that the plutonium in the wells was from the Benham test because 1.3 kilometers is a long distance for plutonium to migrate," says Kersting. She adds, however, that the detected plutonium concentration was extremely small and did not pose a health risk.



Groundwater pumped from wells drilled in Pahute Mesa at the Nevada Test Site showed that small amounts of plutonium traveled surprising distances underground.

The team's findings have important implications for the proposed Yucca Mountain nuclear waste repository in Nevada (see *S&TR*, March 2000, pp. 13–20.) The findings may also be applicable to other DOE sites such as Rocky Flats in Colorado and the Hanford Nuclear Reservation in Washington, although their underground geology differs from the Nevada Test Site's.





Two scanning electron microscope images of mineral colloids (tiny rock particles) containing plutonium filtered from groundwater at (a) the 1-mircrometer scale and (b) the 500-nanometer scale. Mineral colloids consist of clay and zeolites, common secondary minerals found in rocks at the Nevada Test Site. Research by a Lawrence Livermore team suggests that small amounts of plutonium can be transported considerable distances by groundwater by adhering to colloids.

In light of the team's research, Kersting says that models that do not allow for transport of plutonium by colloids may significantly underestimate how far and fast the element can travel. She also notes that colloids may be important in the transport of other actinides. "We want to know how other actinides such as neptunium, americium, and uranium move underground," she says.

Kersting is collaborating with other Livermore geochemists to determine experimentally how actinides are associated with mineral colloids. In addition, she is investigating the importance of colloid-assisted transport of actinides in the vadose zone, or unsaturated subsurface, which is located between the ground surface and the water table. Two-thirds of the underground nuclear tests were detonated in the vadose zone at the Nevada Test Site. The research is taking place in tunnels that have been dug at the site's Rainier Mesa, whose vadose zone was previously studied by Livermore scientists.

The colloid discovery, she says, emphasizes the importance of linking precisely controlled laboratory experiments with field studies. "If you only look at results from experiments in the laboratory, you won't necessarily understand what's happening in the field."

From the arid stretches of the Nevada Test Site to physics research laboratories of Russia, Lawrence Livermore researchers are pursuing wide-ranging aspects of actinide science. They are combining theory, fieldwork, laboratory experiments, and computer simulations on scales ranging from atoms to kilometers, all with the aim of uncovering the secrets of the actinides.

—Arnie Heller

Key Words: actinides, colloids, Forensic Science Center, Glenn T. Seaborg Institute for Transactinium Science, Nevada Test Site, plutonium, Stanford Linear Accelerator Center, Stanford Synchrotron Radiation Laboratory, stockpile stewardship, uranium.

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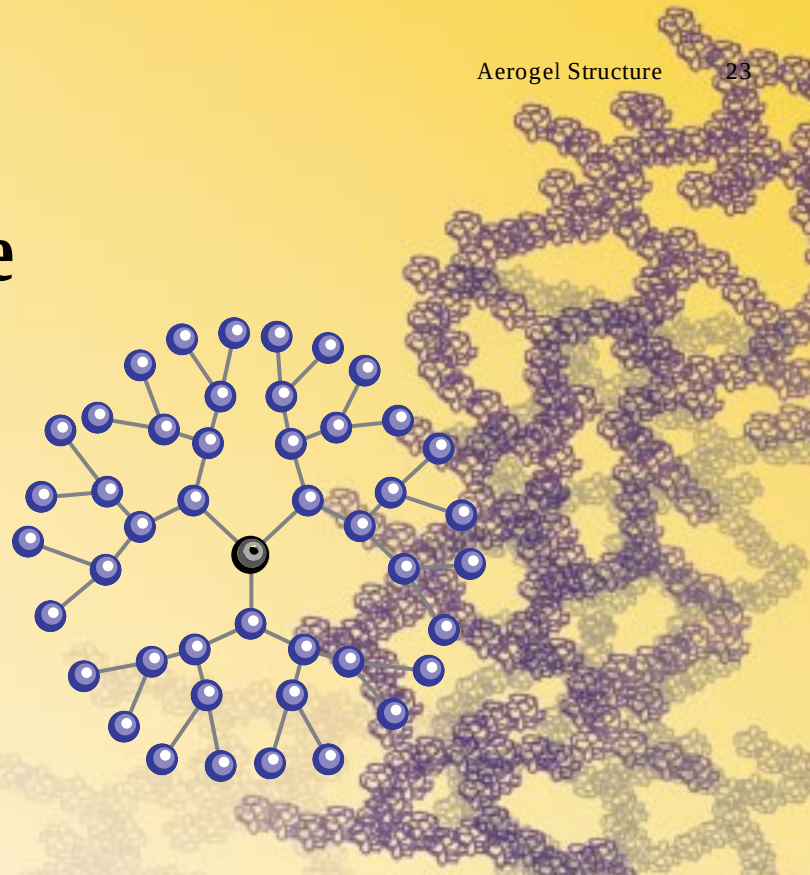
About the Scientist

LOUIS J. TERMINELLO is currently leader of the Materials Science and Technology Division in the Chemistry and Materials Science Directorate at Lawrence Livermore National Laboratory. He is also director of the Glenn T. Seaborg Institute for Transactinium Science at Livermore. He earned his Ph.D. in physical science from the University of California at Berkeley in 1988 and is an adjunct associate professor there. His research interests include solid-state physics, atomic and electronic structure determination of novel materials using synchotron radiation photoemission and absorption, and photoelectron holography and valence-band imaging studies of electronic material surfaces and interfaces.

A Predictable Structure for Aerogels



A Livermore scientist needs a support system with virtually no mass for a project he is working on. He is certain to end up using an aerogel. No mass at all is an impossibility, but aerogels come pretty close. Researchers at Livermore have already synthesized a silica aerogel only twice as dense as air.

Sometimes called frozen smoke, aerogels are open-cell polymers with pores less than 50 nanometers in diameter. In a process known as sol-gel polymerization, simple molecules called monomers suspended in solution react with one another to form a sol, or collection, of colloidal clusters. The macromolecules become bonded and cross-linked, forming a nearly solid, transparent sol-gel. An aerogel is produced by carefully drying the sol-gel so that the fragile network does not collapse.

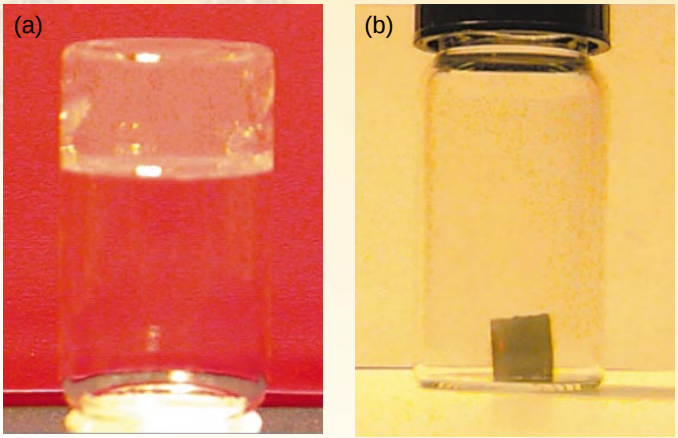
The complicated, cross-linked internal structure gives aerogels the highest internal surface area per gram of material of any known material. Aerogels also exhibit the best electrical, thermal, and sound insulation properties of any known solid.

For about the last 15 years, Livermore has been developing and improving aerogels for national security applications. Livermore scientists have also synthesized electrically conductive inorganic aerogels for use as supercapacitors and as a water purifier for extracting harmful contaminants from industrial waste or for desalinizing seawater. For a time, Livermore was involved with a NASA project in which an aerogel was to be installed in a satellite to collect particles of meteorites as they flew by.

Given aerogels' many sterling qualities, one would expect to find them in use everywhere. Indeed, there has been major industrial interest in aerogels. However, using them in everyday applications presents practical problems, specifically the cost of fabrication and processing. Several years ago, a Livermore team won an R&D 100 Award for developing a new fabrication method that was faster and cheaper. (See *S&TR*, December 1995, pp. 22–25.)

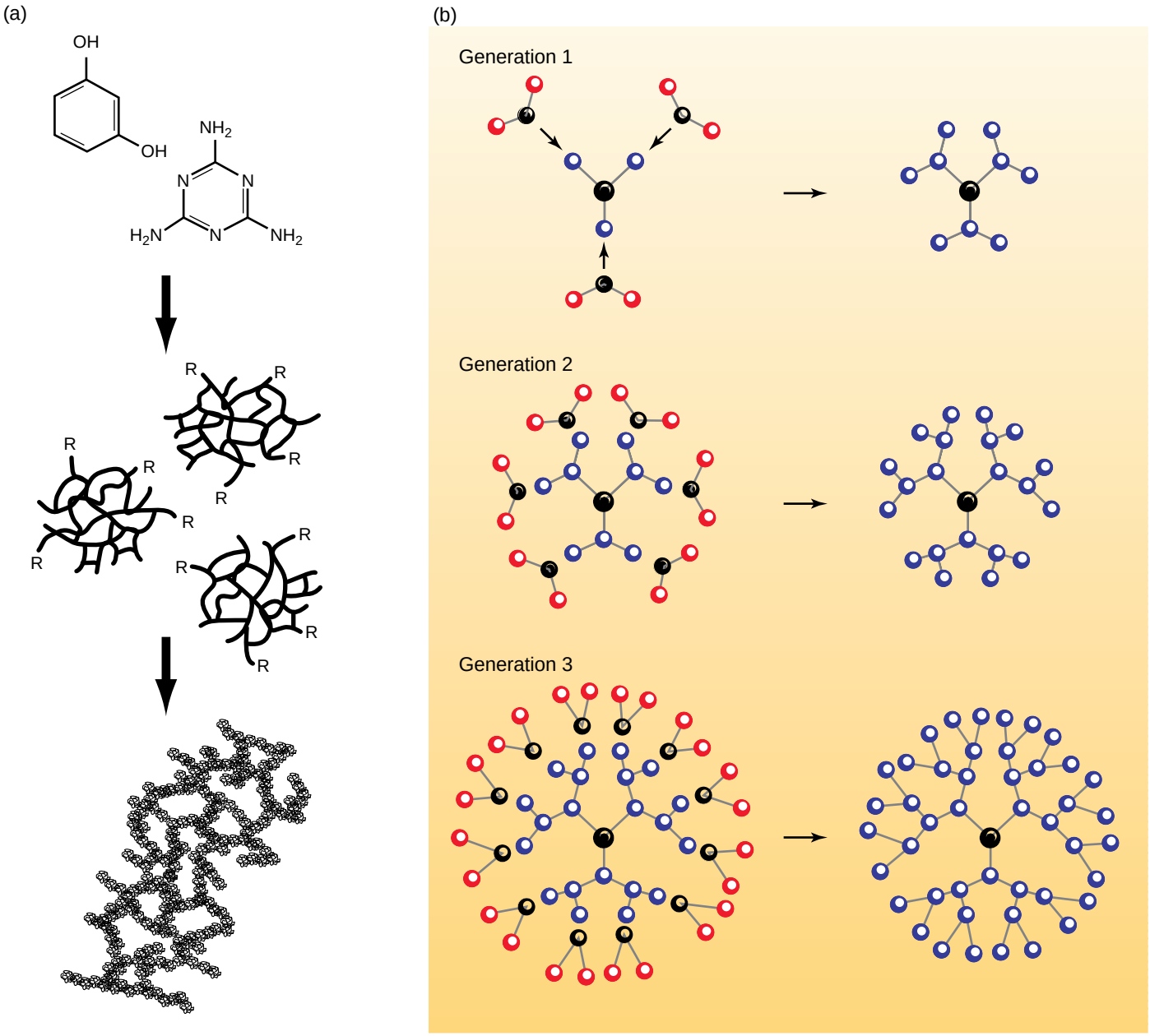
But another problem still stood in the way. Sol-gel polymerization is a bulk process with no way to control the size of the sols or the way they come together. The structure and density of the final aerogel are dictated to some extent by the conditions during polymerization such as temperature, pH, type of catalyst, and so on. But with current fabrication methods, the aerogel's structure cannot be controlled at the molecular level.

Chemist Glenn Fox is leading a project at Livermore that aims to bring more control to the design and synthesis of



A sol-gel polymer (a) in the sol-gel stage and (b) after it has been dried. This particular sol-gel polymer uses dendrimers and is called a dendrigel.

organic aerogels. “Laboratory programs would find many more uses for aerogels if only we could fabricate them to precise specifications,” Fox says. “They could be used as sensors for biological agents, in environmental remediation, as catalysts for chemical reactions, or in experiments on the National Ignition Facility. Aerogels have also been of interest for insulating appliances and homes and for a plethora of other uses. Nanostructured materials are attracting increased scientific and practical interest. But control of the material’s structure all the way down to the



(a) Traditional organic aerogels start out as either resorcinol or melamine combined with formaldehyde. There is no way to control how the cluster formation takes place, and the end result is a cross-linked polymer resembling a string of pearls. In (b), with dendredic polymers, the design and synthesis of reactive, multifunctional monomers can be tailored, with specific sites on the molecules activated for cross-linking. The formation and properties of the resulting gel can thus be carefully controlled.

molecular level is needed first." Fox and a small team obtained funding from the Laboratory Directed Research and Development program to apply a relatively new polymerization method to this problem.

Starting with a Tree

Dendrimers are highly branched, treelike macromolecules that can be synthesized "generationally" to produce perfectly regular structures (*dendron* is the Greek word for tree). Conventional polymers are chains of differing lengths with a range of molecular weights and sizes, while dendrimers have a precise molecular size and weight. Large, multigenerational dendrimers tend to form tidy spherical shapes with a well-defined structure that makes them particularly strong.

Fox's team has begun applying dendritic methodology to the creation of sol-gels and aerogels in the hope of achieving structural control. The Livermore team is one of the first to use dendritic technology in the organic sol-gel process.

Says Fox, "We are trying to understand and control the sol-gel polymerization process on a molecular level. Using dendrimers allows us to separate the clustering and gelling processes when an aerogel is being formed, something that has not been possible before. If we succeed, the payoff for Laboratory programs will be extremely important. We may be able to script the physical properties of the aerogel or build specific tags on molecules in a uniform way."

Organic aerogels are currently formed by combining either resorcinol (1,3-dihydroxybenzene) or melamine (2,4,6-triaminotriazine) with formaldehyde. Fox's team is synthesizing and experimenting with a whole collection of new starting materials that are being assembled into dendrimers. Some are based on resorcinol to take advantage of its well-documented reactive attributes. Another set of new dendrimer systems with rigid cores could give the resulting aerogel greater structural efficiency, improving the ease of processing and lowering the cost of aerogel production. Other experiments involve the synthesis of new organometallic materials and ways to evenly disperse metal ions in an organic aerogel.

These tailored dendritic monomers are being combined with preformed, dendritic, sol-gel clusters whose outer surface has been coated to react with the monomer. Two kinds of dendrimer precursors have been studied, amino-based and aromatic-based, each having different advantages. Amino-based dendrimers are available commercially and have been studied extensively. Reactants can be added relatively easily to their outer surfaces to "functionalize" them, prompting them to cross-link as desired. Benzyl ether dendrimers, on the other hand, are structurally similar to the colloidal sols of the resorcinol–formaldehyde mix. They are not commercially available but can be prepared readily in the laboratory.

Controlling the size and composition of the clusters formed during gelation as well as the type of cross-linking involved should give Fox's team a new-found architectural control over aerogels. Analysis of the structures with infrared spectroscopy, nuclear magnetic resonance spectroscopy, and mass spectroscopy will provide a better understanding of how chemistry can affect the composition and structural efficiency of these nanostructured materials.

—Katie Walter

Key Words: aerogels, dendrimers, polymers.

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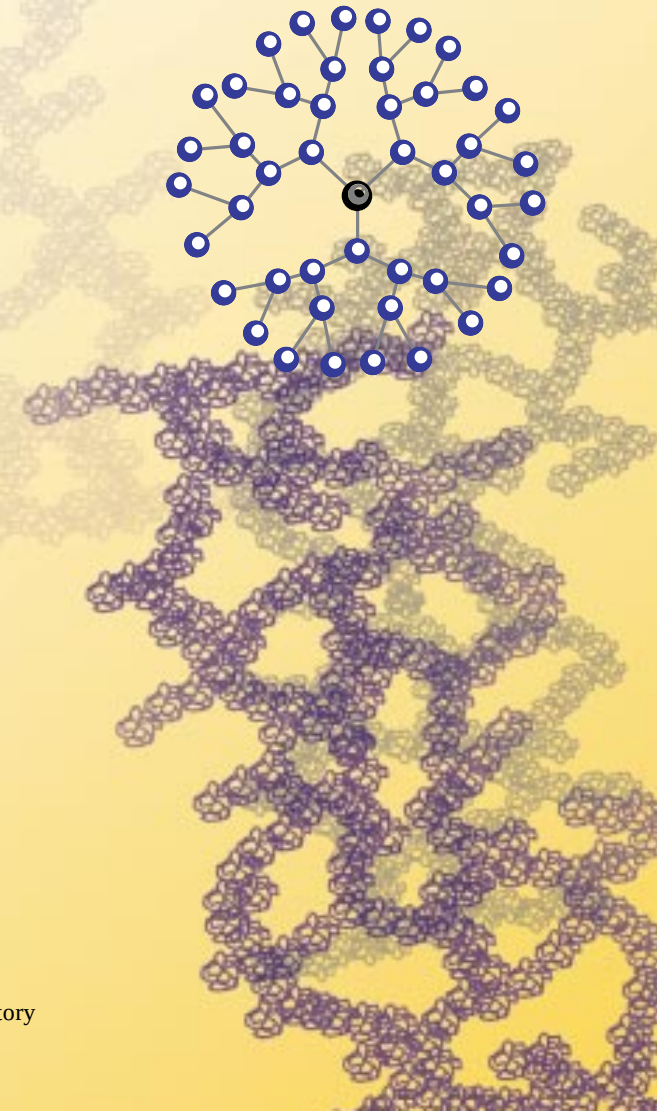
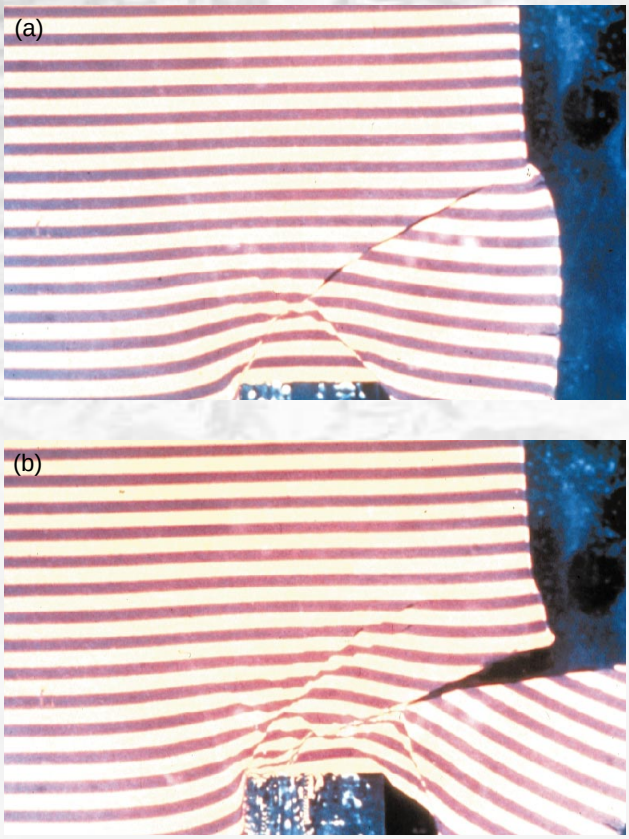


Tibet
Where Continents Collide

THE Himalayas get their height from India, and we aren't talking about genes. About 50 million years ago, the Indian subcontinent collided with Asia, and the two continents continue to converge at a rate of about 5 centimeters every year. The ongoing collision has been violent enough to push up the Himalayas, shove Southeast Asia further and further southeast, and perhaps most impressively, raise the Tibetan Plateau—a landmass as large as two-thirds of the lower 48 states—to an average elevation of 5,000 meters. Uplift of the Tibetan Plateau has been linked to intensification of the Asian monsoon and, by virtue of its erosion products, to gradual changes in seawater chemistry over long time periods. The Indo-Asian collision thus provides not only a natural laboratory for studying the mechanical response of Earth to plate tectonic forces but also an opportunity to explore the links between tectonics, climate, and ocean history.

Livermore geophysicists Rick Ryerson, Jerome van der Woerd, Bob Finkel, and Marc Caffee, along with collaborators from the University of California at Los Angeles and from Paris and Beijing, have been studying this terrestrial wrestling match for several years, making the first-ever measurements of long-term movement along large faults in northern Tibet. The Kunlun, Altyn Tagh, and Haiyuan faults are strike-slip faults that allow blocks of Earth's crust to slide past one another, often with disastrous consequences. All of these faults have experienced large earthquakes ranging in intensity from 7.5 to 8.7.

The function of the faults is a subject of considerable geophysical controversy. Faults may define major discontinuities in Earth's lithosphere (the outer 100 kilometers of the crust that define the plates in plate tectonics) and thus absorb a significant portion of the convergence between India and Asia. Or they may be shallow features that play a secondary role in a more fluid lithosphere. Some research indicates that the Kunlun and Altyn Tagh faults extend to the base of Earth's lithosphere, suggesting that they indeed define continental plates. A first step in deciding the faults' extent and function is to obtain accurate, long-term slip rates at enough sites along the faults to characterize their large-scale behavior.

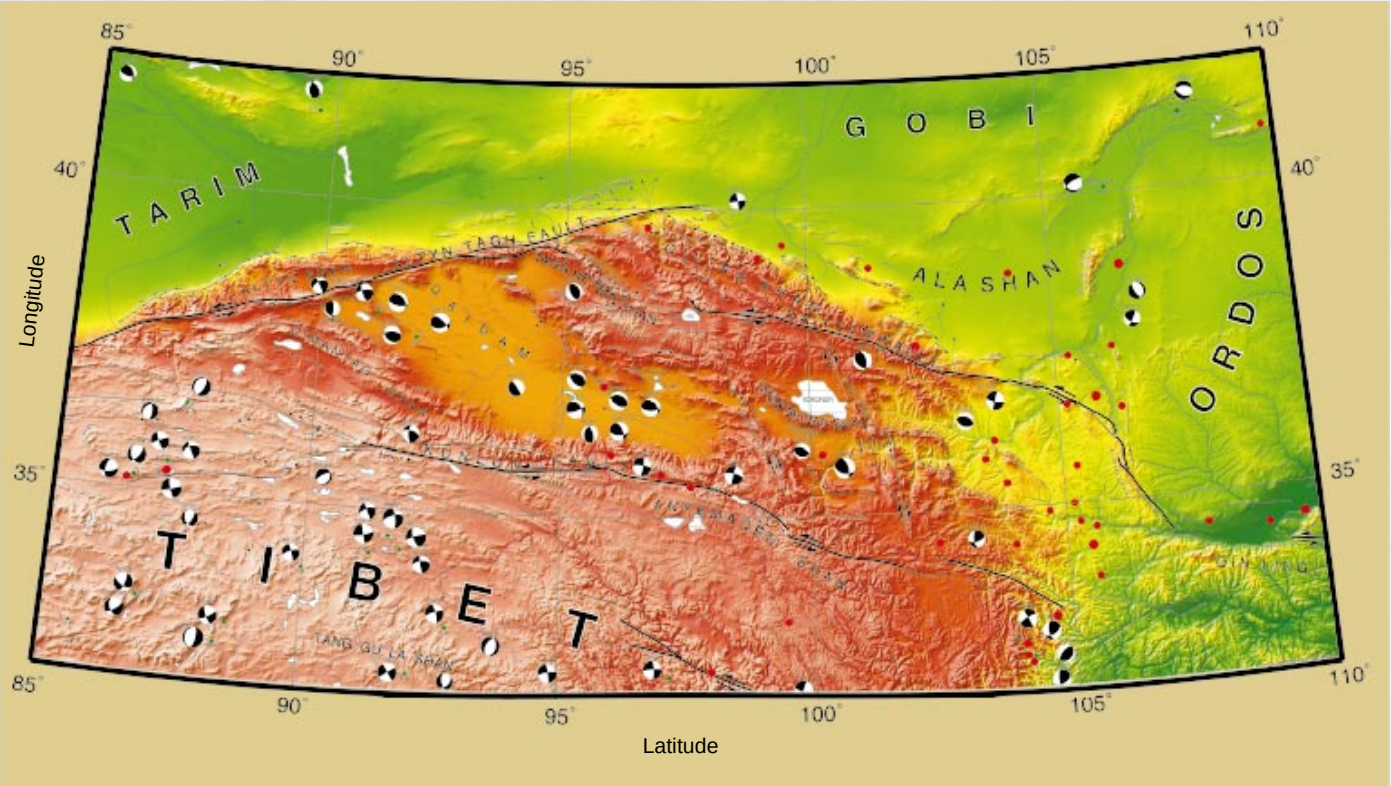


(a) In this plasticine model, the northward movement of a body representing India simulates the creation of faults that have allowed the southeastward displacement of the Southeast Asian landmass, among other features. (b) To accommodate the extrusion of Indochina, the South China Sea opened up to the east. Continued continental collision results in successively younger faults to the north. Paul Tapponnier and Gilles Peltzer of the Institut de Physique du Globe de Paris created this model. They collaborate regularly with Livermore scientists.

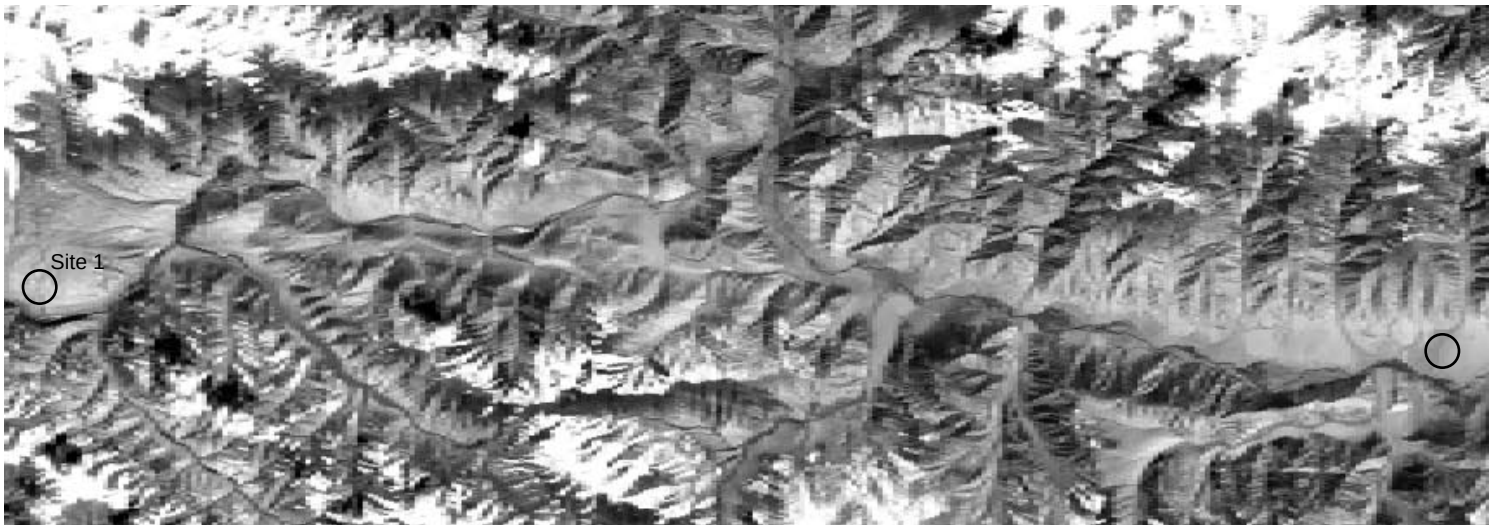
AMS and the Dating Game

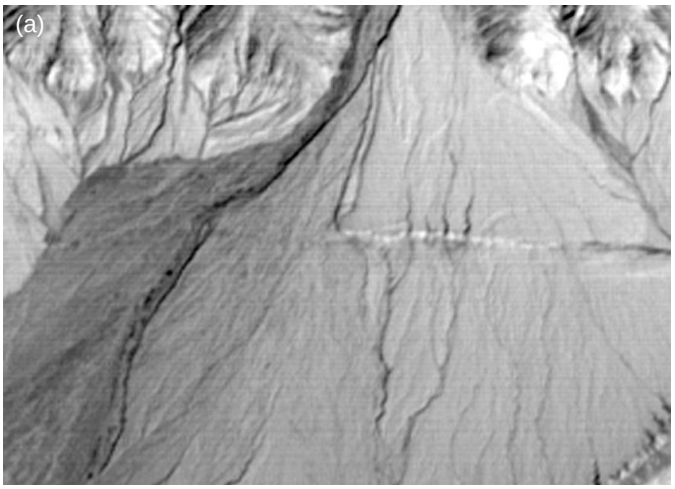
To derive rates of motion along faults, scientists first identify a site where lateral offset has occurred and then measure the offset and determine its age. Commercially available satellite imagery, with resolution to 10 meters, allowed the team to select regions where tectonic offsets are best preserved, such as abandoned stream beds and surfaces formed by glacial action. As shown in the figure on pp. 28–29, the team took measurements at several sites where the faults cross alluvial fans formed by melting glaciers. As a glacier shrinks, the stream running from it becomes narrower, leaving behind an older, wider streambed in a series of terraces. The boundaries between different terrace levels represent lateral offset markers.

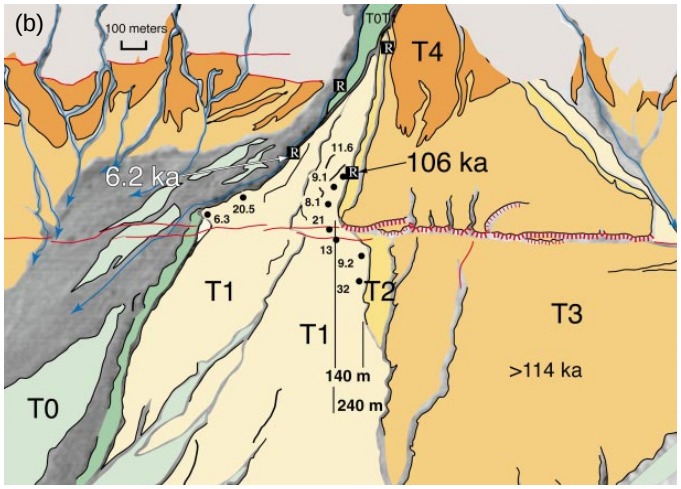
To determine the age of these surfaces and thus a slip rate, the team relied on experts from Livermore's Center for Accelerator Mass Spectrometry. Conventional mass spectrometry measures the concentrations of different isotopes of the same element. Accelerator mass spectrometry (AMS) does the same job but is much more sensitive than conventional mass spectrometry. The most common dating method is to measure carbon-14 relative to other carbon



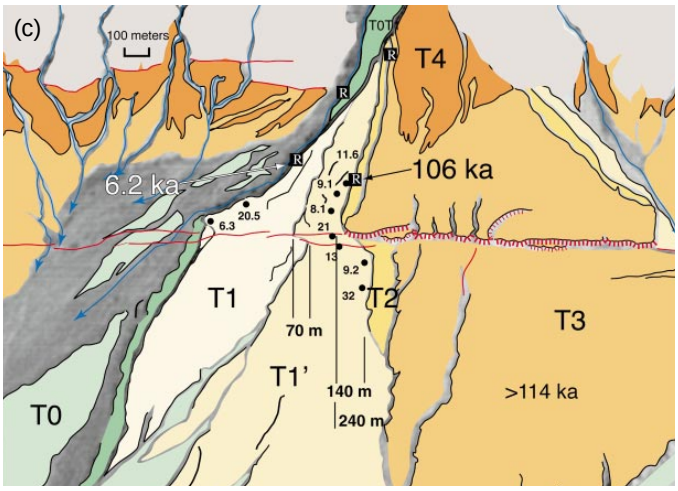
Map of Tibet showing the major faults and geopolitical boundaries for reference.

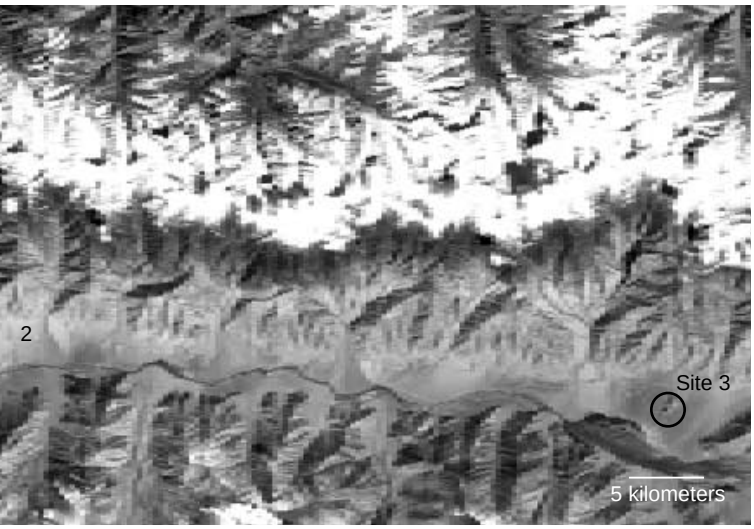






(a) Site 1 on the Altyn Tagh Fault. The fault is illuminated from the south and may be seen as a bright line running across the image. The active streambed is on the left and the older streambed terraces rise sequentially to the right. (b) and (c) Alternative interpretations of the evolution of the various terraces. (ka = 1,000 years)





Three sites studied along the Altyn Tagh Fault are shown. The fault is visible where it crosses several alluvial fans.

isotopes. AMS, for instance, can find one atom of carbon-14 in a quadrillion other carbon atoms, which means that extremely small samples can be studied.

However, in high, arid mountain ranges, fossil organic remains are often hard to find. Moreover, the ages of some surfaces may be too old to measure by carbon-14 methods. Therefore, for its first study, on the Kunlun Fault, the team compared slip rates obtained through radiocarbon dating with those obtained by measuring the cosmogenic nuclides beryllium-10 and aluminum-26 in quartz rock. Cosmogenic nuclides are produced through the interaction of surface samples with cosmic rays. Whereas carbon-14 levels fall over time, the levels of cosmogenic nuclides rise the longer a sample resides at Earth's surface. But the amounts they contain are still small. It has only been in the last 10 years, with advancements in such techniques as AMS, that measuring cosmogenic isotopes has been possible at all.

Under optimal conditions, samples taken from the surface will yield the true age of the surface. But a surface may also contain samples that were previously exposed to cosmic rays. Or rocks may simply roll downhill and contaminate a previously abandoned surface. Scientists must, therefore, collect many samples, both buried and from the surface, to account for all sources of contamination and derive a site's true age.

For the Kunlun studies, slip rates derived from beryllium-10 and aluminum-26 ages compared extremely well with those from radiocarbon dating.

What the Data Say

The figure at the bottom of p. 28, showing one alluvial fan along the Karakax Valley segment of the Altyn Tagh Fault, is an example of the many sites studied on both faults. The fault is clearly visible in part (a) of the figure as is lateral offset of terrace levels along the fault. Parts (b) and (c) show two interpretations of the evolution of this site.

Measurements at 10 sites along the Altyn Tagh Fault yielded slip rates as high as 3 centimeters per year in the west, decreasing to rates below 1 centimeter per year at the fault's eastern end. The rate decreases as lateral movement in the west is transformed into the vertical uplift that has created young mountains in northeastern Tibet. In contrast, using on measurements at six sites along a 600-kilometer length of the Kunlun Fault, the team found a uniform slip rate of about 12 millimeters per year over a time span of 40,000 years.

Comparison of the two faults suggests that the Kunlun Fault may be a more mature version of the Altyn Tagh. While the Altyn Tagh Fault is still in the process of propagating eastward, piling up new mountains along its bow, the Kunlun's movement appears to be fully transferred to other faults to the east. But Ryerson is quick to add, "We don't really understand yet what is happening at the eastern end of the Kunlun Fault."

These data indicate that the birth and growth of strike-slip faults has been moving north with time, suggesting that the northern portion of the Tibetan Plateau has been uplifted by successive episodes of eastward fault propagation coupled with the uplift of young mountain ranges. Sediments from the young mountain ranges accumulate in closed basins that are in turn uplifted by fault movement. Ironically, much of one of the greatest mountain ranges on Earth, the Tibetan Plateau, may have been built not of mountains but of basins.

The relatively high slip rates observed along the Altyn Tagh and Kunlun faults are consistent with the models showing that these faults play an important role in accommodating Indo-Asian convergence. Livermore's data indicate that the models representing the lithosphere as a fluid may be flawed.

The first stage of this work, assessing the slip rates on active faults in northern Tibet, is nearing completion. Barely begun, however, is the next stage—extrapolating these observations of active faulting back to the early history of the collision. Meanwhile, continents continue to collide in Tibet.

—Katie Walter

Key Words: accelerator mass spectrometry, cosmogenic isotopes, dating techniques, faults, plate tectonics, Tibet.

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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

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Peter A. Krulevitch Abraham P. Lee M. Allen Northrup William J. Benett	**Microfabricated Instrument for Tissue Biopsy and Analysis** U.S. Patent 5,985,217 November 16, 1999	A microfabricated biopsy–histology instrument that has several advantages over conventional instruments. These include minimal specimen handling, cutting edges providing atomic sharpness for slicing thin (2-micrometer or less) specimens, use of microliter volumes of chemicals for treating specimens, low cost, disposability, a fabrication process that renders sterile parts, and easy use. The cutter is a "cheese-grater" design comprising a substrate block of silicon that is anisotropically etched to form extremely sharp and precise cutting edges. Tissue specimens pass through the silicon cutter and lie flat on a piece of glass bonded to the cutter. Microchannels are etched into the glass or silicon substrates to deliver small volumes of chemicals for treating the specimens. After treatment, specimens can be examined through the glass substrate. For automation purposes, microvalves and micropumps may be incorporated. Also, specimens in parallel may be cut and treated with identical or varied chemicals. The instrument is disposable because of its low cost and thus could replace current expensive microtome and histology equipment.
Roger D. Aines Kent S. Udell Carol J. Bruton Charles R. Carrigan	**Chemical Tailoring of Steam to Remediate Underground Mixed-Waste Contaminants** U.S. Patent 5,986,159 November 16, 1999	A method to remediate mixed-waste underground contamination such as organic liquids, metals, and radionuclides. It involves chemical tailoring of steam for underground injection. Gases or chemicals are added to a high-pressure steam flow being injected into wells, toward contaminated soil located beyond excavation depths. The additives in the injected steam mobilize contaminants as the steam pushes the waste through the ground toward an extraction well having subatmospheric pressure (vacuum). The steam and mobilized contaminants are drawn in a substantially horizontal direction to the extraction well and withdrawn to a treatment point above ground. The heat and boiling action of the steam front enhance the mobilizing effects of the chemical or gas additives. While being used to remove any organic contaminants, the method may also be used for immobilizing metals. An additive can be used to cause metals to precipitate into large clusters, thereby limiting their future migration.
Layton C. Hale	**Precision Tip-Tilt-Piston Actuator That Provides Exact Constraint** U.S. Patent 5,986,827 November 16, 1999	A device that can precisely actuate three degrees of freedom (commonly referred to as tip, tilt, and piston) of an optic mount. The device consists of three identical flexure mechanisms, an optic mount to be supported and positioned, a structure that supports the flexure mechanisms, and three commercially available linear actuators. Each flexure mechanism constrains two degrees of freedom in the plane of the mechanisms, and one direction is actuated. All other degrees of freedom are free to move within the range of flexure mechanisms. Typically, three flexure mechanisms are equally spaced in angle about the optic mount and arranged so that each actuated degree of freedom is perpendicular to the plane formed by the optic mount. This arrangement exactly constrains the optic mount and allows arbitrary actuated movement of the plane within the range of the flexure mechanisms. Each flexure mechanism provides a mechanical advantage, typically on the order of 5:1, between the commercially available actuator and the functional point on the optic mount. This feature improves resolution by the same ratio and stiffness by the square of the ratio.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Ronald G. Musket	**Sharpening of Field Emitter Tips Using High-Energy Ions** U.S. Patent 5,993,281 November 30, 1999	A process for sharpening arrays of field emitter tips of field-emission cathodes such as those found in field-emission, flat-panel video displays. The process uses sputtering of high-energy (more than 30-kiloelectronvolt) ions incident along or near the longitudinal axis of the field emitter to sharpen the emitter with a taper from the tip, or top, of the emitter down to its shank. The process is particularly applicable to sharpening tips of emitters having cylindrical or similar (pyramidal, for example) symmetry. The process will sharpen tips down to radii of less than 12 nanometers with an included angle of about 20 degrees. Because the ions are incident along or near the longitudinal axis of each emitter, the tips of gated arrays can be sharpened by high-energy ion beams rastered over the arrays using standard ion implantation equipment. While the process is particularly applicable for sharpening arrays of field emitters in field-emission, flat-panel displays, it can be effectively used in the fabrication of other vacuum microelectronic devices that rely on field emission of electrons.
Paul G. Carey Patrick M. Smith	**Method of Fabrication of Display Pixels Driven by Silicon Thin-Film Transistors** U.S. Patent 5,994,174 November 30, 1999	A method of fabricating display pixels driven by silicon thin-film transistors on plastic substrates. The method is useful for active matrix displays such as flat-panel displays. The process for forming the pixels involves a prior method for forming individual silicon thin-film transistors on low-temperature plastic substrates, which are generally considered incapable of withstanding sustained processing temperatures greater than about 200°C. The pixel formation process results in a complete pixel and active-matrix pixel array. A pixel (or picture element) in an active-matrix display consists of a silicon thin-film transistor (TFT); a large electrode, which may control a liquid crystal light valve; and an emissive material (such as a light-emitting diode) or some other light-emitting or attenuating material. The pixels can be connected in arrays wherein rows of pixels contain common gate electrodes and columns of pixels contain common drain electrodes. The source electrode of each pixel TFT is connected to its pixel electrode and is electrically isolated from every other circuit element in the pixel array.
Harley M. Buettner	**Electrical Heating of Soils Using High-Efficiency Electrode Patterns and Power Phases** U.S. Patent 5,994,670 November 30, 1999	Powerline-frequency electrical (joule) heating of soils using a high-efficiency electrode configuration and power phase arrangement. The electrode configuration consists of several heating or current injection electrodes around the volume of soil to be heated and a return or extraction electrode(s) located inside the volume to be heated. The heating electrodes are all connected to one phase of a multiphase or single-phase power system; the return electrode(s) is (are) connected to the remaining phases of the multiphase power source. This electrode configuration and power-phase arrangement can be used wherever powerline-frequency soil heating is applicable. It thus has many potential uses, including removal of volatile organic compounds such as gasoline or trichloroethylene from contaminated areas.
Matthias Frank Carl A. Mears Simon E. Labov W. Henry Benner	**Ultrahigh-Mass Mass Spectrometry with Charge Discrimination Using Cryogenic Detectors** U.S. Patent 5,994,694 November 30, 1999	An ultrahigh-mass, time-of-flight mass spectrometer using a cryogenic particle detector as an ion detector with charge-discriminating capabilities. Cryogenic detectors have the potential for significantly improving the performance and sensitivity of time-of-flight mass spectrometers, and compared to ion multipliers, they exhibit superior sensitivity for high-mass, slow-moving macromolecular ions and can be used as “stop” detectors in time-of-flight applications. In addition, their energy-resolving capability can be used to measure the charge state of the ions, which is valuable for all time-of-flight applications. Used as an ion detector in a time-of-flight mass spectrometer for large biomolecules, a cryogenically cooled niobium–alumina–niobium superconductor–insulator–superconductor tunnel junction (STJ) detector operating at 1.3 kelvin has been found to have charge discrimination capabilities. Because the cryogenic STJ detector responds to ion energy and does not rely on secondary electron production (as in the conventionally used microchannel plate detectors), the cryogenic detector can detect large molecular ions with a velocity-independent efficiency approaching 100 percent.

(continued on p. 32)

(Continued from p. 31)

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
James C. Davidson Joseph W. Balch	**Vacuum Pull-Down Method for an Enhanced Bonding Process** U.S. Patent 6,000,243 December 14, 1999	A process for effectively bonding substrates of arbitrary sizes or shapes. It incorporates vacuum pull-down techniques to ensure uniform surface contact during bonding. The essence of the process for bonding substrates such as glass, plastic, or alloys, which have a moderate melting point and gradual softening-point curve, involves applying an active vacuum source to evacuate interstices between substrates while providing a positive force to hold in contact the parts that are being bonded. The process enables increasing temperature during bonding to ensure that the softening point has been reached and small voids are filled and come in contact with the opposing substrate. The process is most effective where at least one of the two plates or substrates contains channels or grooves that can be used to apply vacuum between the plates or substrates during the thermal bonding cycle. Also, it is beneficial where there is a vacuum groove or channel near the perimeter of the plates or substrates. In both instances, the process ensures bonding at the perimeter and reduces unbonded regions in the interior.

Awards

Jim Bryan, a retired Laboratory engineer, was recently recognized by *Fortune* magazine as one of the six **"Heroes of U.S. Manufacturing"** of 2000 at a ceremony in Chicago, Illinois. Now in their fourth year, the *Fortune* awards are presented annually to innovators who have made a notable contribution to American manufacturing. Bryan is the first award recipient from a U.S. national laboratory.

In the 1980s, Bryan reworked an old British invention called a fixed ball bar by adding a telescoping arm to the instrument. His invention came about, in part, because of the need to produce components with extreme precision for the nation's nuclear weapons. Today, versions of Bryan's ball bar are used around the world to test machine-tool performance quickly.

Used by hundreds of companies to determine if their machine tools are working properly, telescoping ball bars are plugged into a personal computer for tests in which the computer analyzes the deviation of a machine tool's motion from a perfect circle. (Machine tools, such as lathes and milling machines, precisely cut metal to shape.)

During his Laboratory tenure (1955 to 1987), Bryan made wide-ranging contributions to metrology and precision machining. Toward the climax of his career when Bryan was head of the Precision Engineering Group, his team designed, built, and operated the largest diamond turning machine in the world.

Two Laboratory scientists have been elected **fellows** of the **Optical Society of America**.

Stephen Payne, associate program leader in the Laser Science and Technology organization, was recognized for "sustained pioneering contributions to the development of novel lamp and diode-pumped solid-state laser materials." Working with Laboratory colleagues, Payne has developed more than a dozen laser crystals and glasses. A 15-year Laboratory employee, he received his Ph.D. in chemistry from Princeton University. He has 80 refereed journal publications, holds 11 patents, has received four R&D 100 awards, and recently received the Excellence in Fusion Engineering Award from Fusion Power Associates.

Mike Perry, associate program leader for the Short-Pulse Lasers, Applications, and Technology Program, was recognized for "pioneering contributions to the development and use of high-peak-power, ultrashort-pulse lasers" in high-intensity physics research. Areas of investigation include the fast-igniter concept for inertial confinement fusion and materials processing applications in industrial machining and health care. Perry was also key in the Laboratory's development of large-scale diffractive optics for large-area diffraction gratings used to manipulate laser light.

Perry has been at the Laboratory for 17 years, starting with his doctoral work for the University of California at Berkeley in nuclear engineering/quantum electronics. He has contributed to more than 100 scientific papers on materials processing, diffractive and nonlinear optics, and the use of lasers in medicine. He holds patents in areas such as inertial confinement fusion, multilayer dielectric diffraction gratings, and ultrashort-pulse laser machining.

Abstracts

New Day Dawns in Supercomputing

ASCI White—the 10-teraops supercomputer developed by IBM for Lawrence Livermore and due to come online in the summer of 2000—is the latest in a series of ultrahigh-speed computers built for the Department of Energy's Accelerated Strategic Computing Initiative (ASCI). A key component of the DOE's Stockpile Stewardship Program, ASCI has the goal of providing the computational tools needed for running full-scale simulations of nuclear weapons by 2004. Weapon scientists will use these simulations, archived nuclear test data, and nonnuclear experiments to ensure the safety, reliability, and performance of U.S. nuclear weapons. ASCI White is the direct descendant of the ASCI Blue Pacific, a 3-teraops machine. Over the past year, Blue Pacific has successfully run a variety of unprecedented three-dimensional simulations, including the first-ever three-dimensional simulation of an exploding nuclear weapon primary and an award-winning turbulence simulation. Through DOE's Academic Strategic Program Alliance, universities have also used Blue Pacific to research unclassified problems applicable to ASCI research, including the physics of supernovas and fire.

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Uncovering the Secrets of Actinides

The elements from actinium (element 89) to lawrencium (element 103) are known as the actinides. All of the actinides are metals, and all are radioactive. More complete information on actinides is needed to better assess the nation's nuclear stockpile, help stem the clandestine proliferation of nuclear weapons, and gain a better understanding of the use and storage of nuclear fuels such as enriched uranium. A major research focus is on obtaining a better scientific understanding of plutonium, the most complex and perplexing element in the periodic table. The Lawrence Livermore chapter of the University of California's Glenn T. Seaborg Institute for Transactinium Science is attempting to attract and train the next generation of actinide scientists.

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What Shocked Plutonium Can Tell Us

In the remote desert of the Department of Energy's Nevada Test Site, Livermore physicists and engineers are conducting subcritical tests—detonating high explosives and plutonium without sustaining a nuclear chain reaction—to help ensure the safety and reliability of the U.S. nuclear weapon stockpile.

Also in July/August

- *Accelerator mass spectrometry is on its way to becoming a routine tool for biomedical research.*
- *Site-specific seismic analyses help prepare University of California campuses for large-magnitude earthquakes.*
- *Quantum-dot technology yields ever smaller devices emitting more colors of light for various applications.*

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