April 2007

Science & Technology

REVIEW

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Stardust Returns

Also in this issue:

- **Reviving Underground Coal Gasification**
- **Modeling Biological Fluid Flow**
- **Creation of Element 118**
- **Teller's Legacy in Computational Physics**

About the Cover

On January 15, 2006, the National Aeronautics and Space Administration's (NASA's) Stardust spacecraft sped close to Earth (front cover) and ejected its sample return capsule onto the Utah desert. Stardust is the first U.S. spacecraft to return solid space samples to Earth since the Apollo lunar missions. A collector filled with lightweight aerogel safely captured thousands of tiny particles as the spacecraft flew through the tail of the Comet Wild 2 (back cover). As the article on p. 4 describes, a 13-member Livermore team has been examining some of the particles with the world's most advanced analytic instruments. (Images courtesy of NASA.)

Cover design: Amy Henke

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on 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 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Science & Technology REVIEW

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Lawrence
Livermore
National
Laboratory

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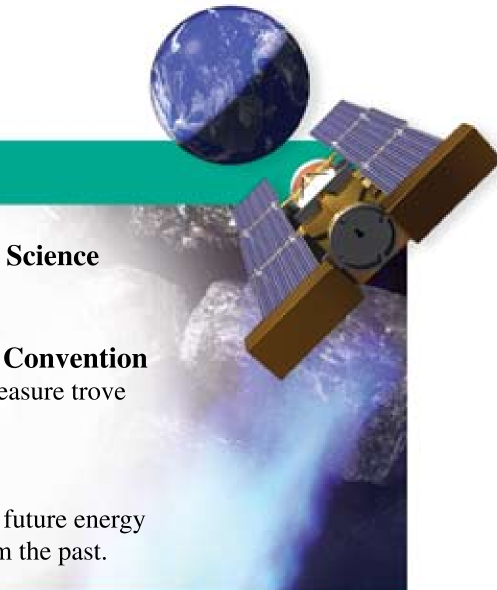

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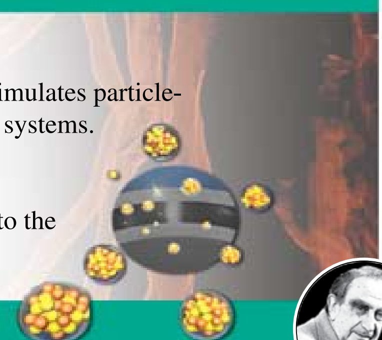

Teller Centennial Highlight

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New tracer better explains bone metabolism

Livermore researcher Darren Hillegonds and retired Laboratory scientist John Vogel of Livermore's Center for Accelerator Mass Spectrometry, with scientists from Belgium, Germany, and Switzerland, have successfully demonstrated that bone calcium can be labeled with the long-lived radioisotope calcium-41. In addition, they found that urinary calcium-41 excretion can be followed over periods of years using accelerator mass spectroscopy (AMS), the most sensitive technique for isotopic analysis at the ultratrace level. The research findings were published in the October 11, 2006, online version of *Analytical and Bioanalytical Chemistry*. The paper won the journal's Best Paper Award for 2006.

This new technique could be used in preventing and treating age-related osteoporosis, which has become a major public health concern because the mean life expectancy has increased three years per decade over the last century—a trend that seems set to continue. A more detailed understanding of calcium metabolism in bone would help to better define the diet and lifestyle strategies needed for osteoporosis prevention. At present, no methodologies allow direct measurement of small changes in bone metabolism with high sensitivity and on a short-term scale. These changes accumulate with time and may play a significant role in maintaining bone health.

For AMS calcium detection, bones are labeled with calcium-41, and bone metabolism is tracked by observing how much of the tracer is lost through urine over time. According to Hillegonds, even a small amount of tracer can sensitively monitor key aspects of bone health over a lifetime.

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Interatomic potential energy surface of bismuth mapped

Laboratory researcher Art Nelson and an international team of physicists have mapped the interatomic potential of crystallized bismuth when it approaches a solid–solid phase transition. The findings were a result of work performed at the Sub-Picosecond Pulse Source at the Stanford Linear Accelerator Center and appeared in the February 2, 2007, issue of *Science*.

Nelson's research experiments, which are supported by Livermore's Laboratory Directed Research and Development Program, are the first to combine the use of a high-brightness linear accelerator-based x-ray source with pulse-by-pulse timing reconstruction for femtosecond resolution. This approach allows for the first quantitative characterization of the interatomic potential energy surface of a highly excited solid. Intense femtosecond laser excitation can produce transient states of matter that would otherwise be inaccessible. At high excitation densities, the interatomic forces that bind solids and determine many of their properties can be significantly altered.

The availability of bright sources of ultrafast hard x rays, such as future free-electron lasers, opens the possibility to follow atomic motion with the spatial and temporal resolution required to study the fastest atomic vibrations and the making and breaking of chemical bonds.

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Shaking the Foundations of Solar-System Science

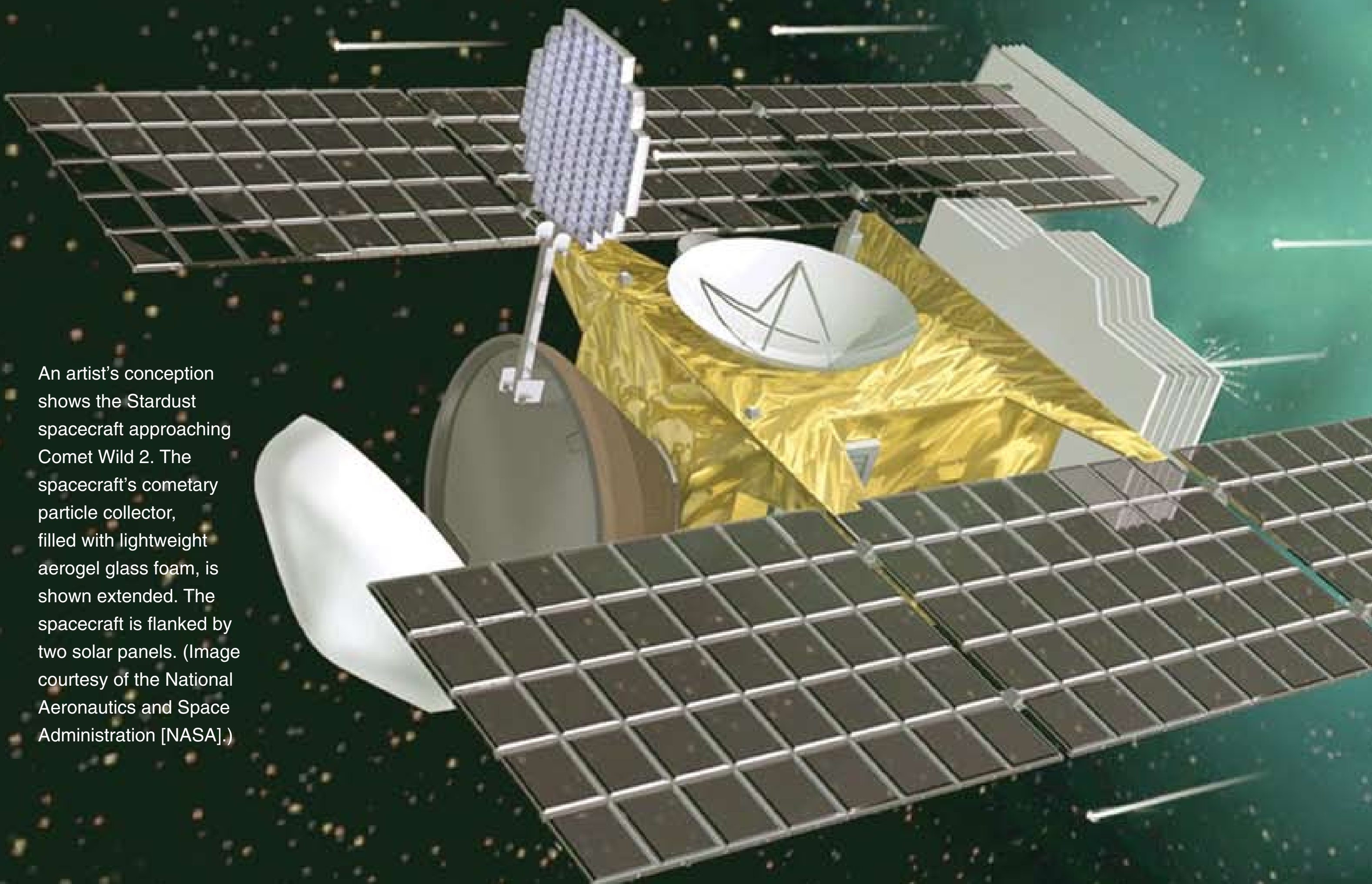
THE touchdown of Stardust in the Utah desert a little over a year ago, after a high-risk, high-velocity flyby of Comet Wild 2, completed the first U.S. sample return from space in more than 30 years. Since then, Stardust particles, mostly nanoscale flakes painstakingly harvested from the spacecraft's aerogel "catcher's mitt," have been analyzed with the world's most advanced analytic instruments at laboratories around the world, most notably here at Livermore. As described in the article beginning on p. 4, the initial results of peering for the first time back to the beginning of our solar system using bits of material carried by this periodic, cometary visitor have shaken the foundations of solar-system science. In December 2006, an entire issue of *Science* magazine was devoted to the findings.

For the National Aeronautics and Space Administration (NASA), it was a high-risk mission. A hit by a single centimeter-size comet particle during the encounter could have destroyed the spacecraft. In addition, debate existed about the use of low-density aerogel for capturing hypervelocity particles. Although similar material had been flown on the European Eureka spacecraft and on Russia's Mir Space Station to capture particles in low-Earth orbit, its efficacy for collecting comet dust was unknown. Even if individual comet grains could be collected in aerogel, it was unclear how they could be recovered. Debate also existed about the scientific significance of tiny, micrometer-size grains. Some among the "old guard" in planetary sciences worried that such samples would simply be too small to provide useful scientific information.

Immediately following the sample return capsule's successful touchdown, Livermore scientists were at Johnson Space Center applying techniques developed at the Laboratory to extract particles from the Stardust payload. Within two weeks, a powerful suite of analytic tools—many not even imagined when the mission launched in 1999—was being used at Livermore to recover the secrets of the early solar system locked away in the tiny particles of stardust. Among these unique tools—spread through the Physics and Advanced Technologies; Chemistry, Materials, and Life Sciences; and Energy and Environment directorates—are the world's most powerful scanning transmission electron microscope (called SuperSTEM), a nanoscale secondary-ion mass spectrometer (called NanoSIMS), a scanning electron microscope, a focused ion beam instrument, and a nuclear ion probe. Each of these tools represents a state-of-the-art Livermore capability; in combination, they have put the Laboratory squarely at the forefront of Stardust sample analysis work.

The Stardust mission has provided a spectacular opportunity for Lawrence Livermore to showcase its capabilities to a global audience. Laboratory staff was on the scene for the first inspection of the Stardust samples in clean rooms at the Curatorial Facility at Johnson Space Center. Livermore-developed technology was used to harvest some of the first comet samples from aerogel collection cells. NASA has recognized Livermore's unique environment and personnel by purchasing the newest advance in STEM instrumentation—the Titan microscope—for the Laboratory. Titan, representing the next generation of aberration-corrected electron microscopes, has already demonstrated subangstrom spatial resolution and 100-millielectronvolts energy resolution, another world-record feat for the Laboratory.

■ William H. Goldstein is associate director of Physics and Advanced Technologies.

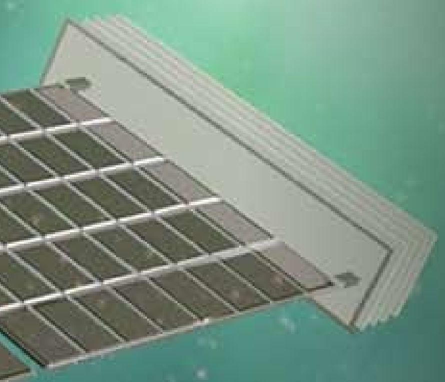


An artist's conception shows the Stardust spacecraft approaching Comet Wild 2. The spacecraft's cometary particle collector, filled with lightweight aerogel glass foam, is shown extended. The spacecraft is flanked by two solar panels. (Image courtesy of the National Aeronautics and Space Administration [NASA].)

Stardust Results Challenge

Astronomical Convention

A Livermore team has discovered plenty of surprises in the first samples captured from a comet.



FORMED in the frozen reaches of the solar system beyond the outer planets, comets have been considered the oldest, most primitive bodies in the solar system. They were thought to be composed of preserved interstellar particles from 4.6 billion years ago, when the Sun and the planets began to form from a primordial disk of dust and gas. However, the first-ever study of material retrieved from a comet is giving scientists, including a team of Lawrence Livermore researchers, new and sometimes startling insights into the makeup of comets and clues that the early solar system was far more active than previously believed.

The particles under intense study were captured in 2004, when the National Aeronautics and Space Administration's (NASA's) Stardust spacecraft flew through the tail of a comet called Wild 2 (pronounced "Vilt 2" after the name of its Swiss discoverer) as it neared the orbit of Mars. As Stardust approached the 4.5-kilometer-diameter comet, the spacecraft briefly extended a collector filled with lightweight aerogel glass foam to safely capture thousands of tiny particles. With its collector stowed, the spacecraft then sped close to Earth and on January 15, 2006, ejected its sample return capsule safely onto the Utah desert southwest of Salt Lake City.

Stardust, which is the first U.S. spacecraft to return solid space samples to Earth since the Apollo lunar missions, also collected dust from a flow of particles that pass through our solar system from interstellar space. Stardust's precious preserved cargo weighed less than 1 milligram; yet, this cometary material is providing more than enough samples to keep hundreds of investigators worldwide busy for decades to come.

The 13-member Livermore team, headed by physicist John Bradley, director of Livermore's Institute of Geophysics and Planetary Physics (IGPP), and Ian Hutcheon, deputy director of the Glenn T. Seaborg Institute, has been feverishly examining some of the particles since shortly after the sample return capsule parachuted to Earth. The team's preliminary data, together with those gathered by their colleagues, were presented in December 2006 at the American Geophysical Union's meeting in San Francisco, California. The results were simultaneously published in the December 15, 2006, issue of *Science*. Livermore researchers were coauthors

John Bradley gives the thumbs-up sign after scientists opened the Stardust sample return capsule in the clean room facility at NASA's Johnson Space Center. In the background, researchers photograph the particle collector filled with aerogel cells that trapped tiny cometary particles.

on all seven *Science* papers detailing the first findings.

The Livermore team includes Giles Graham, Hope Ishii, Zurong Dai, Saša Bajt, Patrick G. Grant, Jerome Aleon (now at Centre de Spectrometrie Nucleaire et de Spectrometrie de Masse in France), Alice Toppani (now at Centre National de la Recherche Scientifique in France), Peter Weber, Stewart Fallon (now at Australian National University), Nick Teslich, and Miaofang Chi. The researchers are from Livermore's Physics and Advanced Technologies; Chemistry, Materials, and Life Sciences (CMLS); and Energy and Environment directorates. The Livermore work is part of the Bay Area Particle Analysis Consortium (BayPAC) established in 2003 to maximize the strengths of San Francisco Bay Area research facilities for examining Stardust particles. BayPAC was recently expanded into the West Coast Consortium with the inclusion of the University of California (UC) at Los Angeles and the University of Washington. Other members include NASA/Ames Research Center, UC Berkeley, Lawrence Berkeley National Laboratory, Stanford Linear Accelerator Center, and UC Davis.

Researchers have long wanted to study cometary samples and determine their chemistry, mineralogy, crystal structure, and trace-element and isotope compositions. The analyses by Livermore and other scientists are providing important new data about the formation of the solar system as well as comets. Preliminary studies show that Comet Wild 2 contains an impressive assortment of materials, many unexpected. In particular, the comet contains an abundance of high-temperature minerals that appear to have formed in the inner regions of the solar nebula. Their unexpected presence strongly suggests that the formation of the solar system included mixing over radial distances much greater than has been generally accepted by scientists in the past.

In the early 1990s, with funding from NASA and the Jet Propulsion Laboratory

The Stardust Mission

The Stardust spacecraft was launched February 7, 1999, embarking on a flight path of three giant loops around the Sun. On January 2, 2004, the spacecraft met Comet Wild 2 beyond the orbit of Mars. While flying through the dust cloud surrounding Wild 2, the spacecraft flipped open a tennis racket–shaped collector that was stashed inside the protective sample return capsule.

The particles impacted the collector at about 6.1 kilometers per second (six times faster than a bullet fired from a gun), but the collector's aerogel cells cushioned their impact and lessened the damage. The spacecraft also recorded in-flight data with its mass spectrometer and particle counter and took detailed pictures of Wild 2's surface, the best photos ever taken of a comet nucleus. The collector then folded down into the capsule, which enclosed the samples for safe delivery to Earth.

The collector had two nearly identical sides. One side of the collector faced toward the particles streaming off Wild 2 in 2004, while the reverse side, with a second set of aerogel cells, was turned earlier to face the streams of smaller interstellar dust particles encountered from March through May 2000.

Comets are relatively small, irregularly shaped bodies that spend most of their existence in the outer reaches of the Sun's influence, which is why so much of their original material is well preserved. When a comet approaches within about 700 million kilometers of the Sun, material on the comet's nucleus heats and begins to vaporize. This phenomenon creates a cloud of dust and ionized gas called the coma and a tail of gases that flows millions of kilometers beyond the nucleus.

Wild 2's nucleus, which measures about 4.5 kilometers in diameter, was probably formed in the Kuiper Belt, far beyond Neptune. Over many millions of years, the comet slowly ventured into the inner solar system, where it had a close encounter with Jupiter in 1974. This encounter placed the comet in its current orbit between Mars and Jupiter, making it an ideal candidate for a National Aeronautics and Space Administration (NASA) mission. Because Wild 2 has not traveled close to the Sun for long, its composition has not changed substantially since its formation billions of years ago.

The Stardust spacecraft is currently orbiting the Sun. NASA is considering a proposal that the spacecraft be sent to fly by Comet Tempel I. In 2005, another NASA spacecraft, Deep Impact, launched an impactor that struck Tempel I and revealed its inner nucleus. With the prospect of visits by future missions, comets will continue to help unravel secrets of the solar system.

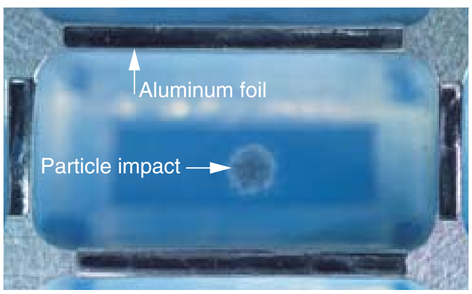
This image of Comet Wild 2 was taken by NASA's Stardust spacecraft on January 2, 2004. The nucleus of the comet (shown here) without its million-kilometer-long tail measures about 4.5 kilometers in diameter. (Image courtesy of NASA/ Jet Propulsion Laboratory– California Institute of Technology [JPL–Caltech].)

(JPL), which manages the Stardust mission, Livermore scientists from the CMLS Directorate developed methods to produce the ultralow-density silica aerogel for Stardust. For more than two decades, Livermore researchers have pioneered the formulation and application of silica aerogels, an extremely lightweight glassy material with ideal mechanical characteristics for capturing ultrafast particles.

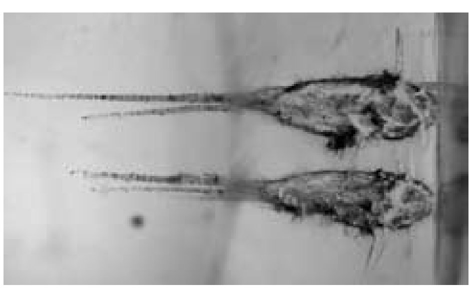
In the late 1990s, physicist Dai, while still at Georgia Institute of Technology, and Bradley used electron microscopes to image interplanetary dust particles captured in Earth's stratosphere by NASA's ER-2 aircraft. At Livermore, Bradley was the principal investigator for a Laboratory Directed Research and Development–funded project to develop technologies for analyzing cometary material from aerogels. As part of this effort, physicist Bajt developed new techniques to characterize particles captured in the stratosphere as well as particles collected by the NASA Orbital Debris Collection Experiment from Russia's Mir Space Station. At the same time, physicist Graham was working with a group in the United Kingdom to conduct experiments that would examine the tracks formed by simulated cometary particles fired at ultrahigh speeds into aerogels.

Working at Johnson Space Center

Livermore researchers were on hand when the sample return capsule arrived at NASA's Johnson Space Center in Houston. The sample tray with aerogel cells was opened in a clean room similar to that used in the semiconductor industry. The 132 aerogel cells, each measuring 2 by 4 by 3 centimeters and mounted in an aluminum structure, appeared largely intact. In fact, so pristine was the collector's appearance, more than one observer worried that it might not have deployed. On closer observation, the researchers made out hundreds of particle impact tracks within each cell. The particles fragmented extensively as they traveled into the aerogel. The tracks measured up to 2 centimeters long, and up to half a centimeter in diameter, and each one contained dozens of tiny particle fragments. Most were smaller than 10 micrometers in diameter, but the largest was visible to the naked eye. Many particles were captured in good condition, although some were coated with a thin layer of melted aerogel.



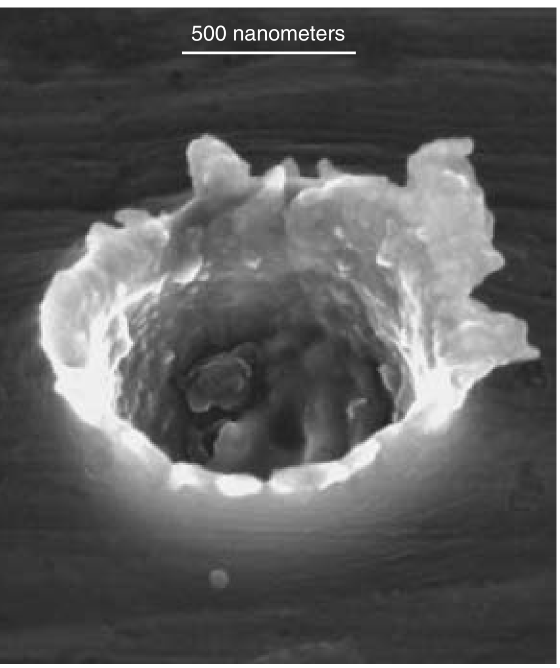
A close-up view shows a trapped cometary particle in an aerogel cell shortly after Stardust's sample return capsule was opened. Also visible is aluminum foil wrapped around the collector grid walls. (Image courtesy of NASA/JPL–Caltech.)



A photo shows tracks left by two cometary particles trapped by aerogel in the collector grid as they entered from the right. The tracks are magnified several hundred times. (Image courtesy of NASA/JPL–Caltech.)

During a heavily attended press conference at Lawrence Livermore, materials scientist Hope Ishii shows reporters a recently returned sample of aerogel containing cometary particles. The plastic barrier protects the sample from contamination.

Livermore played a major role in developing particle extraction technologies adopted by NASA. At the Johnson Space Center, IGPP personnel assisted in some of the first extractions using a tiny knife developed by Ishii, a materials scientist. The knife has a diamond blade that vibrates at ultrasonic frequency to make smooth cuts in aerogel, a difficult task because the brittle material is prone to breaking. The ultrasonic knife is one of several aerogel cutting tools developed to extract cometary particles at the center. Microneedles were also used to extract wedge-shaped aerogel slices called keystones. Each keystone contained an intact particle track. A silicon "microfork" was then used to remove the keystones for further analysis. Both the microneedles and microfork were developed at UC Berkeley.



A scanning electron microscope image shows an impact crater preserved on the surface of a foil.

Many keystones and some of the extracted individual cometary particles were embedded in epoxy, then cut into extremely thin sections with an ultramicrotome stationary diamond blade. Bradley pioneered the use of ultramicrotomy for sectioning extraterrestrial particles in the mid-1980s. Both keystones and isolated particles were distributed to Livermore and other research laboratories around the world. As part of the Stardust Preliminary Examination, samples are often forwarded from one research center to another. For example, the Livermore team has received samples from several centers with the request that Laboratory researchers corroborate or amplify findings.

Some Wild 2 particles were also caught in the high-purity aluminum foils that wrapped around the particle collector's aluminum structure and provided additional security for the aerogel cells. The impacts on the foils produced bowl-shaped craters lined with particles. Graham and Teslich were among the first scientists to detect the craters containing miniscule particles in the collector foils. They used Livermore's focused ion beam to mill away small areas of foil and cut out particle cross sections.

"We thought all the particles caught in the foils would be melted on impact, but some appear to have survived relatively intact," says Graham. "They are proving as important as those caught in the aerogel cells." He notes that particles caught in the foils are localized in the minuscule craters, whereas particles caught in the aerogel cells are arrayed along a track. As a result, the foil-trapped particles are more easily accessed than the particles embedded in aerogel. The foil-trapped particles also are not exposed to contamination from the silicon and oxygen in the melted aerogel.

Advanced Instruments Put to Work

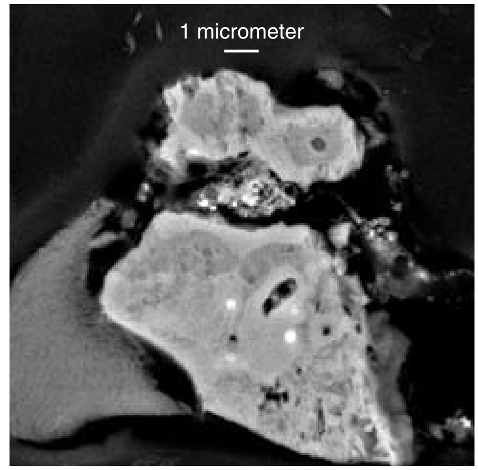
Livermore scientists are characterizing particles extracted from both aerogel and foil with highly specialized instruments such as the super scanning transmission electron microscope (SuperSTEM), nanometer-scale secondary-ion mass spectrometer (NanoSIMS), scanning electron microscope (SEM), and nuclear microprobe. The ability to carry out correlated studies on individual micrometer-size grains using multiple analytic tools is a unique strength of the Livermore team. The researchers also use the infrared microspectroscopy beam line at the Advanced Light Source at Lawrence Berkeley and the x-ray microprobe at the Stanford Synchrotron Radiation Laboratory, a part of the Stanford Linear Accelerator Center.

The highest spatial resolution work is being done using SuperSTEM, the world's most powerful electron microscope. SuperSTEM allows atomic-scale analyses of a particle's composition and produces stunning pictures magnified several million times. The machine has ancillary equipment that corrects images for blurring, yielding striking pictures of a mineral's crystalline structure. "SuperSTEM is invaluable because some of the most significant information contained in the Stardust samples is at the atomic scale," says Bradley.

"We see an extensive variation both from particle to particle and from area to area within each particle on SuperSTEM," says Dai. "In particular, we are seeing many silicate minerals."

Work on SuperSTEM is complemented with a new field-emission SEM, which produces images at magnifications up to about 1 million times. Electrons pass through the sample with SuperSTEM but bounce off the sample with field-emission SEM, yielding different but just as

Zurong Dai uses a transmission electron microscope to take close-up images of cometary dust particles extracted from the aerogel cells.



A scanning electron microscope image shows a calcium aluminum-rich inclusion particle found in a Stardust sample. The particle is made up of several high-temperature minerals. The contrast in the image is caused by differences in atomic weight of the atoms present. Some aerogel is adhered to the particle on the lower left corner.

valuable images. According to Hutcheon, who is chief scientist for Livermore's Forensic Science Center, the SEM is a valuable complement to SuperSTEM because it enables visualization of textural relationships between different minerals.

NanoSIMS is used for the chemical and isotopic analysis of extremely small volumes of material. The machine examines material a few micrometers in diameter and 1 to 2 micrometers in depth. It uses an ion beam (typically oxygen or cesium) to produce plasma of the target material. (See *S&TR*, January/February 2007, pp. 12–20.) Determining the isotope ratios of several key elements has been critical for proving that many of Wild 2's minerals were created close to the Sun.

Ishii is using the x-ray microprobe at the Stanford Synchrotron Radiation Laboratory for generating extremely bright x rays to map the distribution of elements along intact tracks cut out of an aerogel cell. These data contribute to bulk composition estimates for Comet Wild 2 as well as guide future studies on a given impact track. Entire tracks are also analyzed at Livermore's Center for Accelerator Mass Spectrometry. At the center, chemist Grant examines tracks with a nuclear microprobe, which uses a proton beam. Other analysis techniques include scanning transmission ion microscopy, proton elastic scattering, proton backscattering, and proton-induced x-ray emission. Together, these techniques enable Grant to measure the total mass of the particles as well as the elements contained in the particles and tracks.

Bajt uses the Advanced Light Source's infrared microspectroscope to analyze the same small, thin sections required by SuperSTEM as well as entire keystones. The technique uses an intense infrared beam from the synchrotron.

Full of Surprises

"The particles are full of surprises," says Bradley. "They are a remarkable mixture of materials. The biggest surprise is that although comets were formed a long distance from the Sun, far beyond the orbit of Neptune, Wild 2 appears to be full of material from the inner solar system and from close to the Sun. These findings are not what we expected." Extraterrestrial dust particles previously collected in the stratosphere were thought to mostly consist of particles from comets. However, says Bradley, "Wild 2 particles don't look anything like the particles we have captured in the upper atmosphere and have believed to be cometary in origin. In this case, we're seeing large variations from particle to particle."

Another surprise is the scarcity of presolar material, the tiny interstellar grains produced around other stars that existed before the Sun and solar system formed. Except for a single 250-nanometer-diameter grain highly enriched in oxygen-17, the mineral grains have isotopic compositions similar to typical solar system material. However, Wild 2 is full of complex minerals, many of which form only at very high temperatures, presumably near the Sun. For example, a calcium aluminum–rich inclusion has been identified. This inclusion is believed to have been created in the hottest, innermost regions of the gas and dust disk that formed the Sun and planets. Calcium aluminum–rich inclusions are also found in meteorites formed in the asteroid belt. "Calcium aluminum–rich inclusions shouldn't be there," says Hutcheon. "They are the last thing we expected to find." The Livermore team, using the field-emission SEM, provided NASA with a rigorous characterization of the inclusion.

Other high-temperature minerals include olivine and pyroxene (magnesium iron silicates), both associated with igneous rocks on Earth. Olivine is the primary component of the green sand found on some Hawaiian beaches and is among the most common crystalline minerals in the galaxy.

Miaofang Chi, a Student Employee Graduate Research Fellowship participant from UC Davis, performed much of the work using SuperSTEM on the calcium aluminum–rich inclusions to identify osbornite (titanium nitride). "Osbornite is a mineral that forms at about 3,000 kelvins, which means it formed close to the hot, infant Sun," says Chi.

Wild 2's high-temperature minerals were apparently transported from near the Sun to the outer regions of the solar system by a process capable of moving particles at least as large as 20 micrometers, the size of some of the mineral inclusions. The inescapable conclusion is that vastly more mixing of material occurred while the Sun and planets were forming than scientists expected. "The conventional thinking was that the formation of the solar system as we know it was a rather quiet, orderly process," says Ishii. "However, it now appears that the early solar system was a much more dynamic and violent environment than we thought."

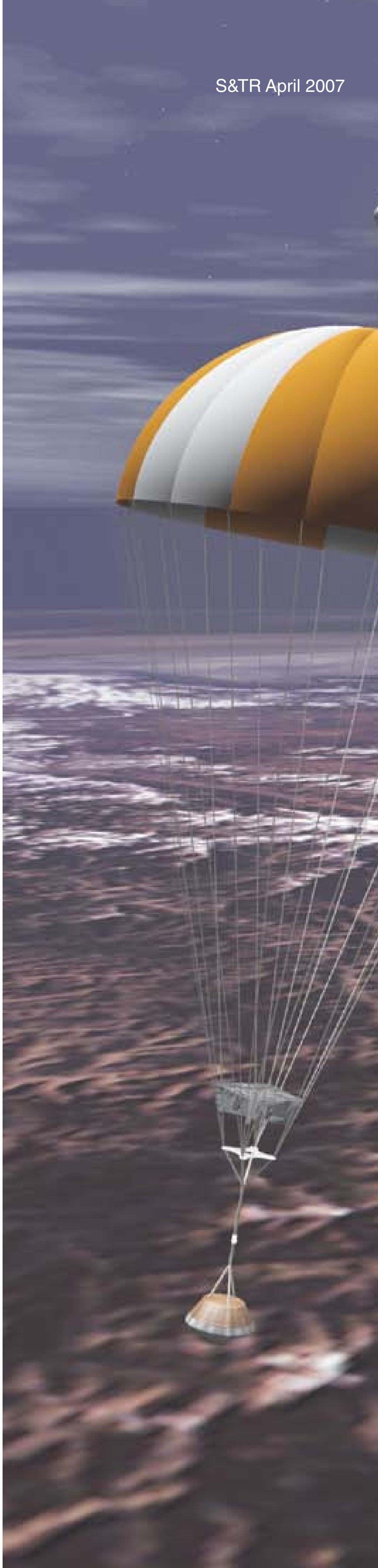
The discovery of high-temperature (refractory) minerals supports the theory proposed in the 1990s that large particles could have been transported by the so-called X-wind from a region surrounding the young Sun. The wind supposedly flowed perpendicular to the disk of hot dust and gas forming the Sun and planets and shot material out hundreds of millions of kilometers in an X shape. Some of the material in the X-wind may have rained into the comet-forming region where it was incorporated into Comet Wild 2.

Rich Diversity of Carbon Compounds

Many of the particles studied thus far contain organic compounds that are surprisingly diverse. The presence of organic compounds in comets is of interest to astrobiologists because the organic precursors of life on Earth may have come from a comet.

Using an infrared microscope at the Advanced Light Source, Bajt detected carbon-rich materials and was the first to chart the distribution of organic compounds along aerogel tracks in a keystone. "Infrared is especially sensitive to organic molecules," Bajt says. "We didn't expect organics to survive the impact with the aerogel during the collection process." However, she found more diversity of organic compounds that were both oxygen- and nitrogen-rich compared with organics identified on the flyby of the Halley Comet, which had an onboard mass spectrometer. Many organic compounds volatilized during impact and diffused into the surrounding aerogel, where they remain.

The comet's organic materials might be more primitive than those seen in meteorites and might have formed in clouds between the stars or in the disk-shaped cloud of gas and dust from which our solar system formed. They may represent a new class of organic compounds not previously observed in other extraterrestrial samples,



Stardust's sample return capsule parachutes to Earth. (Image courtesy of NASA.)

including meteorites and interstellar dust particles.

Bajt notes that infrared spectroscopy allows scientists to image objects exactly as astronomers see them. In this way, her research provides "ground truth" for images of comets, such as Wild 2, taken with infrared terrestrial and space telescopes. Distinguishing carbon contaminants from cometary materials is also important. For example, aerogel consists predominantly of silicon dioxide but also contains a small amount of carbon. However, aerogel carbon is in the form of simple silicon-methyl groups, which are different from the organic compounds found on Wild 2.

Future Plans Look Bright

More than 90 percent of the collected matter remains locked in the aerogel and aluminum foils, archived at Johnson Space Center and stored in dry nitrogen for future researchers. The Livermore team is preparing a second set of papers for publication that will have more detailed results than the initial results published in *Science*.

When the spacecraft was launched in 2004, many of the analytic techniques being used to examine Wild 2 particles didn't exist. "We expect new techniques to come along over the next few years that will provide important additional information," Bradley says. As data accumulate, the results will permit a thorough comparison with samples from asteroids, believed to have been formed in the warmer, inner regions of the solar system, and with interplanetary dust collected from Earth's stratosphere.

The Livermore team is looking forward to analyzing interstellar particles, which were collected by less-dense aerogel cells on Stardust than those that collected Wild 2 particles. In the meantime, an online project called Stardust@Home (http://stardustathome.ssl.berkeley.edu) gives members of the public the opportunity to examine close-up images of the aerogel cells for signs of the dust trails left by interstellar particles, which are smaller than those from Wild 2.

The advanced techniques applied to the Stardust samples have direct benefits to many Livermore programs. For example, the ultrasonic diamond-blade technology developed by Ishii has potential application to other Livermore programs that use aerogels in experiments. In addition, the techniques used to investigate Stardust samples are used to interrogate interdicted materials for nuclear forensic science in support of nonproliferation and national security. Increased expertise with the analytic instruments aids both causes. Bradley says, "The work has been a great example of collaboration across directorates at the Laboratory and has nicely showcased Livermore's superb analytic capabilities. In addition, our Stardust effort has attracted many outstanding young scientists to Livermore who are excited by the rare opportunity to do research on extraterrestrial matter with world-class equipment."

"The Stardust mission has been a stunning success, far exceeding even our most optimistic expectations," Bradley says. Adds Ishii, "This is the opportunity of a lifetime."

—Arnie Heller

Key Words: Advanced Light Source, aerogel, Bay Area Particle Analysis Consortium (BayPAC), Center for Accelerator Mass Spectrometry, Comet Wild 2, Institute of Geophysics and Planetary Physics (IGPP), nanometer-scale secondary-ion mass spectrometer (NanoSIMS), scanning electron microscope (SEM), Stanford Synchrotron Radiation Laboratory, Stardust spacecraft, super scanning transmission electron microscope (SuperSTEM), X-wind.

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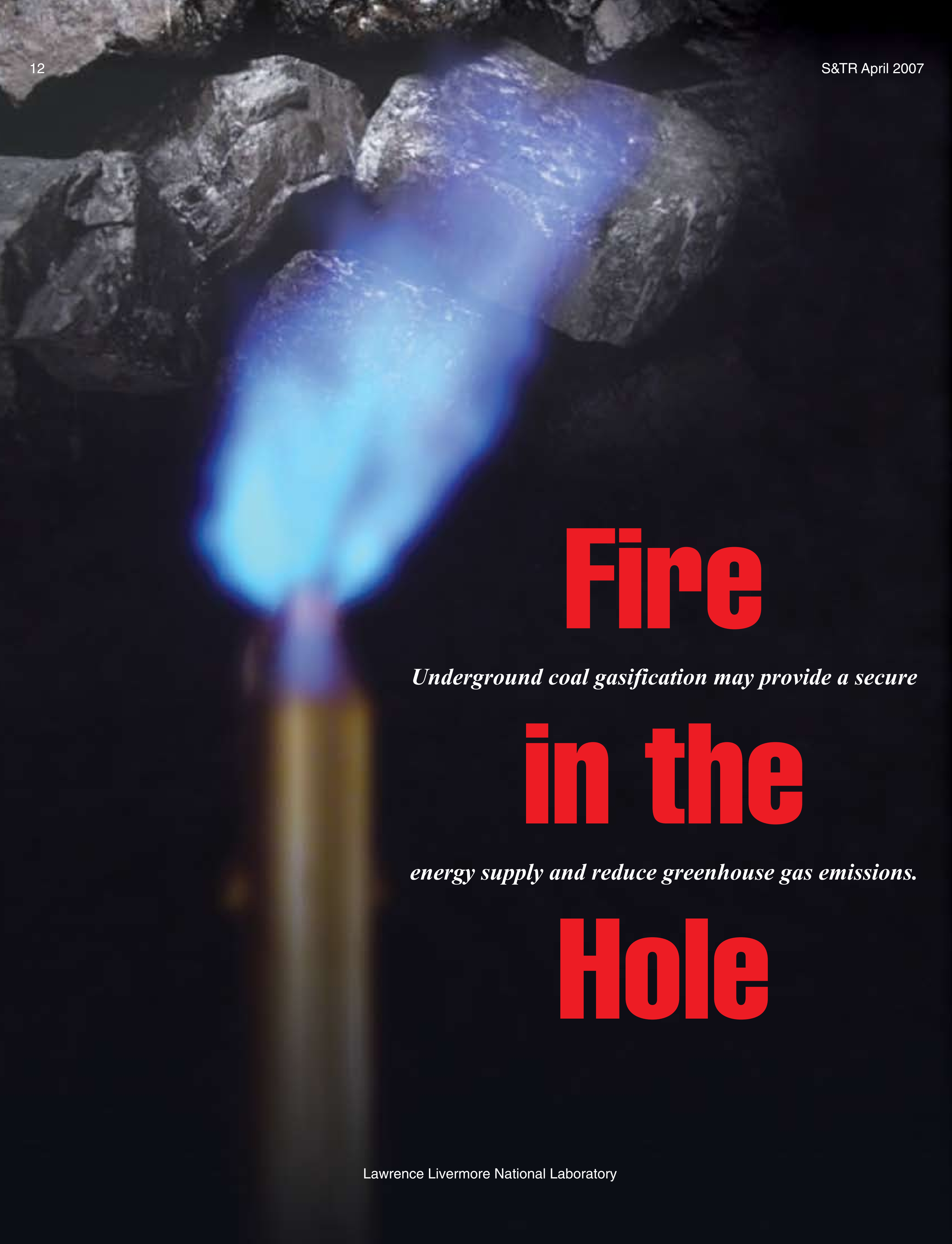


Fire in the Hole

Underground coal gasification may provide a secure energy supply and reduce greenhouse gas emissions.

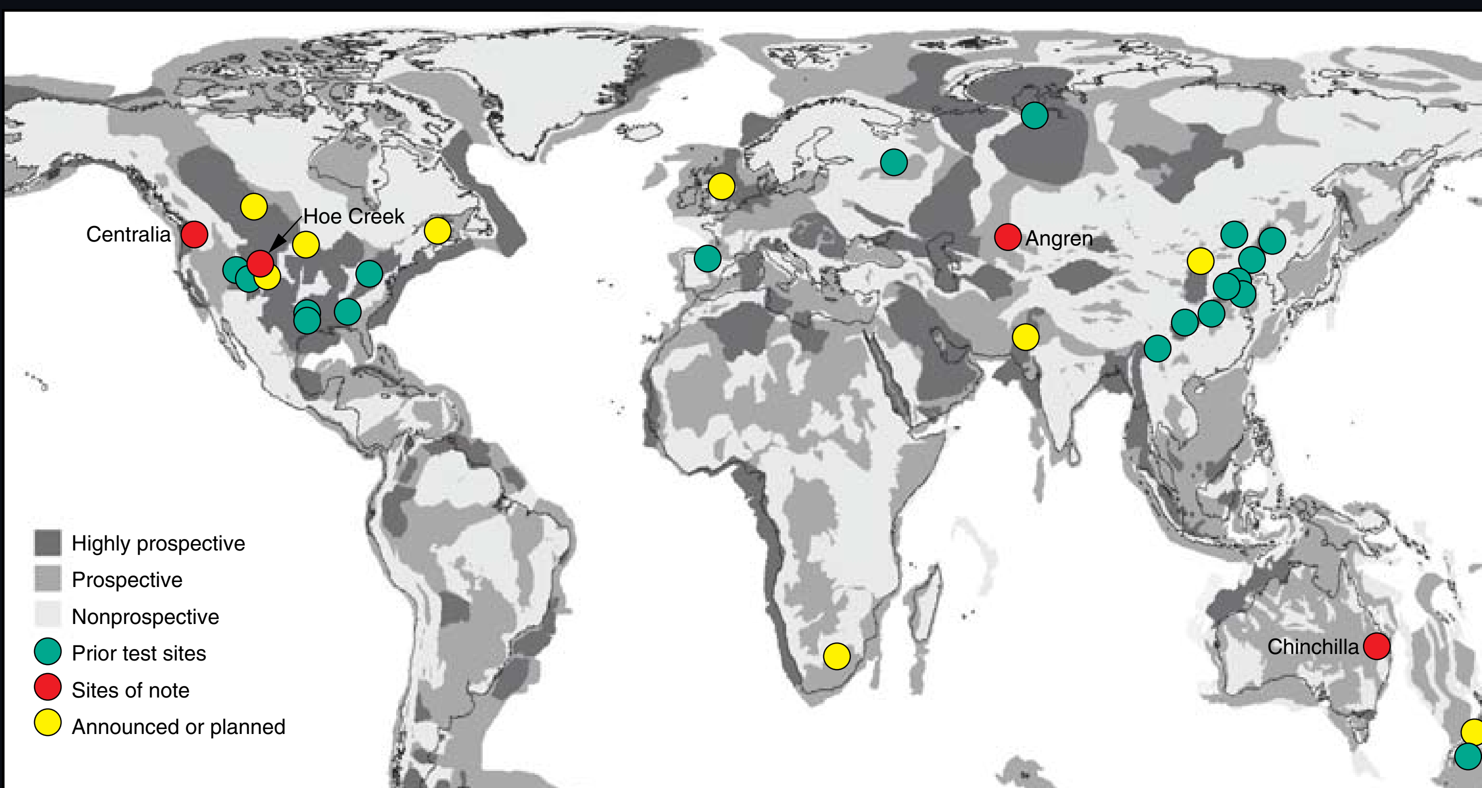
WORLDWIDE coal reserves are vast, over 10 trillion metric tons, but unless cleaner and cheaper ways can be found to convert coal to gas or liquid fuels, coal is unlikely to become an acceptable replacement for dwindling and uncertain supplies of oil and natural gas. Mining coal is dangerous work, coal is dirty to burn, and much of the coal in the ground is too deep or too low in quality to be mined economically. Today, less than one-sixth of the world's coal is economically accessible. However, Livermore is helping to revive an old technology that offers promise to substantially increase usable coal reserves and make coal a clean and economic alternative fuel. Known as underground coal gasification (UCG), this technology converts coal to a combustible gas underground.

In the early years of UCG, the technology gained an "ugly duckling" reputation in the U.S. The UCG process yielded gas of low heating quality with too much hydrogen, and it was considered an environmental risk. But as coal-rich countries now look to replace imported oil with secure domestic energy sources, make hydrogen fuels, and find ways to limit their greenhouse gas emissions, they are rediscovering the potential of UCG.

In the U.S., coal supplies about 50 percent of this country's electricity because it is the least expensive energy source. Coal can be gasified or liquefied to make transportation fuels, natural gas, or chemical feedstocks. Today, the U.S. has only one operating coal gasification plant and no commercial liquefaction operations. However, because of the nation's goal to produce secure and clean energy from its domestic coal reserves, coal-to-gas and coal-to-liquid conversions may become commonplace.

Applying improved UCG technology to gasify deep, thin, and low-grade coal seams could vastly increase the amount of exploitable reserves. The coal could be converted to gas for a variety of uses, and emissions of sulfur, nitrous oxides, and mercury could be dramatically reduced. "UCG could increase recoverable coal reserves in the U.S. by as much as 300 to 400 percent," says Julio Friedmann, who leads Livermore's Carbon Management Program. Another benefit of UCG is that hydrogen accounts for half the total gas product.

As with any hydrocarbon combustion process, UCG generates carbon dioxide



This map shows underground coal gasification (UCG) sites worldwide, including planned sites and prior pilot test sites. The sites of note are Centralia, Washington, and Hoe Creek, Wyoming, which are two Lawrence Livermore test sites; Chinchilla, Australia, where the longest pilot in the Western world was recently completed; and Angren, Uzbekistan, where a commercial UCG plant has operated for 50 years. The underlying gray shading shows potential areas for geologic carbon storage.

(CO_2), a greenhouse gas. Fortunately, potential sites for UCG operations correspond to locations where sites are plentiful for sequestering CO_2 in geologic formations underground. UCG also enhances the storage capacity of the coal seam itself to store injected CO_2. The generated gas, called syngas, would be taken from the ground and the by-products separated out. The CO_2 would then be returned downhole nearby.

Ups and Downs of UCG

The idea for coal gasification, either underground or in aboveground plants using mined coal, has been around for more than 150 years. The technology was first widely used in the U.S. during the late 1800s. Lamplighters made their rounds in many of our largest cities lighting streetlights fueled by "town gas," the product of early and relatively crude forms of coal gasification. Once vast fields of natural gas were discovered and pipelines built to transport the gas to consumers, the use of town gas disappeared.

From the 1930s through the 1990s, the former Soviet Union invested in developing UCG technology at numerous sites and was successful at the commercial scale in several locations. China has been developing the technology since the 1980s and currently has the largest operational UCG program. Their approach uses abandoned tunnels in conventional mines.

During the energy crisis of the 1970s, U.S. interest spiked in all forms of alternative energy, and the Department of Energy (DOE) invested billions of dollars to develop efficient coal-gasification technologies for power generation. Over 30 UCG pilot tests were run across the U.S. At that time, the hydrogen by-product of UCG was viewed as a liability, reducing the perceived quality of the gas. In addition, groundwater-contamination problems resulted at two sites.

The Laboratory, a pioneer in the study of UCG, developed two test sites—one in Centralia, Washington, and the other in Hoe Creek, Wyoming. Livermore researchers also patented a UCG process called Controlled Retraction Ignition Point, which was used in pilot tests performed in Europe during the 1990s. In the U.S., when gas and oil prices dropped in the 1980s and 1990s, efforts to commercialize UCG came to a halt.

Today, high prices have returned for all kinds of fuel, and uncertainties exist about political stability in the Middle East. A renewed U.S. interest in coal gasification is not surprising. Furthermore, hydrogen is now a welcome by-product because of the current interest in alternatively fueled vehicles.

The Majuba UCG Project in Mpumalanga, South Africa, is producing high-quality syngas for power generation. This photo shows the first flare on January 20, 2007, when the UCG plant successfully started operations.

UCG Revives

Four years ago, former Laboratory engineer Ray Smith, who led the Energy Program in the Energy and Environment Directorate, encouraged DOE to revisit UCG as a part of its program to develop hydrogen-from-coal technology. After Smith's retirement a year ago, his team of chemical engineers, geologists, and environmental scientists pursued the revival of UCG through Friedmann's Carbon Management Program. In February 2006, DOE commissioned the team to prepare a document evaluating the current state of UCG technology. *Best Practices in Underground Coal Gasification* was completed at the end of 2006 and is awaiting official release by DOE.

The document explores the UCG efforts that have been undertaken worldwide. Importantly, it also addresses the issues that were problematic in previous UCG operations by evaluating the potential application of technological advances in areas such as environmental risk assessment, combustion-process modeling, geologic subsurface characterization, and geomechanics.

Over the last few years, the number of activities throughout the world focusing on UCG has rapidly increased. The Chinchilla project, operating from 1997 to 2003 in Queensland, Australia, demonstrated the first long-term UCG pilot in the Western world. That project has now advanced to the stage of raising capital for a coal gas-to-liquids pilot that will make ultraclean diesel and aviation fuel. In South Africa, the electricity supply company Eskom is developing UCG at the Majuba Coal Field and achieved ignition in January 2007.

In the United Kingdom, the government undertook a five-year effort to review UCG and study the feasibility of using the technology for exploiting coal on land and offshore. A new UCG partnership, launched in the United Kingdom in 2005, draws its membership from more than eight countries. The partnership hosted its second international conference in February 2007, and Livermore chemist and environmental scientist Elizabeth Burton delivered the keynote address.

In India, interest in the potential of UCG is particularly high. India is the world's third largest coal producer (383 million tons of bituminous coal in 2005) and uses coal for about 60 percent of its own energy needs. Although India has vast coal resources, much of it is low grade, with high ash content. In addition, the coal lies in steeply dipping deposits that are difficult to mine conventionally. India also has a shortage of natural gas.

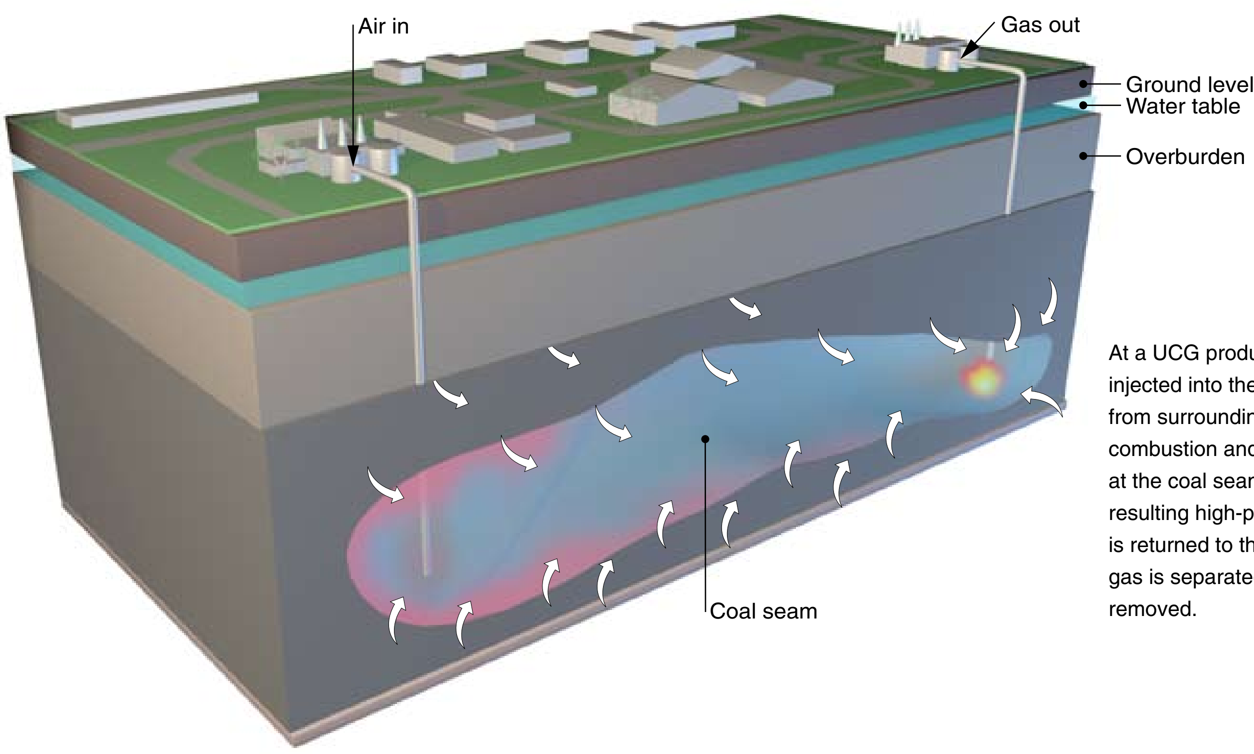
A November 2006 workshop on UCG, hosted jointly by the Indian Ministry of Coal and DOE, was heavily attended by representatives from India's coal industry. At least three pilot projects are now in the planning stages. Livermore, through DOE, is working closely with India on its UCG development. Ravi Upadhye, a chemical engineer who was involved in some of Livermore's early UCG projects, played a major role in organizing the workshop under the auspices of the U.S.–India Energy Dialogue Coal Working Group, with collaboration from governments within the Asian-Pacific Partnership on Clean Development and Climate. Burton represented the Laboratory and made technical presentations at the workshop.

Industry is reengaging with the Laboratory to pursue UCG. On March 30, 2006, Lawrence Livermore signed a memorandum of understanding with Ergo Exergy, which has licensed its proprietary Exergy UCG technology, or εUCG, to clients in Wyoming, South Africa, India, Australia, New Zealand, Canada, and Italy. The two organizations have agreed to cooperate in conducting research on UCG technology, specifically in the areas of process simulation and carbon sequestration, with an emphasis on evaluating the environmental performance of a large-scale operation. In addition, BP (formerly British Petroleum) recently executed an agreement with the Laboratory to develop simulations for optimizing the UCG process as well as tools for drilling, monitoring, and environmental management that are essential for field deployment of UCG.

The Powder River Basin is a massive coal and natural-gas deposit that spans the Montana–Wyoming border. It is the largest source of coal mined in the U.S. and is one of the largest deposits of coal in the world. GasTech, Inc., and the Wyoming Business Council recently completed a feasibility study showing UCG to be a better option with respect to cost, emissions, and environmental effects compared with conventional coal-fired stations and integrated gasification combined-cycle plants. New UCG field pilots are planned for the Powder River Basin. Ergo Exergy Technologies, Inc., will be involved in this test operation.

The UCG Process

In the UCG process, injection wells are drilled into an unmined coal seam, and either air or oxygen is injected into the cavity. Water is also needed and may be pumped from the surface or may come from the surrounding rock. The coal face is ignited, and at high temperatures (1,500 kelvins) and high pressures, this combustion generates hydrogen, carbon monoxide, carbon dioxide, and minimal



At a UCG production facility, air is injected into the cavity, water enters from surrounding rock, and partial combustion and gasification take place at the coal seam face after ignition. The resulting high-pressure syngas stream is returned to the surface, where the gas is separated and contaminants are removed.

amounts of methane and hydrogen sulfide. These products flow to the surface through one or more production wells. As the face is burned and an area depleted, the operation is moved to follow the seam.

Upadhye and chemical engineer Henrik Wallman from the University of California at Berkeley are developing improved combustion process models and a computational fluid dynamics model. Their goal is to optimize the design, operation, and control of UCG processes so that the composition of the product gas can be predicted and, despite variable subsurface conditions, constrained within acceptable limits. Gas composition affects the economic viability of the operation and must stay within the limits of the capabilities of the gas-processing plant at the surface. Thus far, they have developed the essentials of the process model and have integrated it with Aspen Plus, a commercial software package for simulating steady-state chemical processes.

Upadhye and Wallman's simplified model may work for some variables but not for all, as shown in the table below, which compares model results for UCG gas component levels to measurements made during the U.S. field tests in the 1980s. The model quite accurately predicts the hydrogen, methane, and water content of the gas. However, it predicts twice the actual level of carbon monoxide and about two-thirds the actual level of CO_2. "Verification of the model's accuracy can only be done with field experiments," notes Upadhye. "We cannot run laboratory experiments to verify the models. UCG takes place many hundreds of feet underground, and its results can be difficult to measure." Upadhye hopes to test and improve the model using field data from the UCG pilot tests that will occur throughout the world over the next few years.

Meeting Environmental Challenges

The new field pilots will also provide key data for the environmental models being developed by a team of environmental scientists led by Burton at Livermore. Although most of the previous UCG pilots did not produce significant environmental consequences, Livermore's 1970s test site at Hoe Creek, Wyoming, unfortunately resulted in contaminated groundwater, as did one pilot in Carbon County, Wyoming. At Hoe Creek, operation of the burn cavity at pressures higher than that in the surrounding rock strata pushed contaminants away from the cavity, which introduced benzene, a carcinogen, in potable groundwater. The contamination has required an expensive and long-term cleanup effort at the site.

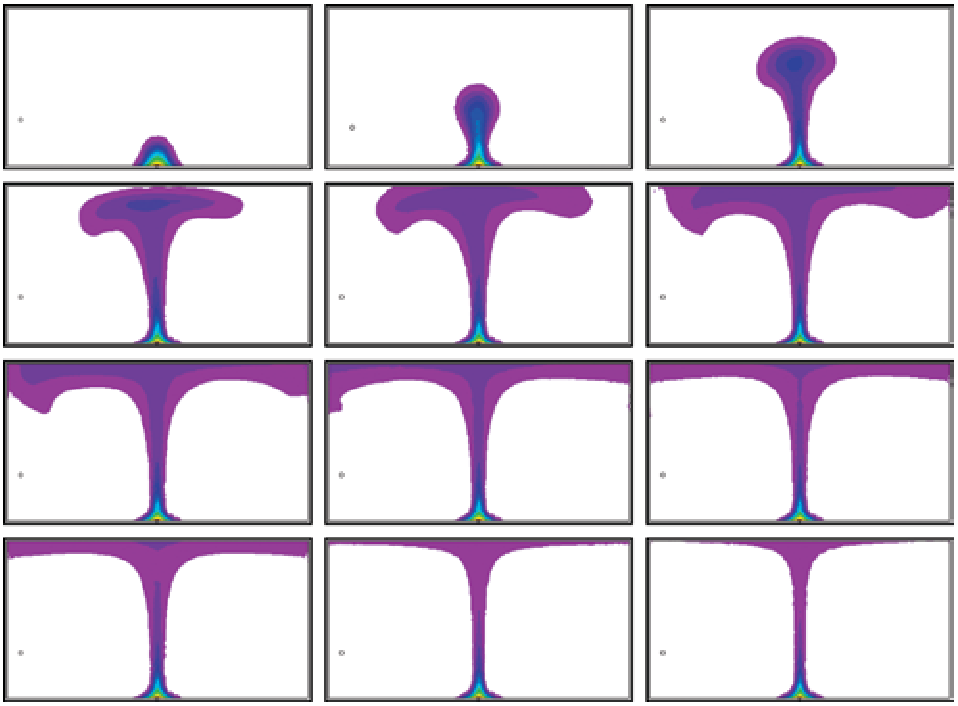
Since these problematic tests in the 1970s, environmental scientists have learned a great deal about the behavior and types of contaminant compounds produced by UCG as well as about contaminant transport and environmental risk assessment. Several steps can be taken to avoid groundwater pollution. One is balancing operating conditions to minimize the transport of contaminants from overpressurized burn zones. Another is to locate a UCG site where natural geologic seals isolate the burn zone from surrounding strata. Isolating the site from current or future groundwater sources and understanding how UCG affects the local hydrogeology are essential. This knowledge greatly benefited the Chinchilla project. "Chinchilla is an excellent example of how to plan a site and operate a UCG plant," says Friedmann. "The operators maintained negative pressure in the combustion cavity so that contaminants could not flow beyond the cavity."

Burton's team is creating the first detailed models of contaminant flow and transport specifically for UCG operations. "The standard types of hydrologic models used for environmental assessments do not consider the full effects of UCG operations," she says. UCG requires integrated simulations that capture the complex geochemical, geomechanical, and geohydrological processes occurring during a burn.

Initially, Livermore groundwater specialists Walt McNab and Souheil Ezzedine created and tested a modified version of the groundwater-modeling tool Flex to generate simple models of contaminant transport from UCG combustion. The models included thermal buoyancy effects on contaminant plume migration.

Model results for UCG gas composition compared with field measurements made during the 1980s Rocky Mountain 1 Controlled Retraction Ignition Point test.

Component	UCG model predictions (percent)	Field measurements (percent)
Hydrogen	27.2	27.3
Carbon monoxide	13.0	6.4
Carbon dioxide	19.4	27.2
Methane	7.4	6.4
Water	33.0	33.0



Groundwater modeling was used to simulate a hypothetical contaminant transport scenario in a subsurface homogeneous aquifer above a UCG coal seam. The model couples flow, heat, mass, and density to calculate changes in the temporal and spatial distribution of contaminants generated by the gasification process. In this simple case, the heat and contaminant sources are modeled for a stationary ignition point, and groundwater flow rates are minimized to highlight the buoyancy effects on the contaminant plume. The contaminant concentrations over time, from top left to bottom right, are shown (purple is lowest, red–yellow is highest).

These first simplistic models used a homogeneous subsurface. The layering and permeability contrasts that characterize natural rock sequences associated with coal seams were ignored. In this way, the researchers could isolate important thermal changes when predicting and assessing UCG environmental effects.

Another environmental concern is that the void created by gasification may cause the land surface to subside. Subsidence is likely to be more of a problem if gasification occurs in a shallow coal seam, closer to the surface. This phenomenon also often occurs above long-wall underground coal mines but is less of a problem if the seam is deep.

Managing Greenhouse Gases

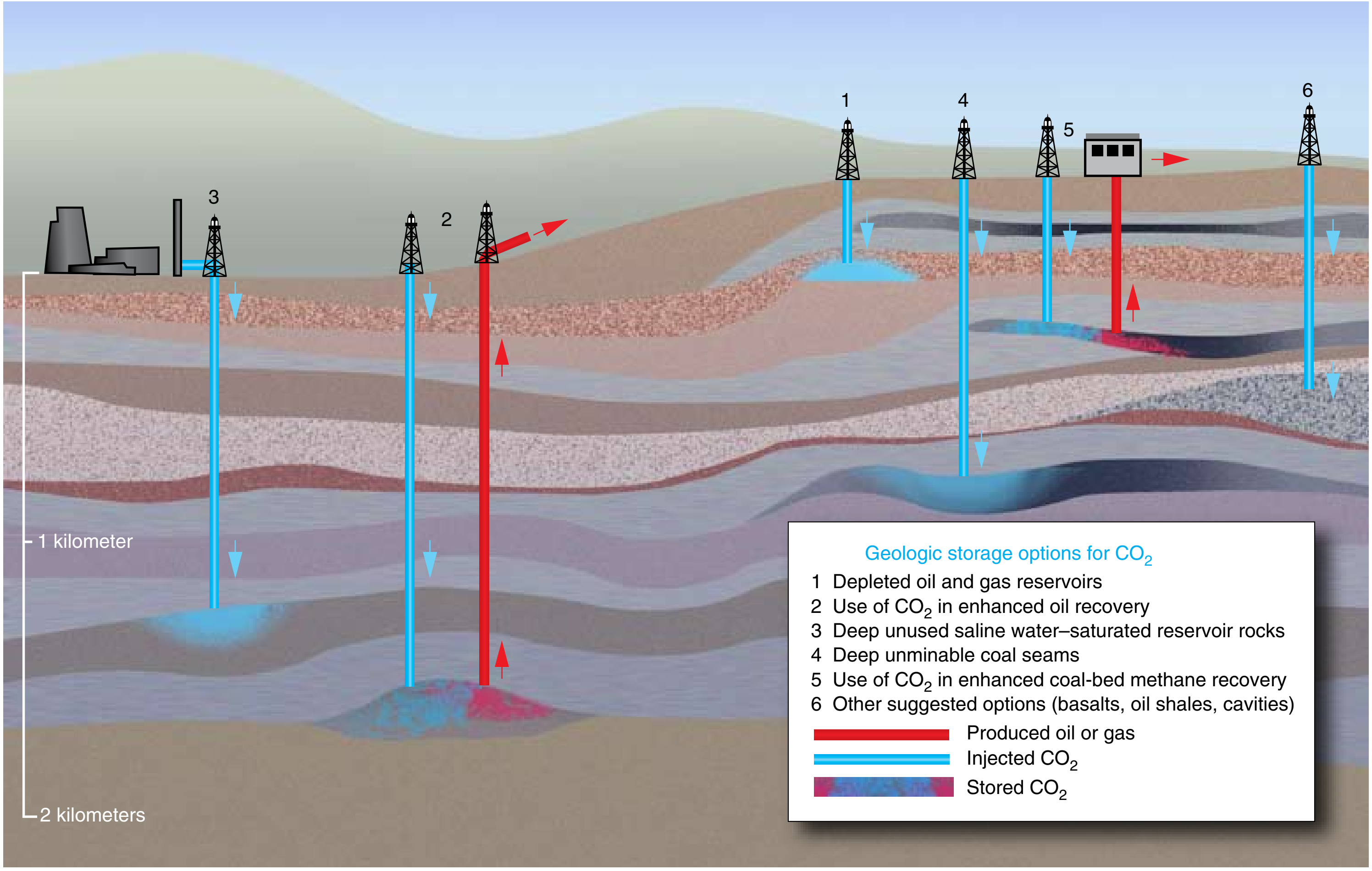
At the surface, the various combustion products are separated out to make the syngas usable. After cooling, the gas is filtered to remove ash and tar particles. Removal technologies are well established for hydrogen sulfide and ash products such as arsenic, mercury, and lead. These compounds are then disposed of safely. Hydrogen can be separated out for use alone, or it can be included as a component in the syngas, which is a mixture of hydrogen and carbon monoxide.

If the CO_2 is to be captured at the surface and sequestered, it must be separated from the syngas. The Laboratory is a leader in the field of carbon management and is developing a number of separation or "capture" technologies. (See *S&TR*, May 2005, pp. 12–19.) At a UCG production site, a significant percentage of the CO_2 would likely be sequestered in the void left by the burned coal seam. Ideally, remaining CO_2 would be sequestered in deep geologic formations nearby.

UCG processes cause thermal, geochemical, and geothermal changes to the surrounding rock reservoir, which may affect the reservoir's ability or capacity for CO_2 storage. Such changes include the effects of heating and quenching on fractures and rock properties. The reservoir may become more porous as acid leaches from ash, tars, char, coal, and rock minerals. Fluid densities in the reservoir may change because of high combustion temperatures. In addition, organic contaminants in CO_2 and metals in acid groundwaters may become more soluble because of UCG. "At this point, CO_2 storage in UCG zones comes with caveats," says Friedmann. Additional research is essential to quantify and characterize the effect of these processes before any CO_2 can be pumped back down near a UCG production facility.

If the CO_2 is not sequestered in place, it can be piped to oil fields. U.S. oil companies can then inject it underground to increase production from oil and natural gas wells, a process called enhanced oil recovery. The U.S. already leads the world in enhanced oil recovery technology, which represents an opportunity to sequester carbon at a lower cost compared with storing it in geologic repositories. Sales of the recovered oil and gas could generate revenues to help offset the expenses of sequestration. The only operating coal gasification plant in the U.S., at Beulah, North Dakota, has been piping its captured CO_2 to oil fields in Canada for years.

Livermore researchers have developed electromagnetic imaging and electrical resistivity tomography to monitor the CO_2 injected underground and ascertain its location over time. Electromagnetic imaging was originally designed as an aid in oil recovery. Electrical resistivity tomography was designed for environmental research but has since been extended for use in oil



Options for storing carbon dioxide (CO_2) in deep geologic formations are represented here. (Courtesy of Intergovernmental Panel on Climate Change, 2005.)

fields. When existing well casings are used as electrodes, electrical resistivity tomography is a nearly noninvasive and low-cost method for monitoring. Three-dimensional modeling at Livermore allows researchers to examine injection scenarios in detail, including those involving enhanced oil recovery, and to "test" monitoring tools in a virtual environment before expensive prototypes are built.

UCG for the Future

Although the potential of UCG as a transformational technology for coal has been rediscovered globally, its future maturation depends on the success of the pilot tests that are just beginning. The U.S. government has declared "clean coal" a critical goal for the near term, and the state of California and other government entities have mandated the reduction of CO_2 emissions. "Current plans are for an additional 120 coal-fired power plants around the world in the next decade," says Friedmann. "UCG could be used to power many of them." Success requires that the right tools are available to accurately assess the economic viability and environmental consequences of UCG in all phases, from planning to operations to site closure.

—Katie Walter

Key Words: carbon dioxide capture and storage, carbon sequestration, hydrogen production, underground coal gasification (UCG).

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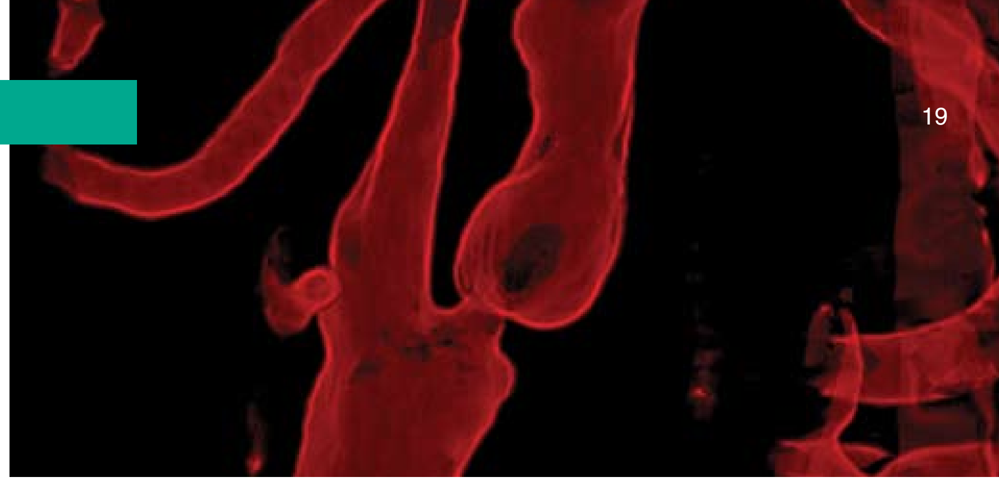


Big Physics in Small Spaces

MODELING what happens to a particle-laden fluid as it travels through the complex channels of a microdevice is not an easy computational task. The dimensions of the device components, such as channel widths, can be nearly as small as the particles themselves. Yet, the details of this fluid flow are important for such applications as designing drug delivery systems, optimizing biosensors, and even determining blood flow.

The difficulties of modeling these flows in confined spaces are a reflection of the scales involved. Several approaches to modeling particle-laden fluid flow exist, depending on the scale to be resolved. For example, continuum models can adequately simulate macroscale properties such as velocity and pressure, while particle methods can simulate individual molecules on the microscale. However, it is difficult to capture both scales in one algorithm that reflects the physics and chemistry of these scales and that runs in a reasonable amount of time—even on a supercomputer.

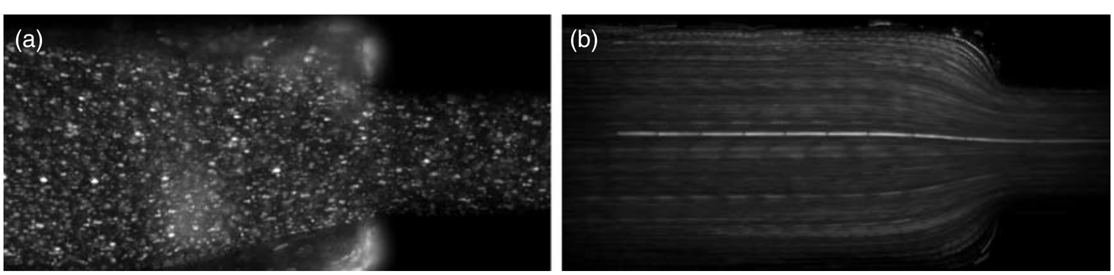
Livermore computational scientist David Trebotich from the Center for Applied Scientific Computing and professor Greg Miller from the University of California (UC) at Davis's Department of Applied Science, along with researchers from Lawrence Berkeley National Laboratory's Applied Numerical Algorithms Group, have developed a multiscale algorithm to better model particle-laden fluid flows. The algorithm can be used to model flow through microscale structures, such as arrays of posts and other complex channels and components inside centimeter-long devices, as well as interactions in biological materials, such as a DNA molecule.

Tiny Flows with Impact

The modeling effort grew out of Trebotich's postdoctoral work at UC Berkeley on microfluidics, in which he explored the fundamental physics of complex flows through microelectromechanical systems (MEMS) devices used in biosensors and drug delivery systems. Trebotich says, "We needed new physical models and advanced numerical algorithms that could accurately simulate the flow of complex fluids containing high densities of biological particles such as DNA in microenvironments."

Livermore's Laboratory Directed Research and Development Program funded Trebotich's project to create a computational design tool for microdevices and components such as those used in pathogen detection systems. "These systems introduce a new flow regime in an already complex biological flow that is not well understood," says Trebotich. "Also, the design and fabrication of bioMEMS devices have been largely a trial-and-error approach. The early devices were certainly not optimal. This project gave us the opportunity to create a computational design tool that would provide critical understanding of the fundamental flow physics in this mostly unexplored regime and provide a predictive capability for designing more advanced microfluidic systems."

Researchers from UC Berkeley's Bioengineering Department performed key validation experiments and proved the hypothesis that a fluid containing even small amounts of long-chain polymers, such as DNA, exhibits both viscous and elastic behavior. "Viscoelasticity is a phenomenon that complicates fluid flow, in general. The difficulty in trying to remove a speck of eggshell from raw egg whites is a practical example of viscoelastic behavior. The eggshell sort of bounces away unless you slowly nudge it toward a surface where there is no flow. If one applies this to macromolecular flow in microdevices where the lengths of the molecules approach those of the flow channels, the behavior becomes even more nonintuitive compared to, say, that of water," says Trebotich. "For instance, if a flow channel contracts sharply, large recirculation zones will appear in the salient corners." If a molecule is caught in such a vortex, it could degrade or possibly break. When the molecule



(a) Experiments show that fluids laden with DNA act in unusual ways when flowing, such as creating large vortices in corners. (b) These behaviors do not occur with plain water. (Images courtesy of Shelly Gulati, University of California at Berkeley.)

reenters the flow near a sensor downstream, it may no longer be identifiable as the original molecule.

The experiments also show that DNA migrates away from regions of high shear, such as close to channel walls, and toward regions of low shear, such as a channel's center. In addition, these molecules stretch out in accelerating flow regions and recoil in decelerating flow or stagnant regions. "This behavior can affect the assumed performance of a biosensor," notes Trebotich. "It's important to be able to not only predict these dynamics in a device for which the objective is to control a biological fluid but also to manipulate and detect biological species in the fluid. Fulfilling these objectives requires using both continuum models to capture bulk properties for flow control and particle methods to represent coarse-grained molecular transport."

Cookie Cutters, Rods, and Beads

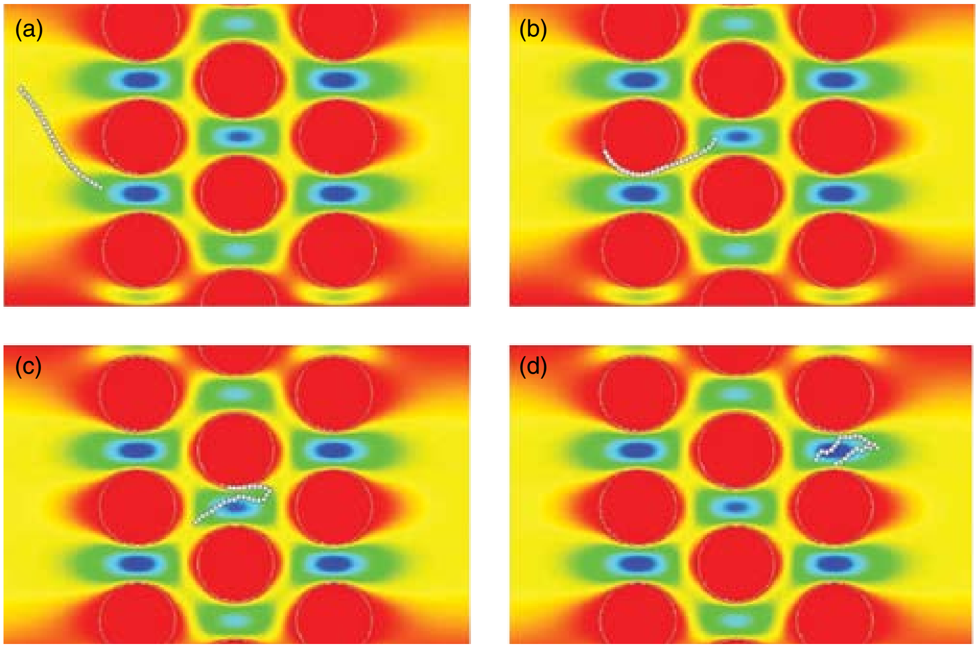
To model the behavior of these unusual flows, Trebotich and Miller created a hybrid fluid–particle numerical algorithm that embraces most scales of interest—from the device scale down to the smallest scale of interparticle interactions. The algorithm is based on discretization of an incompressible Newtonian fluid, such as water, using a high-resolution, finite-difference method. An embedded boundary volume-of-fluid formulation is used near boundaries where the fluid meets structures.

Trebotich and his colleagues chose a finite-difference method on a structured grid because of its simplicity and known numerical properties. However, they found that geometries represented with just squares and rectangles are limited. They then turned to the embedded boundary method, which allows irregular geometries to be represented by overlaying the problem domain on a structured Cartesian grid. In this approach, the irregular boundary of the problem domain cuts through the affected squares on the grid.

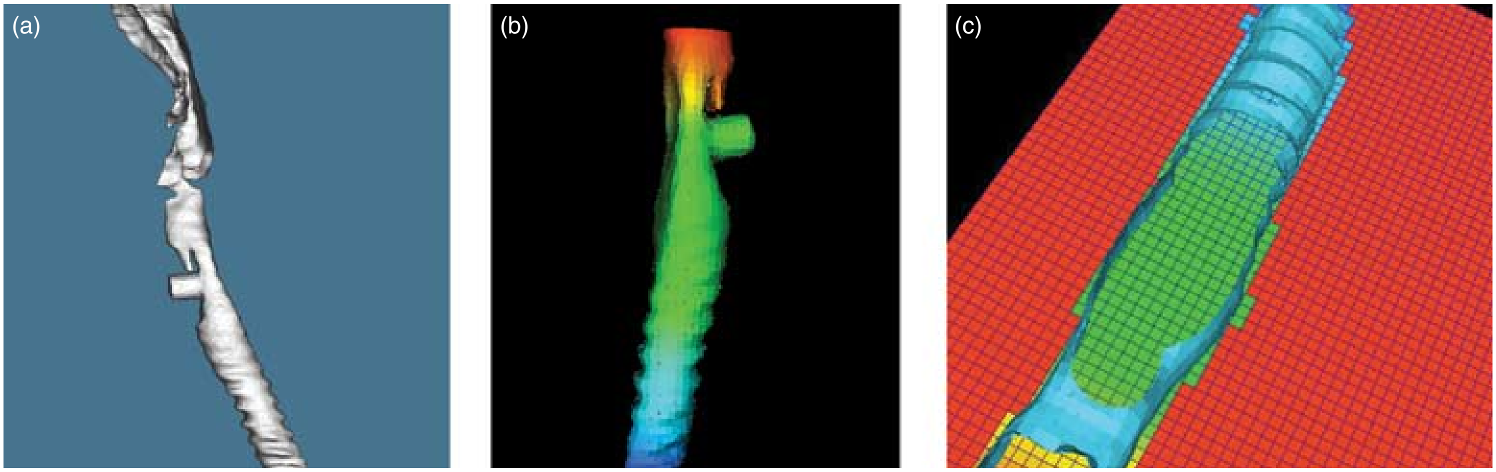
"Think of it," says Trebotich, "as a cookie-cutter approach with the dough spread out on the counter representing a rectangular fluid-flow channel. To represent an obstruction in the flow, such as a post in an array channel, one simply cuts a circle shape out of the dough or domain." The regular grid cells can then be solved with finite-difference methods, and the cut cell can be handled conservatively with a volume-of-fluid approach.

"This approach is an efficient way to solve the problem," says Trebotich. "It uses less computational time than a body-fitted grid approach, particularly when the grid or mesh is moving. The embedded boundary technique itself is specifically intended to enhance parallel scalability and to facilitate adaptive mesh refinement, which focuses computations in areas of interest in the domain. All in all, this approach provides a powerful tool for multiscale, multiphysics computational fluid dynamics."

To represent the DNA and other polymerlike molecules in the fluid, Trebotich and his colleagues use a model of beads connected in a chain by rods or springs. The polymer is then coupled to the fluid through forces representing hydrodynamic drag and stochastic thermal fluctuations. "In this model, the fluid can 'feel' the effects of the polymer molecules, a reverse-coupling mechanism that could prove to be important in simulating more concentrated polymer flows," says Trebotich.



A newly developed algorithm is tested in this simulation of a DNA strand as it flows through an array of posts in a microchannel. (a) The strand begins to wrap around a post. It then is (b) loosened by Brownian and hydrodynamic forces and (c–d) swept through the flow field. Colors show the underlying velocity flow fields: fast (blue) and slow or reversed (red).



(a) A human trachea is shown in this computed tomography scan. (b) Livermore researchers developed a computational tool that uses embedded boundary grids to model fluid flow through a trachea. (c) In this close-up of a three-dimensional simulation, geometric detail is shown in cut cells of a two-dimensional slice.

To increase the realism of the model, the researchers added algorithms that keep the simulated polymers from crossing or "passing through" each other in an unrealistic, ghostlike fashion. "Noncrossing is a constraint frequently ignored in other bead-rod models," says Trebotich. The team developed a novel technique in which the rods elastically bounce off one another without the small time steps typical of particle methods. In a similar way, the model also treats interactions between polymers and surfaces as elastic. "The ability to advance the particles at time steps on the order of the fluid timescale allows us to perform system-level modeling for engineering-scale problems involving particle-laden fluids," adds Trebotich.

Re-creating the Real Thing

The researchers tested their model by simulating a DNA molecule flowing through two microdevice configurations—a microchannel with an array of posts and a small tube packed with microspheres resembling a porous medium. These configurations are similar to those used for extracting DNA in microfluidic-based devices that contain a polymerase chain reaction component. The team used a simple post-array microchannel to hone their algorithm development, model short-range interactions between particles and solid surfaces, and simulate how the rods interact.

"Ultimately, we want to determine if one configuration is better than the other for extracting a molecule," says Trebotich. "In flow-through devices, we want at least one strand of DNA to adhere to a structure so the DNA can be amplified for better signal detection. If the flow rate is too high, the DNA molecule will pass through without being captured. If it's too low, the DNA might not have enough momentum to arrive at the capture point. This effort is an example of how we can help engineers design devices optimized for their purposes."

The algorithms that the team developed are multipurpose. With researchers at Lawrence Berkeley and UC San Francisco, the team examined how realistically its model re-creates flow in a human trachea, which has an intricate anatomical geometry. They used the embedded boundary method to successfully model a trachea from a patient's computed tomography scan, down to the detailed ribbing, where flows can be complex. "The smallest geometric irregularities can alter the flow, causing flow perturbations that other models will not capture if the geometry and mesh obtained from the medical image do not contain enough detail," says Trebotich. "Fluid dynamics can become very complicated when we get down to the details—that is, the smaller scale features." The details are important in certain situations, for example, when a physician needs to know how a tracheotomy procedure could affect the flow of air in a damaged trachea or how a partial blockage in an artery could affect blood flow.

The team's goal is to develop methods to simulate the physics that occur at multiple scales for a variety of flow problems in a time frame that is useful for engineers, physicians, and practitioners in other fields. Trebotich says, "It's an end-to-end endeavor, from model to simulation to analysis, and one that draws on experts in multiple disciplines from throughout the UC system."

—Ann Parker

Key Words: algorithm, biosensor, continuum model, DNA, fluid flow, microchannel, microfluidic device, multiscale computational fluid dynamics, particle model, post array, viscoelastic fluid.

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A New Block on the Periodic Table

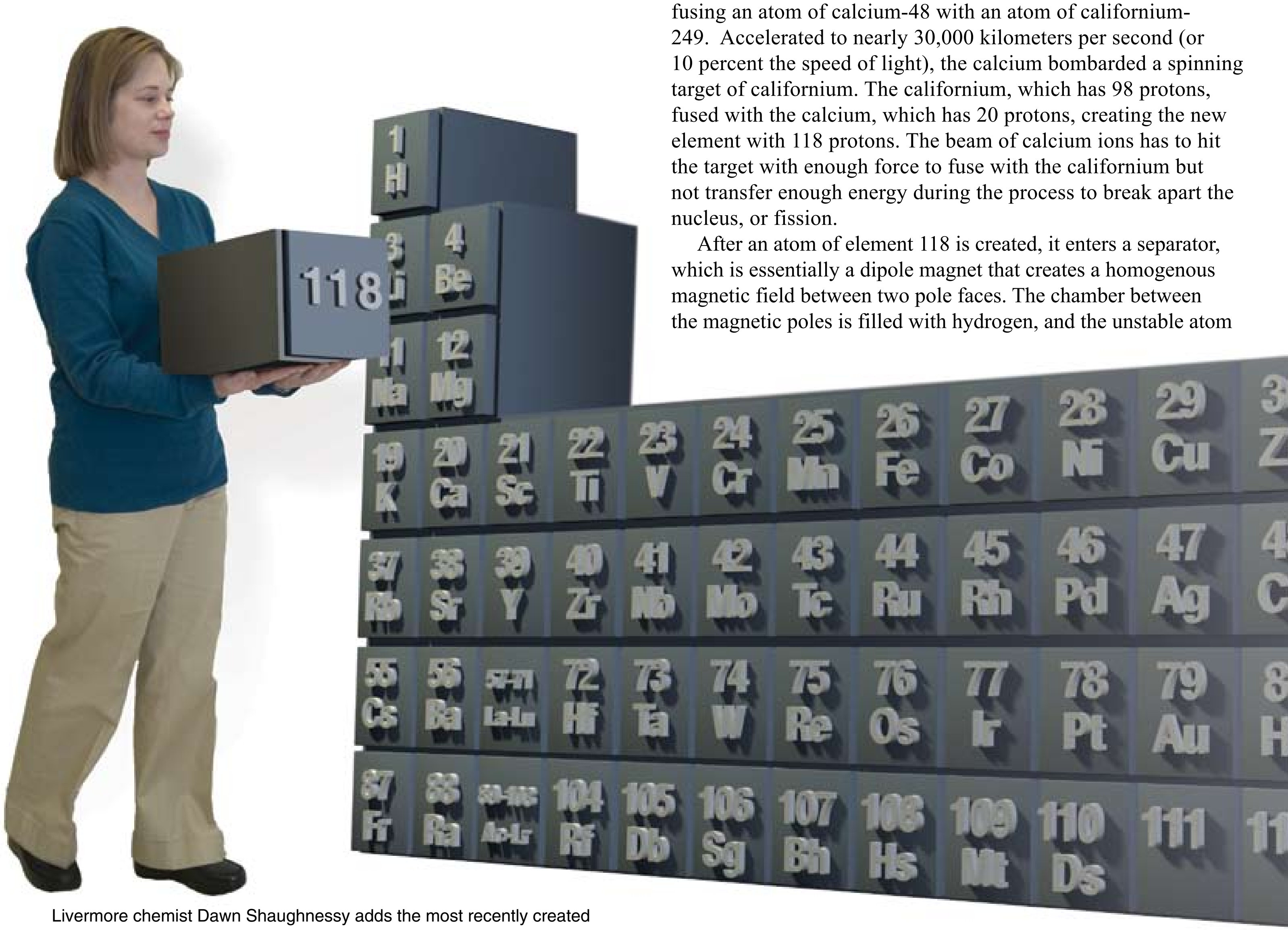
SCIENTISTS from Lawrence Livermore working in collaboration with a team from the Joint Institute for Nuclear Research (JINR) in Dubna, Russia, have discovered element 118, the newest block on the periodic table. Lasting less than a millisecond before decaying and ultimately fissioning, element 118 is the latest element to be synthesized artificially.

Why do scientists work so hard to create new elements that last for such a short time? According to chemist Dawn Shaughnessy from Livermore's Chemistry, Materials, and Life Sciences Directorate, "Each new element we discover provides more knowledge about the forces that bind nuclei and what causes them to split apart. This knowledge, in turn, helps us better understand the limits of nuclear stability and the fission process."

Element 118 under Construction

During experiments conducted in Dubna's U400 cyclotron between February and June 2005, element 118 was created by fusing an atom of calcium-48 with an atom of californium-249. Accelerated to nearly 30,000 kilometers per second (or 10 percent the speed of light), the calcium bombarded a spinning target of californium. The californium, which has 98 protons, fused with the calcium, which has 20 protons, creating the new element with 118 protons. The beam of calcium ions has to hit the target with enough force to fuse with the californium but not transfer enough energy during the process to break apart the nucleus, or fission.

After an atom of element 118 is created, it enters a separator, which is essentially a dipole magnet that creates a homogenous magnetic field between two pole faces. The chamber between the magnetic poles is filled with hydrogen, and the unstable atom



Livermore chemist Dawn Shaughnessy adds the most recently created element to the periodic table.

traveling from the cyclotron into the separator immediately picks up electrons from the hydrogen until it reaches an equilibrium state. The magnetic field is set to recognize this equilibrium state so that, for the most part, only atoms with a matching charge state are passed to a detector. In this way, the few atoms of interest are separated from a flood of interfering particles.

The detector is key to proving the new element's fleeting existence. An atom first passes through a time-of-flight counter, which detects the time the atom enters and its speed. The atom then moves into the detector box and implants itself in one of the silicon walls. The counter sends a signal that helps scientists to identify new and heavier atoms, which travel more slowly, and to ignore unwanted by-products.

The new element undergoes alpha decay almost immediately—that is, it ejects a helium nucleus (two protons and two neutrons) making it element 116. Element 116, in turn, decays to element 114, and then it either undergoes fission or a third alpha decay to element 112. Scientists do not see the element itself—they see only the unique and distinctive alpha decays that prove it existed. Because each of these daughter products is so heavy, they do not travel far between decays, and the signal from the detector shows each one. Only alpha decays within a particular time frame and with certain energy signatures can possibly be emitted from element 118.

Mapping the Island of Stability

Scientists have been creating new elements since 1940, when neptunium and plutonium were created at the University of California at Berkeley. As more elements were created, a pattern emerged: each new element was radioactive, slightly heavier than the one before, and in general, more unstable with an increasingly short half-life. However, in the 1960s, a few scientists theorized that the isotopes of some of the synthesized heavy elements would be more stable, with much longer half-lives. These isotopes would form an "island of stability" in a "sea" of highly unstable isotopes that exist beyond the natural elements. Because those elements would have longer lifetimes, they might be useful for new applications.

Since then, scientists have endeavored to reach this island of stability, constantly pushing the border of what is technologically achievable. To be in the island, the isotopes must have filled or nearly filled nuclear shells. These shells are analogous to the

An artist's conception shows the production of element 118 as it travels through the accelerator to the detector. Three atoms of element 118 are produced when calcium ions bombard a californium target.

Lawrence Livermore scientists (left to right) Jackie Kenneally, Jerry Landrum, Nancy Stoyer, and Ken Moody perform chemical separations on reaction products produced in a cyclotron at the Joint Institute for Nuclear Research in Dubna, Russia. Dubna's U400 cyclotron produces some of the most intense calcium-48 beams in the world and does so for the months required to produce just a few atoms of the superheavy elements.

electron orbitals in atoms. When the shells are filled with the number of protons equal to one of the "magic numbers" of 2, 8, 20, 28, 50, and 82, the nucleons have a greater binding energy and are more stable against nuclear decay. These same numbers and the number 126 are magic numbers for neutrons. The calcium-48 isotope used to create element 118 is "doubly magic" because it has 20 protons (a magic number) and 28 neutrons (also a magic number). Calculations performed in the 1960s indicated that the next magic proton number is 114.

When the Livermore–JINR team earlier created the relatively long-lived elements 114 and 116, they demonstrated that the island of stability exists. (See *S&TR,* January/February 2002, pp. 16–23.) Because element 118 has such a short half-life, it is not likely to have a magic number of protons. Rather, the element's decay properties, and those of its decay daughters, tend to support the view that element 114 contains a magic number of protons. If element 118 were located completely beyond the island of stability, current theory says it would not have lasted as long as it did. The fact that element 118 did not undergo fission immediately was unexpected and suggests that the island of stability is larger than predicted.

Chemist Ken Moody from Livermore's Defense and Nuclear Technologies Directorate says, "Our goal is to create new elements with as many neutrons as possible." However, until technology allows the forcing of more neutrons into the nuclei, no single experiment can prove which is the next magic number. Nonetheless, the discovery of element 118, together with the discovery of elements 113–116, has helped map more of the island of stability and answer some questions.

Applications for element 118 and, indeed, for many other heavy elements, have not yet been pursued. However, several heavy elements do have applications. For example, americium is used in smoke detectors, curium and californium are used for neutron radiography and interrogation, and plutonium is used in nuclear weapons.

Filling in the Periodic Table

Scientists from Livermore and JINR are starting experiments to create element 120. Using a beam of iron-58 to bombard a plutonium-244 target, the team hopes to create element 120 and further map the island of stability. What will be the last block on the periodic table? Although current technology has a limited ability to force more neutrons into the nucleus, future radioactive beam accelerators might produce more intense beams of neutron-rich isotopes. If so, researchers might reach the center of the island. The ultimate goal of the Livermore–JINR team is to fully map the island of stability and develop a comprehensive magic number theory that explains how nuclei bind and how they resist fission.

—Karen Rath

Key Words: element 118, heavy elements, island of stability, Joint Institute for Nuclear Research (JINR).

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A Search for Patterns and Connections

Highlights of Teller's Contributions to Computational and Mathematical Physics

January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the second in a series of 10 honoring his life and contributions to science.

EDWARD Teller began thinking about numbers before he was even five years old. In *Memoirs*, he recalls a game he played as he went to sleep. "I knew that a minute has sixty seconds, and I charged myself to discover how many seconds there were in an hour, a day, or a year." For the rest of his life, he continued to look for mathematical patterns in the physical world around him. And many of his insights led to important methods underlying complex calculations used to model physical processes today.

Teller's career in basic science research coincided with the discovery of quantum mechanics, the mathematical theory that provides a framework for studying atomistic behavior. Quantum mechanics can be used to precisely describe phenomena that classical Newtonian physics cannot account for, such as the stability of matter and the microscopic rules governing the physics of atoms. The discovery of quantum mechanics allowed researchers to precisely connect material behavior at the visible (macroscopic) level with that at the invisible level of atoms, molecules, and their constituents. Quantum mechanical ideas, including much of Teller's best work, thus offer potential new methods to compute the detailed properties of matter.

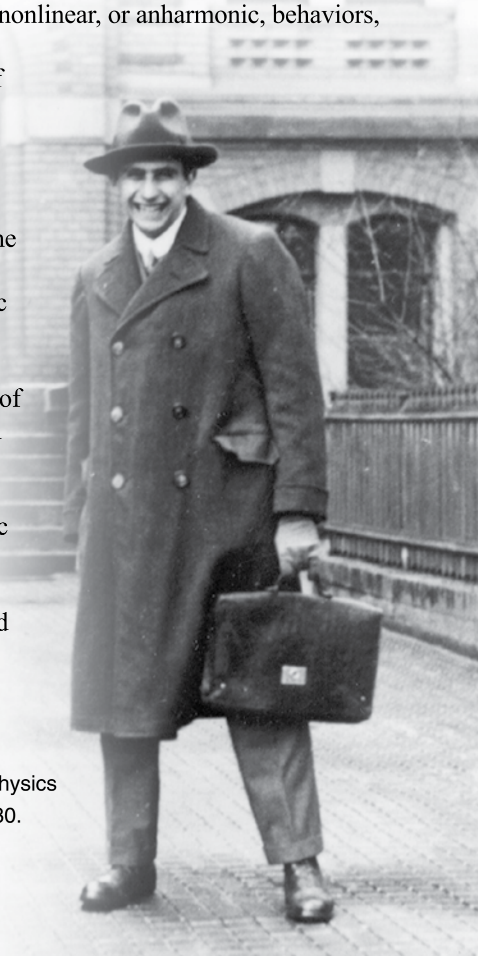
The Metropolis algorithm, which is essential for making statistical mechanics calculations computationally feasible, is perhaps Teller's best-known work in computational physics. (See *S&TR*, January/February 2007, p. 6.) Metropolis resulted from a collaborative effort involving Teller, his former student Marshall Rosenbluth, their wives Mici Teller and Arianna Rosenbluth, and Nicolas Metropolis, who published the algorithm in 1953. Today, it forms a basic part of the arsenal of every computational physicist. Teller was contributing ideas to important statistical mechanics calculations long before his work on Metropolis.

Quantifying Nonlinear Oscillation

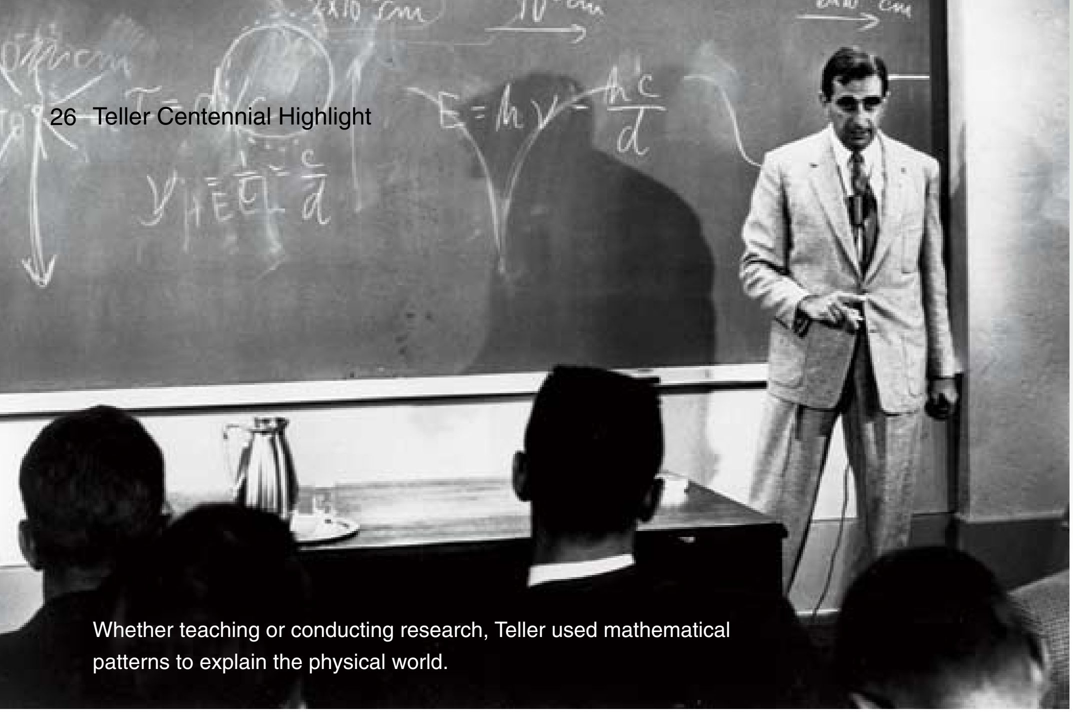
In 1928, Teller transferred from Karlsruhe Technical Institute to the University of Leipzig to study with Werner Heisenberg, a major contributor to the development of quantum mechanics. After receiving a Ph.D. in physics in 1930, he began working at the University of Göttingen, where he applied quantum mechanics to various systems.

Among Teller's many contributions from that time was his work on anharmonic oscillation. A widely applied quantum mechanics calculation describes the dynamics of the harmonic oscillator. Classically, a familiar example is a wire spring, in which the compression or extension is exactly proportional to the force applied. The basic quantum mechanics calculation of this behavior accounts for many of the physical processes occurring in matter, including how the molecular structure of material responds to compression, sound, and heat. However, a harmonic oscillator fails to capture other phenomena such as the expansion that occurs when metal is heated. To model these nonlinear, or anharmonic, behaviors, researchers needed methods to illuminate in detail the effects of the forces between atoms.

At Göttingen, Teller worked with G. Pöschl to study anharmonic oscillators. Their eight-page paper, published in the German journal *Zeitschrift für Physik*, described an anharmonic oscillator that not only could be mathematically solved but also illustrated the detailed behavior of more realistic oscillators. Pöschl and Teller's clever solution was initially thought to be a useful textbook example of anharmonic behavior. Researchers later found it to rely on underlying symmetries that could be applied to physical phenomena from scattering to nonlinear optics.



Edward Teller received a Ph.D. in physics from the University of Leipzig in 1930.



Whether teaching or conducting research, Teller used mathematical patterns to explain the physical world.

for modeling the behavior of atoms, molecules, and condensed matter is the Schrödinger equation, which describes the complete quantum dynamics of electrons and nuclei in matter. This equation involves complex calculations that often do not easily reveal the physics involved. Even with today's supercomputers, only relatively simple systems can be analyzed using the full equation.

Instead, for most problems, computational scientists use approximate methods to examine atomistic behavior. Approximations eliminate unimportant elements of a problem so that, ideally, only the essential features remain, thus reducing computational time and increasing physical understanding. In 1955, J. W. Sheldon published a paper on the widely used Thomas–Fermi approximation that intrigued Teller. Sheldon's analysis indicated that, at this level of approximation to the full Schrödinger equation, the nitrogen molecule would be unstable. Teller wondered if Sheldon's results indicated a general limitation of the Thomas–Fermi approximation. In a concise paper written in honor of his friend Eugene Wigner and published in 1962 in *Reviews of Modern Physics*, Teller showed that the Thomas–Fermi approximation insufficiently captured the physics expressed in the more complex Schrödinger equation. Later, mathematical physicists such as Elliott Lieb used Teller's arguments in explaining how the Schrödinger equation produced stable matter.

An Exact Solution for a Phase Transition

Teller was also interested in the thermodynamics and statistical mechanics of phase transitions, such as the changes occurring in the structure of water when ice melts. In 1925, Ernst Ising developed a mathematical model for studying a similar phase transition in the spins of ferromagnetic materials. These materials will retain an amount of magnetization up to a specific temperature, at which point the magnetism disappears.

Ising was only able to solve his model for spins in one dimension and thus could not illustrate the mechanics of a phase transition. Many physicists then worked at solving the Ising model in two dimensions. Lars Onsager, who won the Nobel Prize in Chemistry in 1968, succeeded in demonstrating a magnetic phase transition by taking advantage of specific symmetries of the model.

Building on the work of Ising and Onsager, Teller suggested that his student Julius Ashkin generalize Ising's model so it would capture more of the physics occurring in ice phases while preserving the symmetries exploited by Onsager's calculations. The two-dimensional Ashkin–Teller model indeed provided an exact solution for a phase transition such as water freezing, and Ashkin's work on this problem became part of his doctoral thesis. For some time, the Ashkin–Teller model was seen as a clever but niche calculation in statistical physics. In the 1960s, scientists began to discover that the Ising and Ashkin–Teller models were examples of a more general class of theories that provide deeper insights to the thermodynamics of phase transitions. More recently, researchers have found that this general class of models is relevant to string theory.

A Limited Approximation

Teller's curiosity also led him to search for a simple understanding of the stability of matter. The rigorous approach

The Quest Continues

Throughout his life, Teller sought simple but incisive explanations to better understand the structure of matter. As these examples show, many discoveries borne out of this quest led to unexpected findings that often had practical applications. One of Teller's many legacies to Lawrence Livermore is the simultaneous pursuit of basic science to understand the physical world and applied science to use that knowledge.

—Carolin Middleton

Key Words: anharmonic oscillator, Ashkin–Teller model, computational physics, Edward Teller, mathematical physics, Metropolis algorithm, Schrödinger equation, Thomas–Fermi model.

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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

Alternating-Polarity Operation for Complete Regeneration of Electrochemical Deionization System

Tri D. Tran, David J. Lenz
U.S. Patent 7,138,042 B2
November 21, 2006
An electrically regenerative battery of electrochemical cells for capacitive deionization (including electrochemical purification) and regeneration of electrodes is operated at alternate polarities during consecutive cycles. In other words, after each regeneration step operated at a given polarity in a deionization–regeneration cycle, the polarity of the deionization step in the next cycle is maintained. In one embodiment, two end electrodes are arranged one at each end of the battery, adjacent to end plates. An insulator layer is interposed between each end plate and the adjacent end electrode. Each end electrode includes a single sheet of conductive material with a high specific surface area and sorption capacity, preferably a sheet formed of carbon aerogel composite. Double-sided intermediate electrodes equidistally separated from each other are placed between the two end electrodes. The electrolyte entering the battery cells flows through a continuous open serpentine channel that is defined by the electrodes and is substantially parallel to their surfaces. Polarizing the cells removes ions from the electrolyte and holds them in the electric double layers formed at the carbon aerogel surfaces of the electrodes. As the electrodes of each battery cell become saturated with the removed ions, the battery is regenerated electrically at a reversed polarity from that during the deionization step of the cycle, thus significantly minimizing secondary wastes.

Silicone Metalization

Mariam N. Maghribi, Peter Krulevitch, Julie Hamilton
U.S. Patent 7,145,229 B2
December 5, 2006
This system provides a silicone layer on a matrix and a metal layer on the silicone layer to produce an electronic apparatus. The apparatus thus has a silicone body with metal features, providing an electronic device.

Composites for Removing Metals and Volatile Organic Compounds and Method Thereof

Paul R. Coronado, Sabre J. Coleman, John G. Reynolds
U.S. Patent 7,148,180 B2
December 12, 2006
Functionalized hydrophobic aerogel–solid support structure composites have been developed to remove metals and organic compounds from aqueous and vapor media. The composite, which can be in molded, granular, or powder form, adsorbs the targeted metals or organics, leaving a purified aqueous or vapor stream. The species-specific adsorption occurs because aerogels are tailored toward specific material. After adsorption, the composites can be disposed of, or the material can be reclaimed or removed and the composites recycled.

Cellular Telephone-Based Radiation Sensor and Wide-Area Detection Network

William W. Craig, Simon E. Labov
U.S. Patent 7,148,484 B2
December 12, 2006
A network of radiation detection instruments, each having a small solid-state radiation sensor module integrated into a cellular phone, provides radiation detection data and analysis directly to a user. The sensor module includes a solid-state crystal bonded to an application-specific integrated circuit readout. This compact, lightweight instrument can detect and measure radiation energies in the local ambient radiation field. In particular, the photon energy, time of event, and location of the device can be recorded at the time of detection and transmitted to a central data collection and analysis system. Data from the entire network of radiation detection instruments are combined by correlation and analysis algorithms, which then map the background radiation and identify radiation anomalies in the region.

Near-Infrared Spectroscopic Tissue Imaging for Medical Applications

Stavros Demos, Michael C. Staggs
U.S. Patent 7,149,567 B2
December 12, 2006
Near-infrared imaging using elastic light scattering and tissue autofluorescence are explored for medical applications. In this approach, cross-polarized elastic light scattering and tissue autofluorescence in the near-infrared region are coupled with image processing and interimage operations to differentiate human tissue components.

Obstacle Penetrating Dynamic Radar Imaging System

Carlos E. Romero, James E. Zumstein, John T. Chang, Richard R. Leach, Jr.
U.S. Patent 7,148,836 B2
December 12, 2006
An obstacle-penetrating dynamic radar imaging system uses several low-power, ultrawideband radar units to detect, track, and image an individual, animal, or object. A radar video system produces a set of return radar signals from a detected object, which are then processed to image the object and track its location.

Autostereoscopic Projection Viewer

John S. Toeppen
U.S. Patent 7,150,531 B2
December 19, 2006
An autostereoscopic viewer is used to produce aberration-corrected images to simulate a virtual presence by using pairs of projector optical components coupled with an image corrector plate and a field lens. Images are designed with magnifications and optical qualities and positioned at predetermined eye zones having controlled directional properties. The viewer's eyes are positioned in these zones. The size of the zones is related to the aperture of the projection lenses, the magnification produced by the Fresnel(s), and the optical properties and position of the image corrector plate.

Radiation Phantom with Humanoid Shape and Adjustable Thickness

Joerg Lehmann, Joshua Levy, Robin L. Stern, Christine Hartmann-Siantar, Zelanna Goldberg
U.S. Patent 7,151,252 B2
December 19, 2006
This radiation phantom has a body with a general humanoid shape, at least a portion of which has an adjustable thickness. In one embodiment, the portion with an adjustable thickness comprises at least one tissue-equivalent slice.

System and Method for Integrating and Accessing Multiple Data Sources within a Data Warehouse Architecture

Charles R. Musick, Terence Critchlow, Madhaven Ganesh, Tom Slezak, Krzysztof Fidelis
U.S. Patent 7,152,070 B1
December 19, 2006
A system and method is disclosed for integrating and accessing multiple data sources within a data warehouse architecture. The metadata formed

by this method provide a way to declaratively present domain-specific knowledge, obtained by analyzing data sources, in a consistent and usable way. Four types of information are represented by the metadata: abstract concepts, databases, transformations, and mappings. A mediator generator automatically generates data management computer code based on the metadata. The resulting code defines a translation library and a mediator class. The translation library provides a data representation for domain-specific knowledge represented in a data warehouse, including "get" and "set" methods for attributes that call transformation methods and derive a value of an attribute if it is missing. The mediator class defines methods that take "distinguished" high-level objects as input, traverse their data structures, and enter information into the data warehouse.

Current-Biased Potentiometric NO_x Sensor for Vehicle Emissions
Louis Peter Martin, Ai Quoc Pham
U.S. Patent 7,153,401 B2
December 26, 2006
This sensor system measures the amount of nitrogen oxide in a gas. A first electrode is exposed to the gas. An electrolyte is positioned in contact with the first electrode. A second electrode is placed in contact with the electrolyte. A means for applying a fixed current between the first electrode and the second electrode and monitoring the voltage required to maintain the fixed current provides a measurement of the amount of nitrogen oxide in the gas.

Target Molecules Detection by Waveguiding in a Photonic Silicon Membrane
Sonia E. Letant, Anthony van Buuren, Louis Terminello, Bradley R. Hart
U.S. Patent 7,155,076 B2
December 26, 2006
Disclosed herein is a porous silicon filter capable of binding and detecting biological and chemical target molecules in liquid or gas samples. A photonic waveguiding silicon filter with chemical or biological anchors covalently attached to the pore walls binds target molecules. The system uses transmission curve engineering principles to allow measurements to be made in situ and in real time to detect the presence of various target molecules and calculate the concentration of bound target.

Method to Detect the End-Point for PCR DNA Amplification Using an Ionically Labeled Probe and Measuring Impedance Change
Robin R. Miles, Phillip Belgrader, Christopher D. Fuller
U.S. Patent 7,157,232 B2
January 2, 2007
Impedance measurements are used to detect the end-point for polymerase chain reaction DNA amplification. A pair of spaced electrodes are located on a surface of a microfluidic channel, and an alternating or direct current voltage is applied across the electrodes to produce an electric field. An ionically labeled probe will attach to a complementary DNA segment, and a polymerase enzyme will release the ionic label. This phenomenon causes the conductivity of the solution in the area of the electrode to change. This change in conductivity is measured as a change in the impedance between the two electrodes.

Awards

The **Optical Society of America** (OSA) has selected two Laboratory scientists as **OSA fellows** for 2007. **Henry N. Chapman** of the Physics and Advanced Technologies (PAT) Directorate was recognized for his "contributions to x-ray microscopy, coherent x-ray imaging, x-ray optics, and EUV lithography." **James Dunn** of PAT was selected for his "important contributions to the development of soft x-ray lasers and optical diagnostics of dense plasmas."

Both scientists attribute their recognition by the OSA to research opportunities at the Laboratory and, in particular, to the support they have received from the Laboratory Directed Research and Development Program.

The OSA limits its number of fellows to 10 percent of the total OSA membership and awards the honor to members who have served with distinction in the advancement of optics.

Electrical engineer **Grace Clark** of Livermore's Engineering Directorate has been named a **Fellow** by the **Institute of Electrical and Electronics Engineers** (IEEE). The total number of IEEE fellows selected in any one year does not exceed one-tenth of one percent of the worldwide IEEE voting membership. With this distinction, Clark becomes one of only three IEEE fellows currently at the Laboratory.

Clark was recognized for her pioneering contributions to the field of block adaptive filtering. Adaptive filters are electronic devices that automatically adjust to time-varying signal and noise environments. Clark's current research focuses on the areas of signal and image processing and pattern recognition applied to acoustics, electromagnetics, and particle physics.

Mount Holyoke College has awarded the **Mary Lyon Award** to Laboratory researcher **Sarah Chinn** of the Chemistry, Materials, and Life Sciences Directorate. The award is given to a Mount Holyoke College alumna who has been out of college 15 years or less and who demonstrates promise or sustained achievement in her life, profession, or community.

Chinn, who attended Mount Holyoke College from 1993 to 1997, focuses her research on nuclear magnetic resonance (NMR) spectroscopy of solid-, liquid-, and gas-phase systems; NMR probe design and hardware development; optically pumped NMR; and optically detected magnetic resonance.

Abstracts

Stardust Results Challenge Astronomical Convention

In 2004, the National Aeronautics and Space Administration's Stardust spacecraft flew through the tail of a comet called Wild 2, capturing thousands of cometary particles with a collector filled with lightweight aerogel glass foam. On January 15, 2006, the spacecraft ejected its sample return capsule safely onto the Utah desert. A 13-member Livermore team has been examining some of the particles with a full array of instruments to determine their chemistry, mineralogy, crystal structure, and trace-element and isotope compositions. The team's preliminary findings show the comet contains many high-temperature minerals that appear to have formed in the inner regions of the solar nebula. Their unexpected presence strongly suggests that the formation of the solar system included mixing over distances much greater than has been generally believed. Many of the particles also contain organic compounds that are surprisingly diverse.

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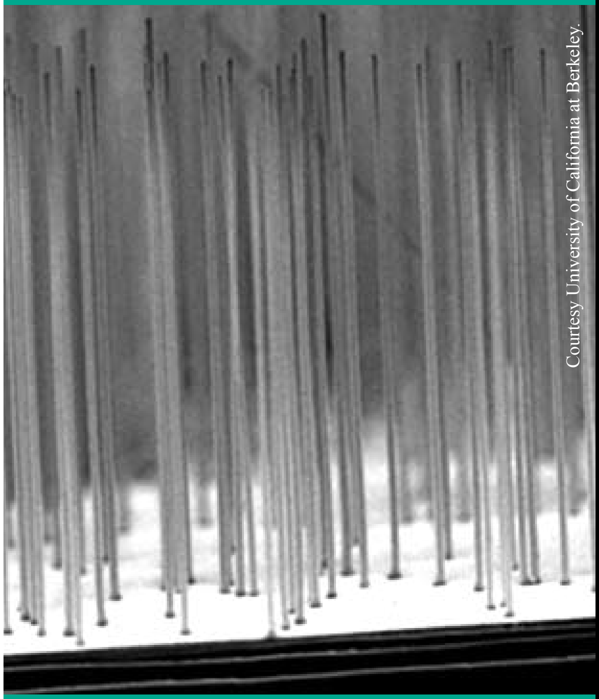
Fire in the Hole

Underground coal gasification (UCG), a process that has been around for 150 years, has shed its "ugly duckling" status and is emerging as a promising new energy source. Earlier problems with contaminating surrounding groundwater can be solved, and the fact that hydrogen accounts for half the total gas product is now considered an asset, not a liability. Because UCG can effectively burn and gasify seams of coal that are too deep to mine or too low in quality to be mined economically, estimates indicate that recoverable coal reserves in the U.S. could be increased by as much as 300 to 400 percent. In countries such as India and China with large reserves of coal and large populations demanding energy, UCG is viewed as a highly promising process. Livermore is a leader among the Department of Energy laboratories in UCG expertise. Laboratory researchers are collaborating with UCG experts around the world to further develop the process.

Contact:
Julio Friedmann (925) 423-0153 (friedmann2@llnl.gov).

U.S. Government Printing Office: 2007/670-074-10027

Quantum Coming of Age



Courtesy University of California at Berkeley.

Livermore scientists are developing quantum molecular dynamic methods to model material processes and evaluate application designs.

Also in May

- *Advances in plutonium science provide researchers with a better understanding of this most mysterious element.*
- *With extremely bright, ultrashort x-ray pulses, researchers can image viruses and complex biomolecules down to the atomic scale.*
- *A Livermore team is collaborating with researchers from the University of California at Davis to examine the growth of raftlike structures in the cell membrane.*

Coming Next Month

University of California
Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551