Developing “Smart” Materials to Treat Aneurysms

Also in this issue:
• Astrophysics Code Helps Solve Puzzle
• The View from Washington, DC
About the Cover

Foam devices made from Livermore-developed shape-memory polymers (SMPs) may offer a custom, nonsurgical treatment for brain aneurysms. The SMP collaborative research team consists of scientists from Livermore, the University of California (UC) at Davis, and UC Berkeley. On the cover, Laboratory scientists (left to right) Jane Bearinger, Ward Small, and Jason Ortega use a crimping machine to compress the foam “plugs” into a shape suitable for maneuvering through a catheter to a patient’s brain. When heated inside the aneurysm, the plug expands back to its original, customized shape. These foam devices may prove to be a safer and more cost-effective treatment option for people with life-threatening brain aneurysms.

About the Review

At Lawrence Livermore National Laboratory, we focus science and technology on ensuring 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 six 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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Contents

Features

3 Biomedical Technology Has a Home at Livermore
Commentary by Cherry A. Murray

4 Shaping the Future of Aneurysm Treatments
Livermore foam devices may offer significant advantages for treating some forms of aneurysms.

Research Highlights

13 Ring around a Stellar Shell: A Tale of Scientific Serendipity
Using a three-dimensional model, Livermore scientists have solved a long-standing puzzle of stellar evolution.

16 On Assignment in Washington, DC
Livermore personnel in Washington, DC, support federal sponsors and become valuable assets to Laboratory programs.

Departments

2 The Laboratory in the News

19 Patents and Awards

20 Abstracts
Global warming threatens West's water resources

Water flow in the western U.S. has decreased for the last 20 to 30 years, but scientists have never understood why. Benjamin Santer of Livermore’s Program for Climate Model Diagnosis and Intercomparison and collaborators from the Scripps Institution of Oceanography have for the first time pinpointed humans as the cause of diminishing water flow on a regional scale. By looking at air temperature, river flow, and snowpack during the last 50 years, the team determined that the human-induced increase in greenhouse gases has seriously affected the water supply in the western U.S. “The water flow decrease is a result of temperature change,” says Scripps colleague Tim Barnett, “and that temperature change is caused by us.”

Santer and Barnett presented the research at the American Geophysical Union Meeting in December 2007. The team scaled down global climate models to a regional level and compared the results to their observations. The researchers found they could use the same models to predict the effects of the increase in greenhouse gases on the western U.S. in the future. By 2040, most of the snowpack in the Sierras and Colorado Rockies would melt by April 1 of each year because of rising air temperatures, causing a shift in river flows. With the existing greenhouse gas in the atmosphere, Earth will continue to warm for the next 80 to 100 years. “We are headed for a water crisis in the western United States, and it has already started,” says Barnett.

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Human activities may shape California climate

Through research funded by the California Energy Commission, scientists from the Laboratory, the University of California at Merced, and the National Center for Atmospheric Research found that temperatures in California from 1915 to 2000 have increased by 1.16°C (2.1°F) statewide. The research, which appeared in the December 19, 2007, online edition of Climatic Change, also suggests that the warming may be related to human activities.

The team used data from up to eight observational records and found that warming has been fastest in late winter and early spring. “The trends in daily minimum and maximum temperatures over the last 50 and 85 years are inconsistent with current model-based estimates of natural internal climate variability,” says Livermore’s Céline Bonfils. “It’s pretty clear the increases are not the result of just natural causes. External factors such as greenhouse gases and urbanization come into play.” However, current climate models have not been effective in explaining California’s summertime trend, where warming mainly occurs at night. Previous research by the team indicates that large-scale irrigation in California has had a cooling effect on summer daytime temperatures, which may have counteracted warming from mounting greenhouse gases and urbanization. If this hypothesis is verified, the acceleration of carbon dioxide emissions combined with a leveling of irrigation may result in a rapid summertime warming in the Central Valley in the near future.

Researchers suggest that greenhouse warming will continue to influence climate and may have significant societal impacts in California. Benjamin Santer, also a member of the Livermore team, says, “Our study represents a credible first step toward identifying the effects of human activities on California’s climate.”

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Stardust samples reveal unexpected results

Laboratory scientists, working with collaborators from other scientific and academic institutions, have unveiled new research on the dust collected from Comet Wild 2 during the Stardust mission. In a surprising turn of events, the research failed to find the primitive materials that had been thought to abound in comets. Rather, the dust from this particular comet formed very close to the young Sun and is more like material in asteroids. The research appeared in the January 25, 2008, edition of Science.

Researchers used Livermore’s aberration-corrected, monochromated, scanning transmission electron microscope known as SuperSTEM to analyze the Stardust samples. The samples were compared to interplanetary dust particles (IDPs) gathered from Earth’s stratosphere. Believed to be cometary dust, these IDPs contain the most primitive starting materials from which the planets in the solar system formed. Researchers were particularly interested in identifying in the Wild 2 dust two silicate materials unique to the IDPs, GEMS (glass with embedded metal and sulfides) and crystalline silicate enstatite (a rock-forming mineral). The team found only a single sliverlike whisker of enstatite, and it was similar to material in asteroids, not IDPs. Objects similar to GEMS were found, but the team determined they were created during the high-speed impact with Wild 2 dust.

The research emphasizes the continuum between asteroids and comets. “Wild 2 doesn’t match our idealized picture of a primitive comet made of ancient, unaltered material,” says Livermore scientist Hope Ishii. “The Stardust mission was a real success because without it, we never would have learned these things about our solar system. The returned sample is enabling us to continue to unravel how our solar system formed and evolved.”

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INNOVATIVE science and the exploration of advanced technologies for biomedical applications are needed to improve human health worldwide and to address the national need of affordable health care for an aging population. When facing these challenges, biomedical research institutions benefit from a variety of research and development activities at Department of Energy (DOE) laboratories, which are sources of special capabilities and expertise. However, at times, the question arises, “Why Lawrence Livermore, a national security laboratory?”

The ties between our national security work and human health have deep roots in the Laboratory’s history. In 1963, Livermore formed a biomedical research program to better understand the effects of ionizing radiation on biological systems—an important issue for worker safety within the nuclear weapons complex and for the resettlement efforts in the Marshall Islands following the end of atmospheric nuclear testing. Research efforts focused on chromosome damage soon led to the development of chromosome sorting technology here and at Los Alamos National Laboratory, culminating in the birth of the Human Genome Project. Today, we are a partner in DOE’s Joint Genome Institute and a developer of advanced biological agent detectors and pathogen signatures used for homeland security and health applications.

In addition, the ties between developing technologies for national security and for biomedical applications are numerous. Livermore’s expertise in accelerator technology and radiography stems from our hydrodynamic testing. Radiography is also important for the nondestructive evaluation of weapons as part of stockpile surveillance programs. We are now working with a licensee to develop the first compact proton therapy system, an accelerator that would fit in any major cancer center at a fifth the cost of larger machines in use today. The accelerator is based on a technology breakthrough made at Livermore and is a result of our continuing interest in compact accelerators for future hydrodynamic testing at the Nevada Test Site.

Laser technologies also bridge national security and biomedical applications. Adaptive optics are key to the design and construction of the National Ignition Facility, and a microelectromechanical adaptive optics system is behind a new ophthalmoscope that won a Laboratory team an R&D 100 Award last year. The ophthalmoscope sharpens images of retinal cell layers, allowing clinicians to diagnose macular degeneration and other retinal diseases much earlier than was previously possible. Lasers also are important components in advanced diagnostics for many nondestructive evaluation applications, and they are the reason for our collaboration with the University of California at Davis’s Center for Biophotonics, Science and Technology—one of our many partnerships with Davis in medical technologies and cancer research.

Materials science research for national security and broader applications is also a Laboratory strength. Recent research includes work on shape-memory polymers (SMPs)—a class of “smart” materials that, as a result of an external stimulus, can change from a deformed shape back to their original shape. SMPs are increasingly used in medical devices, aerospace technologies, and textiles, where their dynamic response can change material performance. They are both inexpensive and easy to manufacture.

The article beginning on p. 4 describes an application using SMPs to improve the treatment of aneurysms. The research team has synthesized new materials with superior properties over those commercially available today and demonstrated biocompatibility and utility. Remarkable progress has been made by combining theory, experiment, and simulation. We look forward to seeing such a promising technology adopted by the medical industry.

This multidisciplinary project—and the application of our technological advances to a broad range of important national needs—exemplifies the mission of the Laboratory and the creativity of our scientists and engineers.

Cherry A. Murray is principal associate director for Science and Technology.
SHAPING THE FUTURE OF ANEURYSM TREATMENTS

Each year, about 30,000 people in the U.S. die or suffer neurological damage from cerebral aneurysms, which form when a weak or thin region on a blood vessel in the brain bulges and fills with blood. An aneurysm can put pressure on a nerve or the surrounding brain tissue. If left untreated, an aneurysm can grow until it leaks or ruptures, spilling blood into the surrounding tissue and causing a hemorrhagic stroke. (See the box on p. 6.)

Stroke is the leading cause of disability in the U.S. and the third most common cause of death, after heart disease and cancer. Although strokes are most common in the elderly, they can occur in people of all ages, including children and infants. Significant strides have been made during the past few decades to lessen the stroke occurrence rate. According to the Centers for Disease Control and Prevention, the number of strokes has decreased steadily since the 1950s, primarily because more people are controlling their blood pressure and taking steps to prevent diseases that can lead to stroke. The decreased number can also be traced to better treatment options for people who have aneurysms.

Lawrence Livermore researchers are collaborating with colleagues from the University of California (UC) at Davis’s Center for Biophotonics, Science, and...

Livermore’s shape-memorizing foams could be key to preventing life-threatening strokes.
Technology and from UC Berkeley to develop safer, faster, and more cost-effective treatments for patients with cerebral aneurysms. The team’s effort is funded primarily through Livermore’s Laboratory Directed Research and Development (LDRD) Program, the National Institutes of Health (NIH), and the National Science Foundation.

Livermore scientist Duncan Maitland, who leads the team of 30, stresses the need for individualized approaches to the problem. “Cerebral aneurysms are not life-threatening until they begin pressing on the brain or burst,” he states. “The problem is that few technical solutions currently exist for treating these aneurysms. Each aneurysm is unique and therefore requires customized treatment. We are widening the range of treatment options.”

**Existing Aneurysm Treatments**

Today, two treatment categories are available for aneurysms: surgical and nonsurgical. The goal of each is to prevent blood from entering the bulged-out section of the vessel, called the sac. Blood flow in this region increases pressure on the weakened vessel wall and heightens the risk of rupture.

Microvascular clipping, introduced in 1937, is the most common surgical treatment for cerebral aneurysms. For this treatment, a section of the skull is removed to expose the aneurysm under a microscope. The aneurysm is then completely closed off with a tiny (1- to 2-centimeter-long) metal clip to prevent bleeding or rupture and thereby protect nearby brain tissue from damage. If the aneurysm has grown enough to severely damage the blood vessel, the surgeon may elect to reroute the blood flow around the damaged area by grafting a piece of blood vessel from another part of the body.

The second procedure, called embolic coiling, is a nonsurgical treatment that was approved in the early 1990s for patients with inoperable aneurysms. For this treatment, a small plastic catheter is inserted in either the femoral (leg) or carotid (neck) artery. A contrast dye injected in the bloodstream through the catheter highlights the normal blood vessels and delineates the aneurysm. Continuous x rays of the patient’s vascular system, provided by an imaging technique called fluoroscopy, help the surgeon maneuver a microcatheter into the aneurysm through the original catheter. Then tiny platinum wires—only slightly larger in diameter than a human hair—are deposited into the aneurysm. Finally, the wires take on a coil shape and induce blood clotting, which reduces or blocks blood flow in the sac.

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**Little Aneurysm, Big Deal**

Cerebral aneurysms occur more commonly in adults than in children, but they can occur at any age and are slightly more common in women than in men. They can result from birth defects, preexisting conditions such as high blood pressure and atherosclerosis (the buildup of fatty deposits in the arteries), or head trauma. Cerebral aneurysms are classified both by size and shape—small aneurysms have a diameter of less than 15 millimeters, while larger ones can exceed 50 millimeters.

“Before a larger aneurysm ruptures, the individual may experience a sudden and unusually severe headache, nausea, vision impairment, vomiting, or loss of consciousness, or the individual may experience no symptoms at all,” says Livermore scientist Duncan Maitland. “A small, unchanging aneurysm will likely produce no symptoms while symptoms of a larger aneurysm usually occur suddenly and without warning. The larger an aneurysm becomes, the more likely it is to burst.” While an estimated 30,000 aneurysms are diagnosed every year, perhaps as many as 10 times more go undetected.

“Our shape-changing foam-plug devices will be competing against the platinum coil technology that is used on 70 percent of treatable aneurysms,” says Maitland. The remaining 30 percent are treated surgically with metal clips. An aneurysm is sometimes considered “untreatable” if it is exceedingly large or in a critical or hard-to-reach area of the brain. According to Maitland, approximately 40 percent of aneurysms are deemed “treatable”—aneurysms measuring outside of the range of 5 to 15 millimeters in diameter are usually not treated.

A brain aneurysm, also called a cerebral or intracranial aneurysm, is an abnormal bulging outward of an artery in the brain. As many as 1 in 15 people in the U.S. will develop a brain aneurysm during their lifetime.
Aneurysms with small entrance points, called narrow-neck aneurysms, are generally treated with the wire coils. A wide-neck aneurysm can also be treated with coils, but a stent or balloon must be used with the coils to prevent them from migrating to the parent vein or artery.

Doctors consider several factors when deciding which treatment option is best for a patient. These factors include the type, size, and location of the aneurysm; risk of rupture; patient’s age, health, and medical history; and risk of treatment. Both surgical and nonsurgical methods have some drawbacks. “Using detachable coils to treat an aneurysm avoids many of the risks associated with surgery, but the treatment is a time-consuming process,” says Maitland. “Because the coils can compact over time in the sac, 40 percent of the patients must have more coils implanted at a later date. In addition, each implanted coil has a 2-percent risk of bursting the aneurysm.”

“Smart” Foams

To address these shortcomings, Maitland’s team developed an alternative treatment that isolates an aneurysm from the rest of the vascular system with one implanted device—a “plug” made from shape-memory-polymer (SMP) foam. SMPs are a class of polymeric materials that remember their primary (original) shape after being molded into a secondary (temporary) shape. Depending on the type of SMP, it can be altered from one shape to the next using heat, moisture, pH, or electric or magnetic fields. The Livermore-developed SMP foam plug is altered with heat.

Researchers first cut a plug out of the foam material to match the contours of an aneurysm. Then a crimping machine with heated blades compresses the foam plug into a stable secondary shape that can be fed through catheters via a fiber-optic cable to the aneurysm sac. Once the plug reaches the sac, it is heated with diode-laser light through the fiber-optic cable. Heating time could range from as little as 10 seconds to several tens of seconds, depending on the temperature at which the foam plug is designed to fully expand to its primary shape. As the plug expands, it absorbs blood, which congeals and forms clots to stop blood flow inside the aneurysm.

Although foam plugs have not been directly compared with platinum coils in statistically significant trials, studies with an in vitro aneurysm model demonstrated that the technology is efficient in filling the aneurysm sac. Livermore chemical engineer Thomas Wilson, a polymer materials expert, says, “A key feature of
Livermore’s SMP foam formulas is an open-cell structure, which makes the foam very porous and absorbent. We can make a foam plug that expands 80 to 90 times its compressed secondary shape.

**Foam Versus Platinum**

If Livermore’s foam-plug procedure is approved for clinical trials, it could lead to a new, nonsurgical treatment option for patients. Wilson is optimistic because the foam plugs offer several advantages over platinum coils, including faster and more complete occlusion of the aneurysm and lower and more uniform stresses to the aneurysm wall, thereby decreasing the risk of hemorrhage.

“A doctor may have to add 20 platinum coils, one at a time, to fill the volume of an aneurysm that would require only one or two foam plugs to fill,” says Maitland. “If the coils become compacted, the already vulnerable aneurysm wall may be reexposed to blood flow. We want to eliminate the need to treat an aneurysm more than once during a patient’s lifetime.”

The foam plugs may also prove safer than platinum coils, which can unravel and migrate into the blood vessel, potentially increasing the risk for aneurysm regrowth and rupture. “The foams are softer and have more tissuelike mechanical properties, so they are less likely to injure surrounding arterial tissue,” says Wilson. What’s more, each plug device can be customized to fit the distinct contours of the aneurysm being treated and is therefore more likely to stay in place.

In addition, unlike platinum coils, Livermore’s foam plugs could be made from bio-absorbable material, which could help to heal the aneurysm. “We hope to develop a foam plug that can biodegrade into small molecules and be safely absorbed,” says Wilson. “Over time, the device would essentially disappear and be replaced by human tissue.”
Chemistry and Dynamics

The Livermore SMP foam plugs are composed of four materials: hexamethylene diisocyanate; 2,2,4-trimethyl hexamethylene diisocyanate; 2-hydroxypropyl ethylenediamine; and triethanolamine. By adjusting the relative amounts of these materials, Wilson has developed three foam “recipes,” which respond to various ranges of temperatures.

The temperature at which a compressed foam plug resumes its primary shape is called the glass transition temperature \( T_g \). Foams with a low \( T_g \) expand to their primary shape when heated from a cooler temperature to below normal body temperature (37°C); foams with a mid-range \( T_g \) expand when heated to 45°C; and foams with a high-range \( T_g \) expand when heated to 60°C and above. Wilson can alter each recipe to allow for greater heating and cooling margins as necessary.

When the \( T_g \) of a foam plug is above normal body temperature, a laser or other heating mechanism is required to restore the foam’s primary shape.

The Livermore group is working with UC Berkeley to develop a measurement system that records aneurysm-wall temperatures during laser delivery of the implanted plug devices. The system will help researchers assess the effects on arteries from heating the foam plugs internally. “Foams with a transition temperature just above normal body temperature are optimal because they won’t require much additional heat to expand,” explains Wilson. “The goal is to reduce the foam’s transition temperature to minimize internal damage to tissue.”

Livermore mechanical engineer Jason Ortega is conducting computational fluid dynamics simulations, which will answer questions about the foam-plug implant procedure. Specifically, the simulations give researchers a look at the interaction of the foam plug with the artery wall. Ortega has modeled blood flow within a simulated aneurysm before, during, and after treatment with an SMP foam plug.

He has obtained detailed information about the velocity, pressure, and traction force that the fluid (blood) exerts on the adjacent artery wall. Ortega notes, “This type of high-resolution, instantaneous data cannot be obtained from current in vivo measurement techniques such as computerized axial tomography and magnetic resonance imaging.”

Wilson says, “The simulations give us information that would be experimentally difficult, time-consuming, and potentially impossible to obtain otherwise. They also help us address the concerns of grant reviewers, veterinarians, and physicians prior to beginning animal and clinical studies.” The simulations, in combination with animal testing, should help demonstrate that Livermore’s expandable foam technology is a better alternative to platinum coils.

Prototype Testing

Bioengineer Ward Small IV leads Livermore’s prototype-testing efforts. In a preliminary study, he used a silicone rubber model fabricated by the Engineering Technologies Division to simulate an aneurysm and the surrounding arrangement of blood vessels, or vasculature. (See the figure on p. 10.) Water was used to simulate the blood flow. Small was successful in deploying a single SMP foam plug to occupy a 11-millimeter aneurysm. His study also showed that varied flow rates affected foam-plug deployment. Low flow resulted in slow, full expansion with minimal temperature increase at the aneurysm wall, while high flow resulted in incomplete expansion. Future efforts are planned to resolve these expansion issues.

According to Maitland, the foam plugs will require modifications before they are ready for clinical trials. In particular, an effort is under way to design lower density foam plugs.
At this time, the foam plugs measure 1,800 micrometers in diameter when compressed to the secondary shape—too large to be delivered through a typical microcatheter with a diameter of 300 to 600 micrometers. If additional volume is removed (for example, from holes, dimples, and channels in the foam), Maitland says that foam devices capable of filling a 10-millimeter aneurysm could possibly be compressed to 500 micrometers in diameter without sacrificing clotting performance.

Small also tested a Livermore-developed stent and plug device designed to treat fusiform, or wide-neck, aneurysms. These aneurysms pose a problem for wire-coil and foam-plug treatments alike because the implanted devices can easily dislodge through the wide-neck openings. Small’s prototype consists of a stent, or tube, on which a foam plug has been grafted. After deploying the device into an in vitro aneurysm model, Small observed that the foam-plug portion of the device successfully expanded and filled the fusiform aneurysm, while the stent prevented the plug from migrating out of the aneurysm. At the same time, the stent maintained an open channel for fluid to flow in the blood vessel.

Wilson has also been working with researchers from UC Davis to test the biocompatibility of the SMP foams with pig and human blood. Both blood types were shown to be compatible with the foams.

**Years of Research**

The Livermore group was formed in 1996 to work with Micrus Endovascular Corporation, a U.S.-based neurointerventional device company. The purpose of this effort was to develop a device that could quickly release platinum coils inside an aneurysm and prevent a hemorrhagic stroke. The researchers created a device called an SMP microgripper, which was successful in clinical tests. In 1999, the group was one of 15 in the nation to receive an award that recognizes federal laboratory employees who have accomplished outstanding work in the process of transferring a technology to the commercial marketplace. It also received LDRD funding to continue working on applications for treating both hemorrhagic (aneurysm-induced) and ischemic (blood-clot-induced) strokes.

In 1999, while Maitland was using a plumber’s snake to unclog a drain in his house, he came up with an idea to develop a mechanism that could work similarly on blood clots in the brain. In 2000, he received a grant from the Department of Energy’s Office of Biological and Environmental Research to fund the research and development of a corkscrew wire made of SMP materials. This device for spearing a blood clot is designed to
enter the body through a catheter as a straight wire. The wire is then heated with a laser, which causes it to recoil. As the wire is withdrawn through the catheter, it “grips” the clot to remove it from the blood vessel. Tests showed the wire could hold a clot securely against a flow of liquid more than 10 times the blood pressure normally found in the brain. Maitland’s team successfully took the corkscrew through pilot animal studies and is currently developing an advanced version.

In 2002, the team shifted its focus from treating blood clots back to treating aneurysms when Wilson began developing SMP foams using commercial formulas. The National Institute of Biomedical Imaging and Bioengineering at NIH funded the initial research and development of these expandable foams in 2003. However, after two years of experimenting with commercial SMP formulas, the effort was abandoned in 2005 when Wilson and Livermore biomedical engineer Jane Bearinger began developing novel SMP formulas for bulk materials. A subset of these SMPs were then developed into foams that could expand 80 to 90 times their compressed volume—far exceeding the expandability limits of commercial formulas, which could only expand to 30 times their compressed volume.

Maitland points to the synergy between SMP foam research and homeland security, a major Livermore mission. “Our expertise in the fabrication of complex devices and in energy–materials interactions can transfer into biosecurity and sensor applications relating to nuclear weapons.”

**Shape-Changing Team Dynamics**

In 2008, the team received five years of NIH funding to test Livermore’s plug devices on animals at Texas A&M University. As a result, Wilson will continue leading the team’s research efforts.
Shape-Memory Polymers

Cerebral aneurysms are an undertreated medical problem. Our new foam technology has the potential to make dramatic gains in survivability and quality of life.

—Kristen Light

Key Words: aneurysm, embolic coiling, foam, hemorrhagic stroke, laser, shape-memory polymer (SMP).

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Lawrence Livermore National Laboratory
Using a three-dimensional (3D) model run on some of the fastest computers in the world, Laboratory astrophysicists have cracked a mystery of stellar evolution that has puzzled the astronomical community for nearly four decades. For years, physicists and astronomers theorized that low-mass stars (one to two times the mass of our Sun) produce great amounts of the helium-3 isotope. According to this theory, as these stars evolve, they eventually exhaust the hydrogen in their cores before violently igniting their helium-rich cores in a “helium flash.” That process, carried out by billions of stars over billions of years, should have resulted in an interstellar medium enriched with the light helium-3 isotope, adding to the helium-3 created during the big bang. Accepted calculations indicate that the big bang produced mostly hydrogen, mixed with about 0.001 percent helium-3 and 4 percent helium-4. Later, low-mass stars should have increased the helium-3 amount in the interstellar medium to 0.1 percent. But observations show that it remains at 0.001 percent, raising the question of where is the missing helium-3?

Using Djehuty, a Livermore-developed 3D astrophysics code, Laboratory scientists Peter Eggleton and David Dearborn uncovered a mixing mechanism that not only accounts for the mysteriously missing helium-3, but also could explain an equally mysterious overabundance of carbon-13. Eggleton and Dearborn’s discovery came out of a 3D-simulation study, supported in part by the Laboratory Directed and Research Development Program, exploring the helium flashes that occur when a low-mass star evolves into a red giant.

Flash Leads to Insight

A star that has a total mass equal to or less than the Sun will burn hydrogen at its core for nearly 10 billion years, turning that hydrogen into various isotopes of helium. When the hydrogen supply is exhausted, the core contracts, raising the star’s temperature and density to the point where the core begins to burn helium. This dense core, where the nuclear burning takes place, is surrounded by a large, low-mass convective envelope that is a mixture of hydrogen and the “missing” helium-3.

“In a helium flash, the star’s core ignites under high densities and temperatures,” explains Eggleton. “This ignition leads to more nuclear reactions in the core as the helium rapidly converts to carbon.” Most one-dimensional (1D) and two-dimensional (2D) simulations show that these reactions are plentiful and rapid enough to be explosive. “However,” says Eggleton, “the fact we observe stars that have passed through helium flashes indicates a flash is not extremely violent.”

Eggleton, Dearborn, and John Lattanzio from Australia’s Monash University decided the helium flash would be a good test problem for Djehuty, which simulates the evolution and structure of stars. Djehuty is designed for 3D stellar modeling on massively parallel supercomputers. (See S&TR, May 2002, pp. 4–10.) In general, astrophysicists depend on 1D and 2D codes for much of their stellar modeling. “Because a star is often assumed to be a sphere, what happens in one dimension along the radius should apply in all directions,” explains Dearborn. “For some conditions, that assumption holds. However, for unstable conditions in which material mixing occurs, we need a 3D code for our simulations.”

“When we looked at the helium flash evolving in three dimensions, we expected the simulation to show what has been

The most exciting phrase to hear in science, the one that heralds new discoveries, is not “Eureka!” but “That’s funny.”
—Isaac Asimov
observed: rapid expansion but no explosion,” says Eggleton. They ran the helium-flash simulation using up to 10 million mesh points with time steps corresponding to one-tenth of a second. The simulation ran on 351 processors and modeled reactions occurring over 10,000 seconds, which translates to modeling a little more than 2.5 hours in the life of a red giant star. This simulation took a few days to run on the Laboratory’s supercomputers.

While examining the results of the simulation—which did, indeed, show a rapid expansion with no explosion—Dearborn noticed something strange. “We saw an unexpected shell of matter deep inside the star, just outside the hydrogen-burning layer on top of the helium core,” says Dearborn. “None of our 1D or 2D models has shown this ring.”

“When he pointed the shell out, it was an ‘ah-ha’ moment for us both,” notes Eggleton. The shell is evidence of a molecular-weight inversion—a thin layer of helium-3—surrounding a lighter weight hydrogen layer. “This inversion set up a classic Rayleigh–Taylor situation,” explains Eggleton, “similar to trying to float water on top of oil. The heavier material on top of a lighter material created a very unstable situation. In a 2D or 3D simulation, we would expect the heavier elements to be driven to the core by the enormous pull of the star’s gravity—but that’s not what the simulation revealed.”

The 3D simulation showed that the burning shell of helium-3, just outside the lighter weight hydrogen layer, created a turbulent mixing motion, much like a stellar lava lamp. During this mixing process, bubbles of material substantially depleted in helium-3 float toward the surface of the star. Helium-3-enriched material from above the thin shell moves in the opposite direction, sinking farther into the core and then burning. In this reaction, two helium-3 atoms form a single helium-4 atom and two protons. Thus, the rapid mixing process effectively destroys helium-3 in the star, explaining why so little of this isotope appears in the material ejected during a helium flash. This mixing and burning process occurs on a very short time scale for stellar evolution: in a few hundred to a thousand years, compared with the tens to hundreds of millions of years it takes for a star with the mass of the Sun to evolve into a red giant.

The Carbon-13 Conundrum

The deep mixing that occurs inside low-mass stars as they evolve into red giants could also solve another astrophysical puzzle: the question of why so much carbon-13 is observed in these stars. “According to earlier theoretical models,” says Eggleton, “old, low-mass stars during their evolution into red giants should have increased amounts of carbon-13 in their spectra, on the order of two
to three times more. Yet, observations show that carbon-13 in these stars is commonly enriched by a factor of 10 to 20. This incongruity has perplexed scientists since it was first observed.”

Deep mixing uncovered in the Djehuty simulation offers an explanation for the discrepancy between theory and observation. When large reservoirs of burnt helium-3 (that is, protons and alpha particles) bubble upward and mix with the carbon-12 in the convective envelope, carbon-12 is mixed downward to the hot helium-3-burning layer. In this layer, the carbon-12 can be burned to carbon-13 and then mixed upward again. Eggleton says, “This deep mixing thus not only accounts for the ‘missing’ helium-3 but also could account for the overabundance of carbon-13. In a way, Djehuty has allowed us to deal a blow to two odd birds with a single stone.”

Robert Kraft, University of California (UC) at Santa Cruz professor emeritus and an expert in stellar abundances and evolution, agrees that the Djehuty 3D stellar modeling may help solve the carbon-13 mystery. “Many researchers are specifically looking at the stellar abundances of carbon-12 compared to carbon-13,” he explains. “Spectral observations are ongoing at the largest telescopes in the world, including UC’s Lick telescope, the 10-meter Keck telescope in Hawaii, and the European Southern telescope in Chile. We know from these observations that more carbon-13 exists than can be accounted for. The 3D modeling achievable with Djehuty may clear up this mystery.”

**Power of Three Dimensions**

Moving forward from this serendipitous discovery, Eggleton plans to tackle other thorny issues with Djehuty. His current project involves examining surface convection in low-mass stars. “With the resolution available on Livermore’s supercomputers, Djehuty can model the convection of a low-mass star but not of a star such as our Sun,” says Eggleton. “The Sun has a narrow but intense convection layer near the surface, requiring a much higher resolution.” Modeling the Sun’s convection layer would require a minimum of a hundred billion mesh points. Low-mass stars with their more spread-out convection layers require a billion mesh points, an amount achievable on Livermore’s supercomputers. “We’ll ‘see’ into the surface layers using Djehuty,” says Eggleton. “We can transfer this information to our 1D codes, which are much faster and require less computer power than the 3D Djehuty code. The end result will be more accurate 1D codes.”

Other projects Eggleton hopes to explore with Djehuty include investigating core convection in massive stars, with and without rotation; surface convection in a binary system of evolved red giants, where two stars are so close that they share a common surface layer but have separate cores; and various types of supernova explosions. “Who knows what wonderful discoveries we might find along the way,” says Eggleton.

—Ann Parker

**Key Words:** Djehuty code, helium-3, helium flash, stellar evolution.

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The hours are long, the weather can be harsh, and the commute may be lengthy. But the work is rewarding, the environment is dynamic, and the experience is one-of-a-kind. Welcome to being on assignment in Washington, DC.

Since the early 1990s, hundreds of Livermore scientists have accepted off-site assignments in Washington, DC, providing technical high-level support to federal agencies. Approximately 30 assignees are in Washington at any given time, serving in advisory roles at the Department of Energy (DOE), the Department of Defense (DoD), the Department of Homeland Security (DHS), in the intelligence community, in the White House, or on Capitol Hill. “Laboratory managers across the directorates and programs recognize Washington assignments as valuable to our institutional strategy as well as to the career growth of assignees,” says T. R. Koncher, head of the Laboratory’s off-site personnel program. Koncher, who is also deputy principal associate director for strategy and policy in the Global Security Principal Directorate and director of Livermore’s National Security Office, notes, “Assignments are not entry-level. Employees in their mid to late careers are needed for technically focused positions, and senior-level personnel are needed to lead organizations.”

Program participants say the world looks different from Washington. “One sees the bigger national security picture,” says Susan Hurd, a Laboratory employee currently on assignment at DoD. In addition, assignees learn about the workings of federal agencies and congressional committees, building programs, developing budgets, and communicating with Congress. Many assignees describe the environment as “intense” but consider the experience rewarding and beneficial to themselves, the sponsor, and the Laboratory.

From the Hill to the Pentagon

In most cases, off-site positions arise in response to a request from a federal agency. An individual is then selected for his or her related knowledge and experience. Assignments are generally processed as a change-of-station, a Laboratory policy that enables employees to move their residence and work location with minimal personal financial impact.

Many program participants are sent to Washington through Intergovernmental Personnel Agreements, which authorize Laboratory personnel to act as federal employees. Other assignees serve in advisory roles, without federal employee responsibilities or authorities. In either capacity, individuals are on assignment to fully support the agency.

Larry Ferderber, Livermore engineer and chief of staff for the Laboratory Director, is one of the few Laboratory employees who has worked in Congress. In 1993, Ferderber was selected to be an advisor to Nevada Senator and current Senate Majority Leader Harry Reid. As a result of the nuclear testing moratorium issued by President George H. W. Bush in 1992, the future of the Nevada Test Site was uncertain. Ferderber, then deputy associate director of nuclear test and experimental science, had the expertise to advise the senator on test site and other DOE-related issues.

According to Ferderber, “Working as a congressional advisor provides a unique perspective on what it is like to be an elected official and allows one to see the difference between technical and political decision making. One gains a much greater appreciation for what happens in Congress.”

Nancy Suski, deputy program director for domestic security in the Global Security Principal Directorate and two-time Washington
assignee, agrees, “In Washington, I developed a huge appreciation for the sponsor, what they have to deal with, and how responsive they must be to the political climate.” Suski’s first Washington assignment changed her career path. In 1992, she left her position as a project engineer at Livermore to establish and then run the Laboratory’s Washington-based uranium enrichment program office. “There was a lot of turmoil in DC at the time,” says Suski. “The White House was going through an administration change, and the Soviet Union had fallen the year before.” In addition, the United States Enrichment Corporation had recently been established with the goal of privatizing the government’s uranium enrichment operation for nuclear power plants. Suski’s experience working with Livermore’s Atomic Vapor Laser Isotope Separation—a uranium enrichment process that uses lasers—made her a perfect fit for the assignment. Four years later, she returned to the Laboratory as a program leader.

In January 2003, Suski again took a Washington assignment, this time through an Intergovernmental Personnel Agreement to help establish DHS. She was assigned to DHS’s Science and Technology Directorate as director of the portfolio for Emergency Preparedness and Response. Her responsibilities included assessing the needs and capabilities of first responders and developing ways to improve their emergency-response capabilities. This experience was very different from her first Washington assignment. During Suski’s second term, she worked in a federal capacity, justifying budgets, speaking to Congress about the portfolio, and dealing with controversies in the decision-making process. “Acting as a federal employee, I had to decide what is best for the federal government to support,” says Suski.

Suski is one of several Livermore employees who have worked in DHS. Mike Carter, deputy principal associate director for programs in the Global Security Principal Directorate, went to Washington in 2002 as a technical advisor for the White House Transition Planning Office to help establish DHS. He subsequently moved to DHS’s Science and Technology Directorate in March 2003.

In 2005, Carter was designated the deputy director of DHS’s Domestic Nuclear Detection Office, an interagency office that incorporates staff from DOE, DoD, Department of State, the National Regulatory Commission, and other DHS groups. In this assignment, he was routinely involved in the high-level interactions of DHS and the Office of Management and Budget. Carter recalls the time when he was asked to give a half-hour briefing about the Domestic Nuclear Detection Office to the new Secretary of Homeland Defense, Michael Chertoff. During the briefing, Secretary Chertoff unexpectedly asked Carter to give him a tutorial on the physics of nuclear detection.

Carter believes that spending time in Washington is essential training for future leaders of the Laboratory. “Building programs, developing budgets, and learning how priorities are set in DC made me more effective back at Livermore,” he says.

Laboratory assignees also help strengthen communication between national laboratories and Washington officials. Hurd believes one of her most important tasks is to help effectively present programs of Lawrence Livermore and other laboratories. Hurd has had the opportunity to take three assignments in Washington. She initially served as a scientific advisor in DoD’s Office of Nuclear Matters and was later recruited by the National Nuclear Security Administration, where she helped develop the strategy for transforming the nuclear weapons enterprise. For her third assignment, she returned to DoD, where she currently works for the Office of Strategic Warfare. “The work is hugely rewarding,” says Hurd. “Washington assignments provide a unique opportunity to serve the Laboratory, a federal organization, and the nation, all at the same time.”
In an effort to stay connected to Washington assignees, one or two Livermore managers, typically associate directors or principal associate directors, travel to Washington each quarter. “It’s part of good management to keep track of how the assignees are doing,” says Ferderber. In addition, some assignees periodically return to Livermore to take part in the Laboratory’s seminar, “The View from Washington,” where they describe their assignments and interact with colleagues.

Everybody Wins

“Off-site personnel assignments are an all-around good idea,” says Ferderber. “Each individual brings the skills, knowledge, and abilities to fulfill a particular sponsor’s needs. At the same time, the assignments afford personnel an opportunity to learn how government works, how decisions are made, and how information must be presented to be effective.” In addition, when assignees return to the Laboratory, they are valuable assets to programs because of their insight into the workings of federal agencies and congressional committees. “Personnel who have been on assignment in Washington have seen how government works and know how the Laboratory can better relate to the customer,” says Ferderber.

Off-site assignments do involve some sacrifice. Carter says, “The hardest part about working in Washington is juggling the family and the job.” Relocating across the country can be difficult for one person, but it is even more complicated when moving a family, especially when the family includes school-age children. The combination of family circumstances and the mental and physical demands of the job can make working in Washington a challenge.

Despite these personal obstacles, participants believe the experience is highly beneficial. “When the Laboratory has the right people, doing the right job, at the right time in Washington, it can develop solid programs that withstand the test of time and benefit the sponsor,” says Carter. In addition, employees who spend part of their careers in Washington often return to the Laboratory in higher-level positions.

As a telling example, in 1989, Livermore’s current Director, George Miller, was asked to go to Washington by DOE to work for Secretary of Energy Admiral James Watkins and with senior members of DOE’s defense programs. Miller says, “It was a rewarding experience in terms of making personal connections and being more closely exposed to the issues that affect the Laboratory. I strongly support having employees take a Washington assignment. These assignments are valuable to an individual’s career development and to the Laboratory.”

Overall, participants in the off-site personnel program understand the importance of what they do and how it benefits the nation. As Koncher says, “Having people in DC is important to the future of the Laboratory. Success of the program is really all about the people.”

—Caryn Meissner

Key Words: change-of-station; Intergovernmental Personnel Agreement; off-site assignment; Washington, DC.

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Each issue 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**

**Nanosensors Based on Functionalized Nanoparticles and Surface Enhanced Raman Scattering**
Chad E. Talley, Thomas R. Huser, Christopher W. Hollars, Stephen M. Lane, Joe H. Satcher, Jr., Bradley R. Hart, Ted A. Laurence
U.S. Patent 7,301,624 B2
November 27, 2007
Surface-enhanced Raman spectroscopy (SERS) is a vibrational spectroscopic technique that uses metal surfaces to enhance signals by several orders of magnitude. When molecules of interest are attached to designed metal nanoparticles, a SERS signal is attainable with single-molecule detection limits. This technique provides an ultrasensitive means of detecting molecules. With selective chemistries, metal nanoparticles can be functionalized to provide a unique signal on analyte binding. With measurement techniques, such as radiometric received SERS spectra, metal nanoparticles can be used to monitor dynamic processes and static binding events. Accordingly, nanoparticles can be designed as nanosensors for a wide range of chemicals in fluid, gaseous, and solid form; as environmental sensors for pH, ion concentration, and temperature; and as biological sensors for proteins, DNA, and RNA.

**High-Resolution Ophthalmic Imaging System**
Scot S. Olivier, Carmen J. Carrano
U.S. Patent 7,303,280 B2
December 4, 2007
This system produces a retinal image with improved resolution. An imaging camera captures the image. A computer system connected to the camera produces short exposures of the image and uses speckle processing to improve resolution.

**Nanostructured Materials for Hydrogen Storage**
Andrew J. Williamson, Fernando A. Reboredo
U.S. Patent 7,303,736 B2
December 4, 2007
This hydrogen storage system comprises hydrogen absorbed on the surfaces of porous nanostructured semiconductor material.

**UWB Communication Receiver Feedback Loop**
Alex Spiridon, Dave Benzel, Farid U. Dowla, Faranak Nekoogar, Erwin T. Rosenbury
U.S. Patent 7,305,052 B2
December 4, 2007
This system maximizes the extraction of information from reference pulses for ultrawideband (UWB) transmitted reference (TR) receivers. The system efficiently processes an incoming signal to suppress different types of UWB and non-UWB interference prior to signal detection. The system adds a feedback loop to enhance the signal-to-noise ratio of reference pulses in a conventional TR receiver. Sampling the second-order statistical function, such as the autocorrelation function (ACF) of the received signal, and matching it to the ACF samples of the original pulses for each transmitted bit, provides a more robust UWB communications system in the presence of channel distortions.

**High Resistivity Aluminum Antimonide Radiation Detector**
John W. Sheroehman, Arthur W. Coombs III, Jick H. Yee
U.S. Patent 7,309,393 B2
December 18, 2007
Bulk aluminum antimonide–based single-crystal materials have been prepared for use as ambient (room) temperature x- and gamma-ray radiation detection.

**Microelectromechanical Systems Contact Stress Sensor**
Jack Kotovsky
U.S. Patent 7,311,009 B2
December 25, 2007
This contact stress sensor includes a microelectromechanical silicon body. A recess is formed in the silicon body, and a silicon element extends into the recess. The silicon element has limited freedom of movement within the recess. An electrical circuit in the silicon element includes a piezoresistor material that allows for sensing changes in resistance proportional to bending of the silicon element.

**Deposition of Dopant Impurities and Pulsed Energy Drive-In**
Paul Wickboldt, Patrick M. Smith, Albert R. Ellingboe
U.S. Patent RE39,988 E
January 1, 2008
A semiconductor doping process enhances the dopant incorporation achievable using a gas-immersion laser. First, a thin layer of dopant atoms is deposited on a semiconductor surface. Then the surface is exposed to one or more pulses from either a laser or an ion beam. These pulses melt a portion of the semiconductor to a desired depth, thus causing the dopant atoms to be incorporated into the molten region. After the molten region recrystallizes, the dopant atoms are electrically active. Plasma-enhanced chemical vapor deposition or other known deposition techniques are used to deposit the dopant atoms.
Laboratory physicists Peter Celliers, Jim De Yoreo, and Denise Hinkel have been named Fellows of the American Physical Society (APS). The APS recognizes those who have made advances in knowledge through original research or significant innovative contributions in the application of physics to science and technology.

Celliers of the Science and Technology Principal Directorate was recognized for improving ways to measure shock waves used to study material states. He developed variations and improvements of existing diagnostic methods to make them work with laser-driven shock waves.

De Yoreo, now at Lawrence Berkeley National Laboratory, was honored for his work in biomineralization. His citation reads, “For his pioneering work using in situ force microscopy to understand the physical principles underlying biocrystallization, particularly the control of biomolecules and other modifiers on energy landscapes, step dynamics, and morphological evolution during crystal formation.”

Hinkel, who works in the Weapons and Complex Integration Principal Directorate, currently leads a simulation effort on beam propagation in ignition targets designed for the National Ignition Facility. She was cited for her extensive contributions to laser–plasma interaction physics and radiation hydrodynamic testing of inertial confinement fusion targets and to the fundamental physics of linear and nonlinear wave propagation in plasmas.

Diane Spencer, a safety analysis engineer in the Operations and Business Principal Directorate, has been named a Fellow of the American Institute of Chemical Engineers for her constant advocacy on behalf of her profession. Spencer has played an instrumental role in pulling together a support coalition for chemical engineers and now serves as a delegate for the California Legislative Council of Professional Engineers. She has spent time in Sacramento educating legislators about the profession and seeking changes in current laws that limit the role of chemical engineers in the state.

Lisa Poyneer of the Engineering Directorate received the Jain Prize from the University of California (UC) at Davis for her dissertation entitled, “Signal Processing for High-Precision Wavefront Control in Adaptive Optics,” which she completed in June 2007. The annual award recognizes the best Ph.D. dissertation in the UC Davis Electrical and Computer Engineering Department.

Poyneer joined the Laboratory in 2001 as a signal-processing engineer. She began her Ph.D. program through Livermore’s Education Assistance Program in 2003. Poyneer’s research, which focused on applying signal-processing techniques to adaptive optics, helped the Laboratory secure a $24 million contract to build the Gemini Planet Imager. The new techniques described in her dissertation will be used in that instrument.

Employees from several national laboratories, including Lawrence Livermore, have assisted Russian officials in developing a national accounting system for civilian nuclear material. Rose Babcock of the Global Security Principal Directorate was honored in February 2008 by the National Nuclear Security Administration for her role in helping “build a flexible and sustainable system and earning the respect of Russian counterparts.”

Babcock served as the project leader for the Federal Information System at Russia’s Federal Atomic Energy Agency for seven years. “We were able to establish a partnership through which the federal managers in Russia believe in the accounting system,” says Babcock. “The system has been successfully implemented and provides annual reports of the location and amount of civilian nuclear materials in Russia.”
**Shaping the Future of Aneurysm Treatments**

Laboratory scientists have created an expandable foam device that can be implanted in the brain to isolate an aneurysm and prevent it from rupturing and causing a stroke. These devices are made from Livermore-developed shape-memory polymers, which change size and shape in response to an external stimulus. Each foam device, or “plug,” is cut into a primary shape to match the contours of an aneurysm. The plug is then compressed into a smaller secondary shape so it can be maneuvered through a catheter into the brain and deposited inside the aneurysm. Once inside, it is heated with a diode laser, which causes the plug to expand back into its larger primary shape to fill the volume of the aneurysm. The plug absorbs the existing blood and blocks additional flow inside the aneurysm to prevent it from growing and possibly rupturing. Researchers are hopeful that the foam devices will be a safer, more efficient, and more cost-effective treatment option for people with life-threatening brain aneurysms.

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**Also in July/August**

- Laboratory scientists are designing the next generation of weapon sensors.

- Advanced antineutrino detectors help safeguard fissile materials created within a nuclear reactor’s core.

- Using computer simulations, researchers are interpreting results from Livermore experiments on membrane proteins and nanolipoprotein particles.