October 2000

Science & Technology
REVIEW

Getting the Big
## Computational Picture
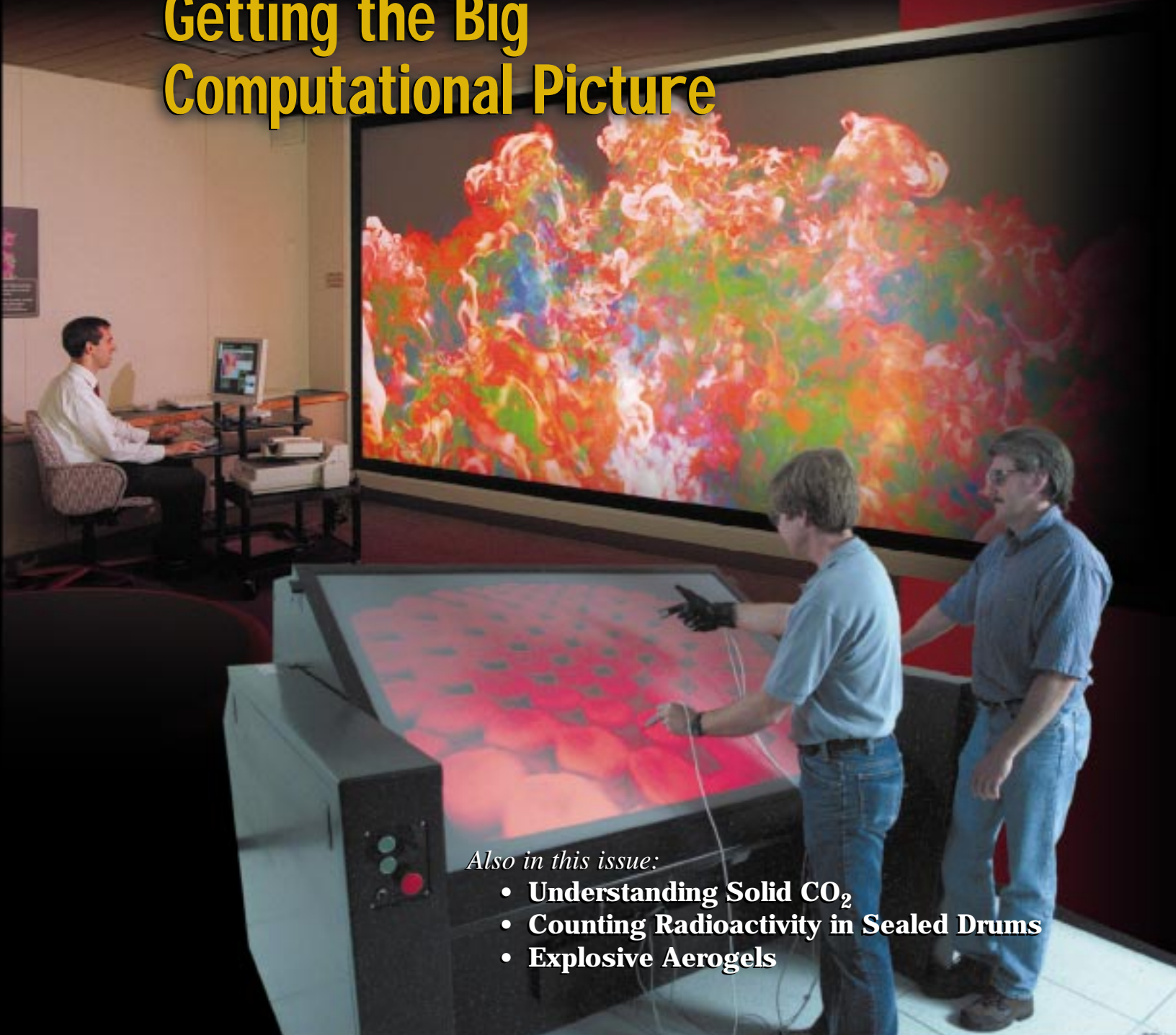
Also in this issue:
- **Understanding Solid CO$_2$**
- **Counting Radioactivity in Sealed Drums**
- **Explosive Aerogels**

About the Cover

The Assessment Theater at Lawrence Livermore features a 5-meter-wide, 2.5-meter-tall power wall (in background), one of the largest interactive displays ever built. The wall transforms reams of supercomputer data into clear and detailed images. It was developed by Livermore's Visual Interactive Environment for Weapons Simulation (VIEWS) program, which supports DOE's Accelerated Strategic Computing Initiative. In the foreground, VIEWS team members are testing data gloves that allow a user to reach out and "touch" three-dimensional images. A new generation of software and hardware tools is making supercomputer data readily understandable. These tools are described in the article beginning on .
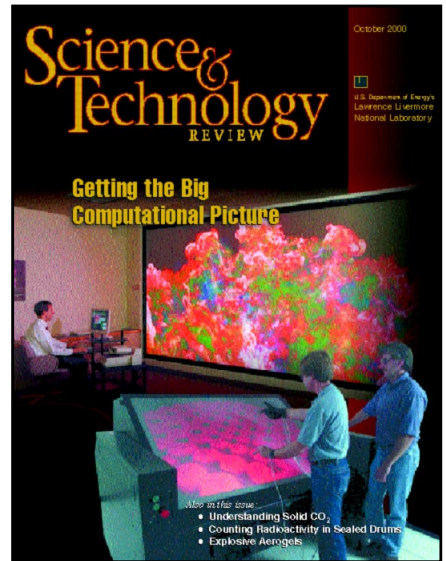
About the Review

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

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str/.

Science & Technology REVIEW

Contents

Features

Research Highlights

Departments

The National Ignition Facility gets go-ahead from DOE

On September 15, 2000, the Department of Energy released a rebaseline report for the National Ignition Facility (NIF) confirming that construction of the project could "move ahead with confidence." NIF is one of five key elements in the science-based Stockpile Stewardship Program to assure the safety and reliability of the nation's nuclear arsenal without nuclear testing. A 192-beam laser, NIF will be one of the world's largest lasers once it is completed. It has been under construction since 1997.

The DOE rebaseline report included the conclusions of an independent review of the project, known as the Carlson-Lehman Review, which occurred at Lawrence Livermore during the week of August 7, 2000. Some forty experts with experience in industrial project management, lasers, accelerators, and procurement heard dozens of presentations on virtually all facets of NIF. The Carlson-Lehman Review concluded that the NIF project can be completed successfully within the total cost and schedule defined by the revised baseline.

"We are pleased that the Department of Energy has validated the go-forward plan for NIF and reaffirmed the importance of the facility for the nation's Stockpile Stewardship Program," said Director Bruce Tarter. "The Department has submitted the new baseline to Congress with supporting documentation, including the very positive results of the Carlson-Lehman Review. This review, recommended by the Government Accounting Office and the Secretary of Energy's Advisory Board, was an independent, high-quality, intensive and rigorous process.…[It] concluded that the project plan was credible, that we have an outstanding technical and management team, and that the cost and schedule proposal is valid."

The DOE report confirms a construction cost of $2.5 billion and completion of the project by September 2008. "This is great news for everyone who works on the National Ignition Facility and the Lab," said NIF project manager Edward Moses. "It is proof that there is a talented team in place to see this project through commissioning and operation." Tarter concluded, "The entire NIF team and the Laboratory is eager to move forward to finish this strategic national asset."
Contact: Susan Houghton (925) 422-9919 (houghton3@llnl.gov).

Russian technology for plutonium immobilization

As they were touring the Russian Scientific Research Institute of Atomic Reactors (RIAR) in May 1999, Lawrence Livermore researchers Les Jardine and Mark Bronson noticed an intriguing piece of machinery. It was a plutonium oxide saltwasher, something that will be useful to U.S. scientists preparing plutonium for immobilization in a ceramic matrix.

Plutonium from dismantled nuclear weapons must be disposed of safely and prevented from falling into the wrong hands. The Laboratory is leading the DOE's research, development, and testing of plutonium disposition by immobilization. The RIAR system that intrigued Jardine and Bronson fits inside a glovebox and is used to wash plutonium oxides free of contaminating chloride salts, which hinder the ceramification process. And while the system removes the chloride salts, it deliberately leaves other contaminants behind, making the plutonium less attractive for proliferation.

The Laboratory recently purchased the RIAR machine and is in the process of modifying and testing it before installation in Livermore's plutonium facility. Says Bronson, the associate program manager for plutonium processing, "We think this will be a big help. It's an automated system, which means it will be faster and more efficient than our own current methods." The Laboratory has relied on a series of beakers and flasks used inside a glovebox to wash, filter, and dry plutonium. The plutonium oxide saltwasher does all three tasks more quickly and with less risk of radiation exposure.

"This is the first known piece of plutonium processing equipment from Russia slated to be used for our own plutonium operations," says Jardine. He adds that the collaboration with Russian scientists to get the system built for use in the U.S. shows "the level of commitment, technical expertise, and quality control that exists in Russia. This equipment shows that their technical people are competent, capable, and dedicated to efficiently handling the plutonium fissile materials."

The DOE has a national effort to treat and immobilize about 13 metric tons of plutonium, which come from Rocky Flats, Hanford, and other DOE sites. The treatment will take place in a new facility to be constructed at DOE's Savannah River site. Once the plutonium is immobilized and turned into disks the size and shape of hockey pucks, it can be sealed inside canisters and stored in a waste depository.
Contact: Les Jardine (925) 423-5032 (jardine1@llnl.gov).

Visualization Tools Take On Supercomputing Challenges

ONE of the most challenging scientific tasks is simulating, in three dimensions, the complex physics of a nuclear explosion. Such simulations are now possible for the first time, thanks to the massively parallel supercomputers of the Department of Energy's Accelerated Strategic Computing Initiative (ASCI).

However, that possibility presents yet another major challenge: understanding the enormous amounts of data generated by the supercomputers and the advanced codes running on them. As described in the article beginning on , personnel from Livermore's Computation Directorate have taken on the task of developing new tools for managing, sharing, and comprehending three-dimensional ASCI simulation data. Much of the effort in this activity is focused on data and visualization corridors. These corridors represent paths through which data rapidly flow, permitting users to easily interact with each other and with their data. In this way, scientists can readily analyze and understand the simulations and their implications for the nation's nuclear stockpile.

Constructing data and visualization corridors requires changes in networking, systems architecture, large-scale data management, and the way in which people interface with computers. A major focus of these changes is on achieving better ways to transform raw data into richly detailed graphical representations from which the human brain can find patterns, spot anomalies, and draw inferences.

Until recently, the development of advanced visualization tools was a modest effort scattered across many organizations nationwide. What's more, few commercial products were available to handle the data generated by computers the size of the ASCI systems. As a result, the DOE national laboratories have embarked upon a program to develop new data manipulation and visualization systems.

As part of the overall DOE effort, Livermore computer scientists are pioneering new approaches to computing, information handling and storing, and communications—all requiring advances in both software and hardware. Among their successes to date are the giant Assessment Theater housed in one of Livermore's building complexes, the large flat-panel displays now being installed in scientists' offices, dedicated visualization servers, and software programs that allow users to sift through reams of data and focus on areas of greatest interest.

Lawrence Livermore's effort involves collaborations with other national laboratories, U.S. industry, University of California campuses, and other universities. Perhaps the most important collaboration, however, is with the weapon scientists who are the end users of the new tools.

Although the work centers on developing tools for the nuclear weapons program, one can expect the advances to benefit other fields of scientific inquiry that use supercomputers for large-scale simulations or for analyzing large amounts of experimental data. Understanding protein folding and its effects on drug interactions, modeling long-term global climate change, modeling materials, designing for automobile and aircraft safety—all could be uses for the new supercomputing tools. Clearly, advanced visualization techniques can assist a host of major scientific disciplines and challenges.
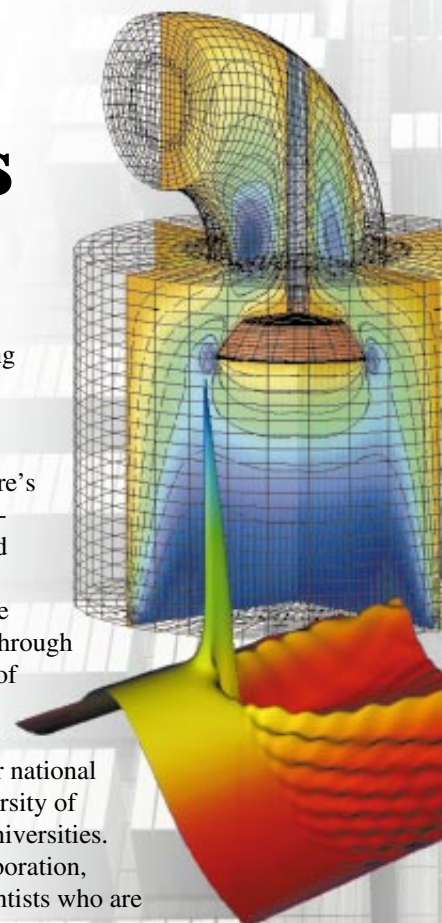
n David Cooper is Associate Director, Computation, and the Laboratory's Chief Information Officer.

A New World of Seeing

Livermore hardware and software tools allow users to more clearly visualize and hence better understand vast amounts of supercomputer data.

L AWRENCE Livermore scientists using the world's most powerful supercomputers are turning to another computational engine—the human visual system—to make sense of the huge volumes of data produced by the giant computers. Increasingly, advanced three-dimensional visualization tools are seen as key to gaining greater insight from the reams of computer data that can easily overwhelm scientists.

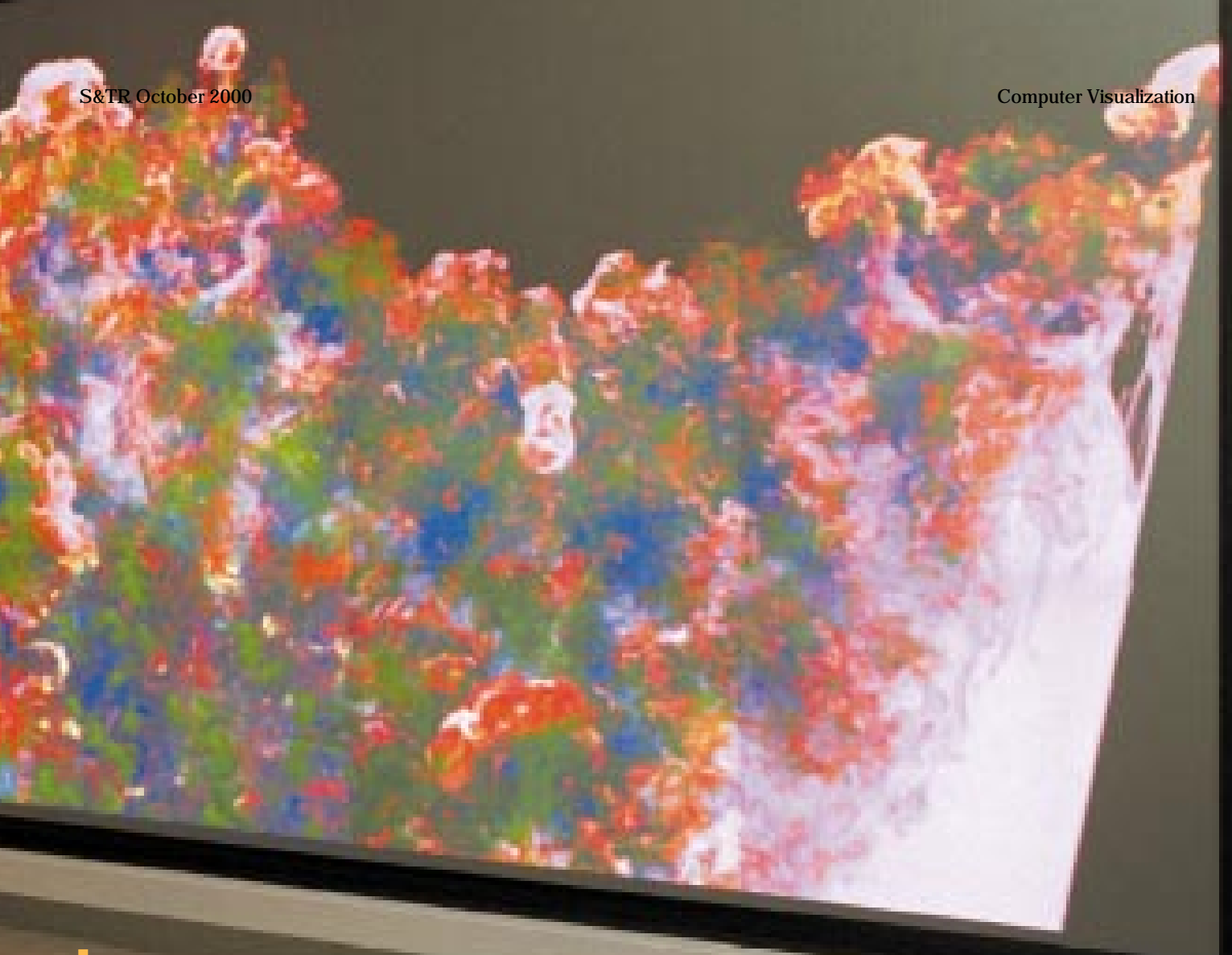Developing the new generation of visualization and data management tools is the task of a program called VIEWS (Visual Interactive Environment for Weapons Simulation) that is part of the Laboratory's Computation Directorate. Formed in 1999 by combining several related activities, VIEWS integrates hardware (storage, networking, and visualization) and software (data exploration and management) to help interpret the supercomputer data

generated in the Department of Energy's Accelerated Strategic Computing Initiative (ASCI) program. VIEWS researchers also explore innovative visualization approaches such as stereo display goggles and advanced human–computer interfaces.

"See and understand" is the mantra of the 40 VIEWS computer scientists and electronics engineers, according to computer scientist and program leader Terri Quinn. The program's new visualization tools, she says, together open a larger, clearer window into ASCI data that promotes greater understanding by relying on the human eye to discern subtle changes among colors and patterns. In this way, scientists can compare the results of different codes, compare code results to experimental results, and spot errors in new codes.

ASCI was established to develop computer tools to help validate the safety, reliability, and performance of the nation's nuclear stockpile in the absence of nuclear testing. The massively parallel ASCI supercomputers employ thousands of processors that work in unison to generate terabytes (trillions of bytes) of raw data. Advanced visualization techniques allow scientists to track physical parameters such as temperature, pressure, and velocity shake by shake (a shake is 10 nanoseconds) as they follow the detonation of a nuclear device. Seeing events proceed in three dimensions is necessary because component aging and manufacturing variations introduce asymmetries whose effects on performance must be understood.

Lawrence Livermore National Laboratory

The VIEWS effort includes collaborations with a number of University of California (UC) campuses, the University of Utah, and the Supercomputer Centers at the University of Illinois and UC–San Diego, as well as colleagues at other DOE national laboratories. Much of the research is conducted at the Laboratory's Center for Applied Scientific Computing, which maintains strong links to the nation's academic community.

Quinn says the work demands close relationships with physicists from the Laboratory's Defense and Nuclear Technologies Directorate, who develop and use ASCI codes. Says Quinn: "Working with 3-D simulation data is new to everyone, and we don't know how best to go about it. We speculate on how best to view 3-D data sets and then we develop solutions. We share our solutions with the physicists to obtain their reactions." She also notes that the group must "run as fast as it can" to meet physicists' demands for faster

and easier ways to access the terabytes of ASCI data.

The hardware backbone supporting the advanced visualization tools includes an expanding network of graphics workstations, two visualization servers (called TidalWave and EdgeWater), a separate video delivery network using optical fibers, and accompanying storage systems. All elements are connected to ASCI computers via the Laboratory's classified network of high-speed optical fibers.

Numbers Are Transformed

The visualization servers free the ASCI supercomputers to do what they do best: sheer number crunching. The servers use dedicated microprocessors, "graphics pipes" (sophisticated graphics cards that support high-end graphics techniques), and several terabytes of disk storage to transform reams of numbers from ASCI runs into graphical objects. The servers are capable of redrawing complex objects interactively many times every second and delivering

the resulting imagery to a growing number of scientists' offices and to a 15-projector display wall.

Quinn says that visualization techniques (2-D simulations, graphs and charts, and low-resolution 3-D views) that were developed for earlier generations of computers can't handle the scale and complexity of ASCI calculations. For example, the first-ever 3-D simulation of a nuclear weapon's primary (the first stage of a hydrogen bomb) was completed last November using Livermore's Blue Pacific supercomputer. The simulation used a mesh composed of tens of millions of cells, hundreds of times more than a comparable 2-D simulation. The simulation ran a total of 492 hours on 1,000 processors and used 640,000 megabytes of memory in producing 6 million megabytes of data contained in 50,000 graphics files.

"With 3-D we appeal to the mind's ability to see patterns," says Livermore physicist Jim Rathkopf. He explains that stockpile stewardship involves "a lot of

The TidalWave visualization server drives Livermore's Assessment Theater as well as advanced displays in individual offices. TidalWave and its newer companion, EdgeWater, use dedicated microprocessors, "graphics pipes" (both contained in stacked units on the left), and over 20 terabytes of disk storage (on the right) to transform ASCI data into graphical objects.

physics happening simultaneously." A major advantage of 3-D visualization is the ability to display several physical parameters, such as pressure, temperature, and density. New methods of visualizing those parameters are being devised to indicate the direction of fluid flow in time and space.

Livermore physicist Steve Langer notes, "People are still learning how to explore the 3-D nature of their data. We're finding out what kinds of visual information are useful and what kinds aren't." Three-dimensional visualization is particularly useful to Langer because he simulates the compression of tiny fusion capsules by the National Ignition Facility, now under construction at Lawrence Livermore as a key stockpile stewardship asset. Advanced visualization permits Langer to follow a simulated imploding capsule in time to determine how spherical it will remain as it is compressed.

Quinn says that terascale data visualization makes unprecedented demands on display resolution and leads to a quest for ever-more pixels. "If you put lots of pixels on a screen, you can more easily pick out small anomalies in performance that could turn out to be critical," she says. "Having more pixels and a method to display them—without choking the rest of the system—is important."

Pixel is short for picture element, a single point in a computer display of a graphic image. (On color monitors, each pixel is composed of three dots—red, blue, and green— that appear to converge into one.) Computer monitors divide the screen into thousands (or millions) of pixels, arranged in rows and columns. The quality of a display largely depends on its resolution, that is, the number of pixels.

Physicists can now follow in three dimensions a simulated imploding laser target capsule to learn how to control deviations from the desired spherical shape.
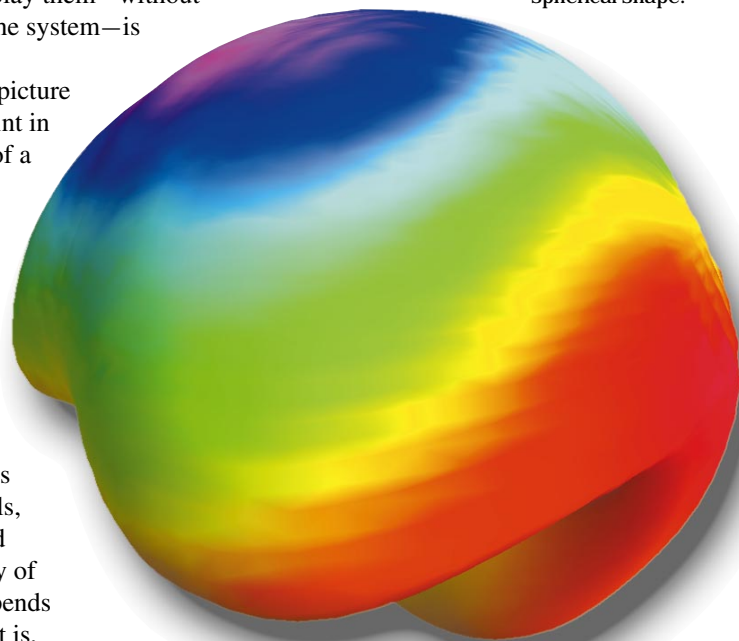
The power wall in the Assessment Theater (left) permits physicists to see ASCI codes in detail. On its screen is a simulation of two gases intermixing after being hit by a shock wave. At right, an operator uses projectors arranged in a 5 by 3 array to create and control the large, clear display.

A resolution of 1,024 by 768 has nearly 800,000 pixels, a resolution of 1,280 by 1,024 has about 1.3 million pixels, and a resolution of 1,600 by 1,200 has nearly 2 million pixels.

The more pixels, the greater the picture detail, and often, the greater the insight on the part of the user. In response to the need for greater resolution, VIEWS staff have begun an effort to develop "personal" displays that have far more pixels than common computer monitors. They have also built one of the largest interactive displays ever, called the Assessment Theater.

A Wall Projects an Eyeful

The Assessment Theater is the most striking example of Livermore's new

Arrays of flat-panel displays are being installed in individual offices of ASCI scientists.

visualization world. Here, scientists follow computer-generated ASCI movies of unprecedented image quality on a 5-meter-wide by 2.5-meter-tall projection screen called a power wall. First installed in December 1998, it was upgraded substantially in 1999.

The power wall currently uses 15 state-of-the-art projectors arranged in a 5 by 3 array to create a large-scale display with great detail and clarity. Each projector is driven by a visualization server to generate an image with a 1,280 by 1,024 resolution, similar to that of a high-end monitor. The overall display has a total resolution of 6,400 by 3,072, or nearly 20 million pixels, giving it a resolution 15 times better than that of a typical desktop display.

The projectors must be kept in sync, particularly in edge-matching each projected image to its neighbor without overlapping pixels or creating separation lines between the tiled projections. Thankfully, the liquid-crystal-display projectors have a single lens that can be adjusted for exact pixel positioning without moving the projector body. Once again, the human eye comes into play because, says computer scientist Randy Frank, "The human eye is particularly adept at detecting image edges and color gradients." The projector's color output, which varies as the projectors' xenon lamps age, must also be properly calibrated. Livermore experts are developing a computerized system to automatically adjust each projector's color output.

Electronics engineer Bob Howe, who leads the deployment of new VIEWS systems, says the power wall is an essential tool for answering the basic question, "What on earth can we learn from all of this data?" He says that by using the power wall, a large group of scientists can collectively view simulations (at rates up to 20 frames per second) and then stop or zoom in on specific features. In this way, many scientists can work together and share their interpretations and insights.

The power wall is often the only way to view a simulation when very fine detail needs to be scrutinized. Simulations are based on meshes of millions of individual cells, and a power wall permits the clear visualization of individual cells. On a typical desktop monitor, individual cells can be visualized, but it's easy to lose sight of what is happening in the tens of thousands of surrounding cells. "Details we see on a power wall simply get lost on a typical computer monitor. To see the context, we need larger displays," says Livermore physicist Tom Adams.

Although scientists are still gaining experience in using the power wall, they are pleased with the results thus far. One physicist had spent several days

searching in vain on his desktop monitor to locate an error he knew resided in his newly written code. It didn't take more than a few minutes viewing the simulation on the power wall when he jumped out of his seat and pointed to a section of the display containing a deformed cell. "That's it!" was his exhilarated response.

More Tools for Scientists

Another power wall, a smaller 4 by 2 array, will be housed in the Visualization Work Center, now under construction and scheduled to debut by late December. While the Assessment Theater's single large room is suitable for team visualizations and for formal presentations, the Visualization Work Center is designed to allow small teams and individual users to work simultaneously. For example, a team of scientists could divide the wall into two 2 by 2 displays to simultaneously compare two simulations. The center will have several rooms with advanced visualization equipment, including arrays of flat-panel displays connected by high-speed optical fibers to the visualization servers. "We want to make advanced visualization tools ever more accessible to scientists," says Rathkopf.

Smaller aggregations of 17-inch, high-resolution (1,280 by 1,024), flat-panel displays in 2 by 1 and even 2 by 2 configurations are being installed in the offices of ASCI scientists. Connected to the visualization servers, the displays provide a new level of resolution for an individual office.

Users have the choice of using the flat-panel displays on a desk or hanging them on the wall. They can choose to have the panels tiled as a mini power wall or have each monitor assigned to different software windows. Still other scientists are opting for more traditional cathode-ray-tube monitors that measure 64 centimeters diagonally and have a resolution of 1,920 by 1,600 (3 million pixels).

Despite the introduction of these new monitors, VIEWS staff are not satisfied with current display technologies. They are working with the Laboratory's Information Science and Technology Program to encourage companies to produce better monitors. The Digital Display Integration project, headed by electronics engineer Norm Bardsley, is evaluating a new generation of flat-panel displays that exhibit more than 5 million full-color pixels. Bardsley says flat-panel displays, with their inherent sharpness, have the best potential for achieving ever higher levels of resolution.

The display project is also working to speed the transition from the traditional analog interface between computer and monitor to the new digital interface standard. Digital interfaces make far more efficient use of flat-panel displays. In like manner, Bardsley and colleagues are working to implement digital

connections that will greatly speed data transfer for ASCI applications using the newest optical-fiber technology.

Software Advances to Keep Pace

Trying to keep pace with the explosive growth of new visualization hardware are software tools that allow scientists to more easily store, retrieve, and search ASCI data. Many of the tools are developed by Livermore's Scientific Data Management (SDM) project. "We want scientists to more efficiently use the power of ASCI machines and quickly zero in on data they want to retrieve for further analysis," says computer scientist and group leader Celeste Matarazzo.

The group's work focuses on the creation and use of metadata, which are data describing the contents or relevance of a computer file. (Matarazzo compares metadata to sticky notes on the outside of a file folder.) In this case,
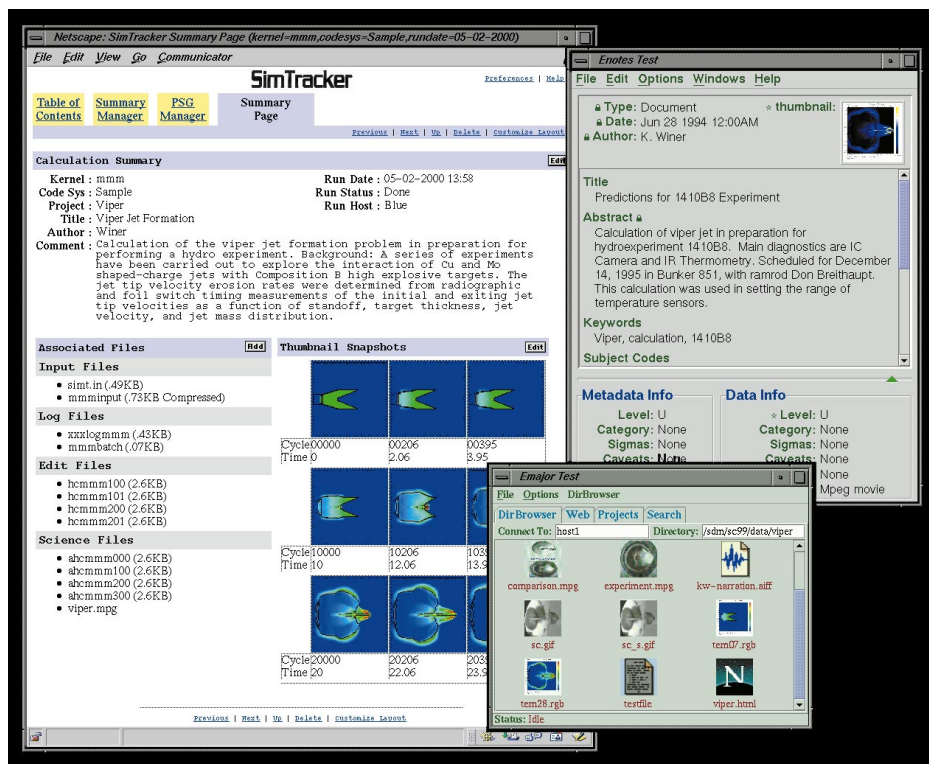
New software tools such as SimTracker (left) and a companion annotation editor and viewer (right) help scientists keep track of and access files used in ASCI analyses.

metadata ranges from a scientist's brief notes on a particular simulation to system-level documentation on the size, type, and creation date of a set of data.

SDM project members developed SimTracker, a secure Web-based metadata tool that keeps track of files used in a simulation and summarizes the results. SimTracker automatically generates summaries that provide a quick overview and index to archived simulation results. The summaries provide convenient access to the data and analysis tools, graphical snapshots, links to files, and assorted annotations. SimTracker is used not only at Livermore but also at Sandia and Los Alamos national laboratories and has drawn interest from the Department of Defense and the larger scientific community. The group has also developed Enotes, a metadata editing and browsing tool that works like an online notebook, as a companion to SimTracker.

The workhorse software for visualizing and analyzing ASCI data is a program called MeshTV. The program visualizes data for 3-D meshes ranging in size from hundreds of thousands to hundreds of millions of cells. It can present results from a host of displays varying from a power wall to a desktop monitor. It handles many different mesh types, provides many different ways of viewing the data, and is virtually independent of the hardware being used. Mesh cells are all independent, and one cell can contain multiple types of materials for realistic simulations.

MeshTV provides data comparison through multiple side-by-side graphics windows, overlaying of images, and simultaneous display of data from
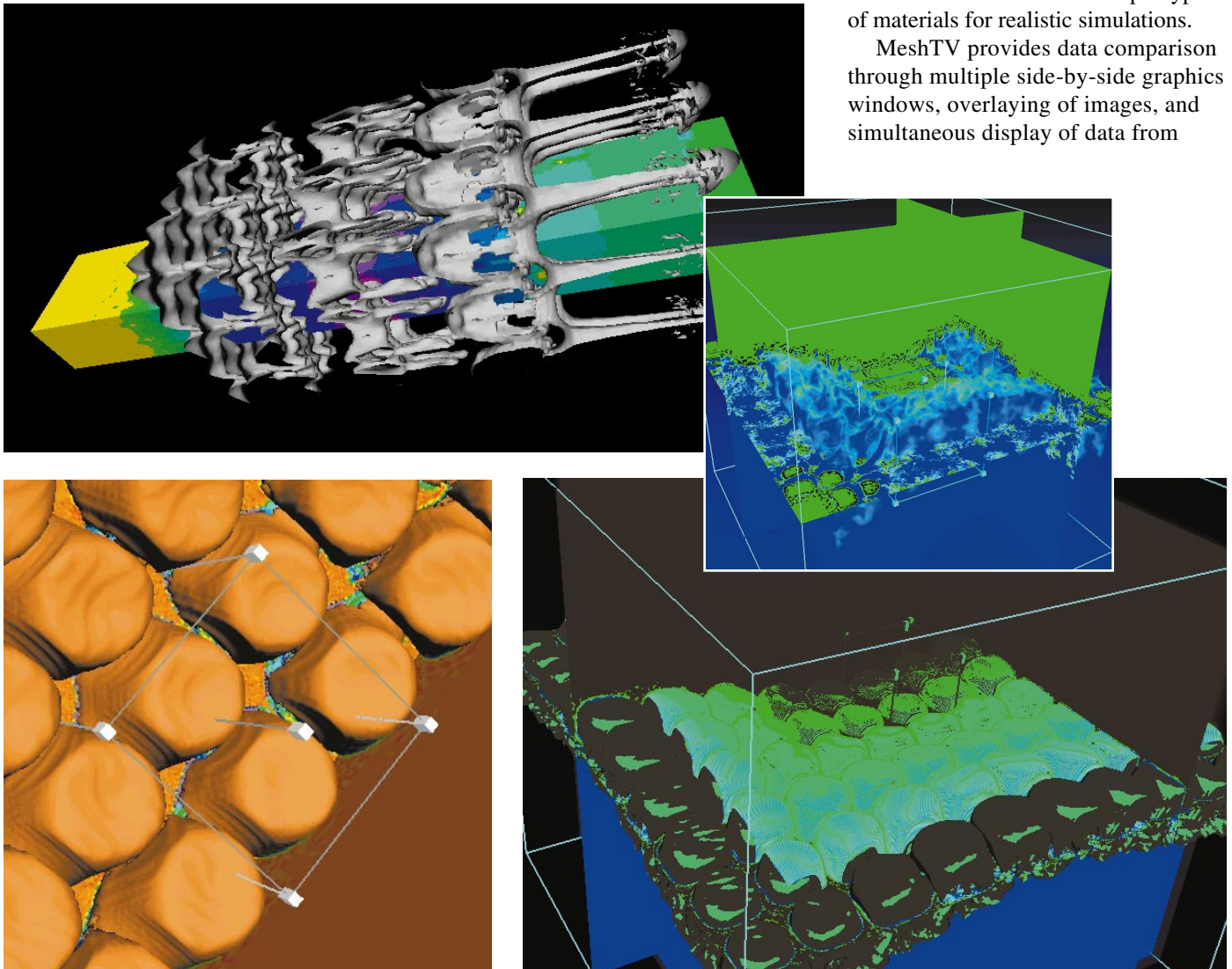
The Terascale Browser easily deals with terabytes of data and produces images like these before "handing off" the task to MeshTV.

different files or different data from the same file. It can play an animation of the user's data changing over time. A user can rotate, zoom, or pan an object while the movie is playing.

The program was originally developed in the early 1990s by Livermore computer scientists Jeff Long and Eric Brugger to help scientists analyze data produced by codes much less sophisticated than today's. It was modified to take advantage of the power of ASCI's massively parallel supercomputers. With this modification, typically hundreds to a thousand of the more than 5,000 processors in an ASCI supercomputer work together to display changes in a mesh. The program has also been enhanced to run on a power wall.

New Browser for Terascale Data

A VIEWS visualization project headed by Randy Frank is developing even newer ways to explore the volumes of ASCI data. One important tool, the Terascale Browser, made its debut in July. The program can be used on the desktop as well as on a power wall. "No commercial visualization software exists that can handle terabytes of information," says Frank. "Some give up, while others can take hours to redraw."

The Terascale Browser rapidly investigates large data sets by providing an easy-to-navigate overview of a simulation. It is not intended to be a full-featured visualization tool, but rather a system to allow scientists to explore an entire terabyte data set to find areas of

interest that they can then pursue in greater detail with full-featured tools like MeshTV. The software creates new images in less than one second by making use of specific features of ASCI hardware. In particular, it uses what Frank terms "terascale technologies," which include speculative techniques that make assumptions about what the user might want to see next.

The group has also produced a software program called X-movie for playing ASCI animations at 20 frames per second (similar to video) on the nearly 20-million-pixel power wall. "Displaying images 20 frames per second is not hard to do if your pixel count is small," says Quinn. "Displaying 20 frames per second when you have 20 million pixels is quite

Livermore computer scientists test the usefulness of "data gloves" that allow the user to reach out and seemingly move and examine images. The gloves are being tested with a novel desktop display that is also under evaluation.

an accomplishment." The program permits users to zoom in and out of selected areas and move forward and backward in time, in addition to providing VCR-like controls; it is ideal for power-wall presentations.

Research in Goggles and Gloves

Frank's group tests new commercial visualization hardware, from power walls to stereo display goggles, in a laboratory near the newly arrived ASCI White supercomputer (see *S&TR*, June 2000, pp. 4–14). The group is currently exploring the effectiveness of goggles that give the illusion of 3-D objects popping out of a computer monitor. The goggles have liquid crystal shutter lenses. In conjunction with specialized software, the goggles alternate between left- and right-eye-specific images on a monitor 120 times a second. With each eye seeing a different perspective, on-screen objects appear to have real depth and texture. "Although this technology is not new, applying it to large scientific simulations is still under investigation. The resolution of these immersive-type displays is still lower than what we would like," says Quinn.

A new generation of projectors might also allow stereoscopic eyewear to be used with a power wall. Livermore experts are also testing the combination of the goggles and "data gloves." The gloves, electronically attached to a workstation, allow the user to reach out and seemingly move and examine the 3-D images.

In a related research effort, Livermore computer scientists are exploring new ways to allow users to interact with their data in a more intuitive manner. For example, power-wall users must currently enter commands using a workstation and a mouse. One promising technique would allow users to stand directly in front of a power wall while a camera tracks and translates their hand gestures into computer commands. A sweep of a hand, for example, might be a signal to play an animation, while a hand held up might be a stop command.

The group is also keeping a watchful eye on the rapid evolution of personal computer technology, particularly graphics cards for PCs. One idea is to use networks of hundreds of PCs to achieve the same performance as a vastly more expensive visualization server. The Laboratory is funding a research group at Stanford University to determine if such an idea makes both practical and economic sense "We're taking advantage of the tremendous growth in the PC game industry and using the same advanced graphics cards game that players use," says Quinn.

Quinn says that both VIEWS developers of new visualization tools and early users among ASCI scientists are true pioneers in the new world of visualization. Both groups have much to learn about how best to present, store, and analyze ASCI data. However, the many successes to date show that Lawrence Livermore researchers are on the right track as they help to assure that the nation's nuclear stockpile remains safe, secure, and reliable.

—Arnie Heller

For further information contact
Terri Quinn (925) 423-2385
(quinn1@llnl.gov).

About the Scientist

TERRI QUINN is the assistant department head for Scientific Computing and Communications in Livermore's Computation Directorate. She leads the Visual Interactive Environment for Weapons Simulation (VIEWS) program, which is responsible for research and development, deployment, and operations of scientific visualization and data management systems for the high-performance computers developed by the Accelerated Strategic Computing Initiative. She has been a computer scientist and software engineer at Lawrence Livermore for 15 years, working in the Nuclear Weapons Program, Treaty Verification Program, and Yucca Mountain Program. She received a B.A. in mathematics from the University of California at Irvine in 1977, and an M.S. in engineering and applied science from the University of California at Davis in 1984. She was a nuclear engineer in the Naval Sea Systems Command, Division of Nuclear Reactors, in the period between her undergraduate and graduate education.

The Many Faces of Carbon Dioxide

THE only solid carbon dioxide most of us know is the dry ice we use for cooling or in Halloween witch's brew. But researchers have known one other form of it for some time and recently isolated several more in the laboratory. One of the new-found forms is nearly as hard as diamond, and indications are that it will conduct heat just as well, too. Basic research in Livermore's mission-related work has led to yet another surprising and important scientific discovery.

Carbon dioxide (CO_2) is a simple and nearly inert molecule. It is abundant in the atmosphere of Earth and other planets and is also a major byproduct of high-explosive detonations. Understanding how it and the other byproducts of high-explosive detonations—water, carbon, and nitrogen—behave at detonation pressures and temperatures is important for creating accurate models for codes that simulate nuclear weapons performance. Studying the optical, mechanical, and energetic properties of the individual reaction products at high pressures and temperatures provides important experimental data for improving Livermore's models to predict the performance of high explosives.

The split second of a high-explosive detonation may produce temperatures as high as 5,500 kelvin and pressures up to half a million times that of Earth's atmosphere. Chemists and material scientists have suggested a number of molecular phases for CO_2 at various high pressures and temperatures, but their structure and stability have not been fully characterized. That is changing, however.

In experiments using Livermore's diamond anvil cell to slowly increase pressures up to millions of Earth atmospheres, a team led by physicist Choong-Shik Yoo has verified two forms of solid CO_2 never before seen in the laboratory, known as CO_2-IV and CO_2-V. The team also has experiments under way on a third form, CO_2-II, which has weaker chemical bonds. All three forms are very different from one another as well as from the two previously known molecular phases, CO_2-I (dry ice) and CO_2-III.

The phase diagram for carbon dioxide shows the pressures and temperatures at which changes in phase occur for CO_2 based on results to date. All five phases are solid in one form or another, but they differ greatly in their molecular configuration

and crystal structure and, more importantly, in the nature of their chemical bonding and the strength of intermolecular interactions. The intermolecular interactions change from weak quadrupolar interactions in the linear molecular phases (I and III), to relatively strong dipolar interactions in the bent-molecular phase IV, and eventually to strong covalent bonds in the polymeric phase V. (Results of the most recently discovered phase, CO_2-II, are just beginning to be understood.)

The evolving intermolecular interactions are in line with recent theoretical and experimental results that suggest that many simple molecules will become polymeric and even metallic at high pressures and temperatures. These findings have important implications for the chemistry of high-explosive detonations, which entail similar temperatures and pressures.
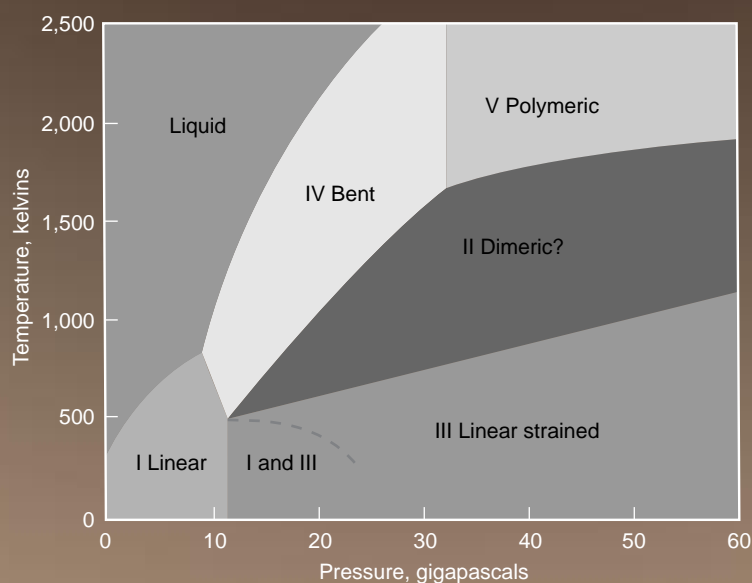
Phase diagram for CO_2, showing pressures and temperatures at which the phase changes.

Carbon dioxide crystallizes into CO_2-I with a pressure of 1.5 gigapascals at room temperature. Increased pressure on CO_2-I produces CO_2-III, which becomes a highly strained, high-strength solid above 20 to 30 gigapascals. CO_2-III is fairly stable at room temperature to about 70 gigapascals.

The Livermore team turned up both the pressure and temperature to isolate CO_2-V, the polymeric solid, using the synchrotron facility at Grenoble, France. They found that CO_2-V has extremely low compressibility, similar to that of cubic boron nitride. This suggests that the carbon dioxide polymer could be used as a superhard material just as cubic boron nitride and diamond are. What is especially interesting about CO_2-V is that it shows nonlinear optical behavior. The frequency of light that passes through it doubles, which may lead to a new class of generating materials for high-power lasers.

More recently, Yoo's team discovered CO_2-IV at pressures between 12 and 30 gigapascals. Its bent molecule is the precursor to polymeric CO_2-V. Also, CO_2-IV has proved to be optically nonlinear.

Crystallizing a Liquid

To create CO_2-V, the team placed a small amount of condensed, liquid CO_2 between the two tips of the diamond anvil cell and squeezed it to pressures of about 40 gigapascals, or 400,000 times the air pressure at Earth's surface. At the same time, they used a neodymium-doped yttrium-lithium-fluoride (Nd:YLF) laser to indirectly heat the CO_2 to 1,800 kelvins.

When the compressed sample was heated, the team was surprised to see a visible emission of green light. The incoming laser light at the infrared wavelength of 1,054 nanometers had been frequency doubled to 527-nanometer light, which is green. The green light being emitted is the second harmonic of the laser light used to heat the sample.

Because CO_2 absorbs the Nd:YLF light poorly, the team heated the sample indirectly by scattering micrometer-sized ruby chips in it and heating the chips with the laser. In other experiments, they used a platinum foil or a rhenium gasket for heating. The experiment was repeated 20 times and yielded the same results each time, regardless of the heating material used. "We wanted to verify that the frequency doubling we saw was not the result of contamination from the heating materials," says Yoo.

The sample, reduced to just a few micrograms, had become an extended solid phase of CO_2. X-ray diffraction, Raman spectroscopy, and other forms of analysis showed that the carbon and oxygen atoms had rearranged themselves in chainlike patterns connected by single carbon–oxygen bonds, a structure similar to that of a high-temperature modification of quartz.

The team found CO_2-IV by laser-heating CO_2-III at pressures between 12 and 30 gigapascals to 1,000 kelvins
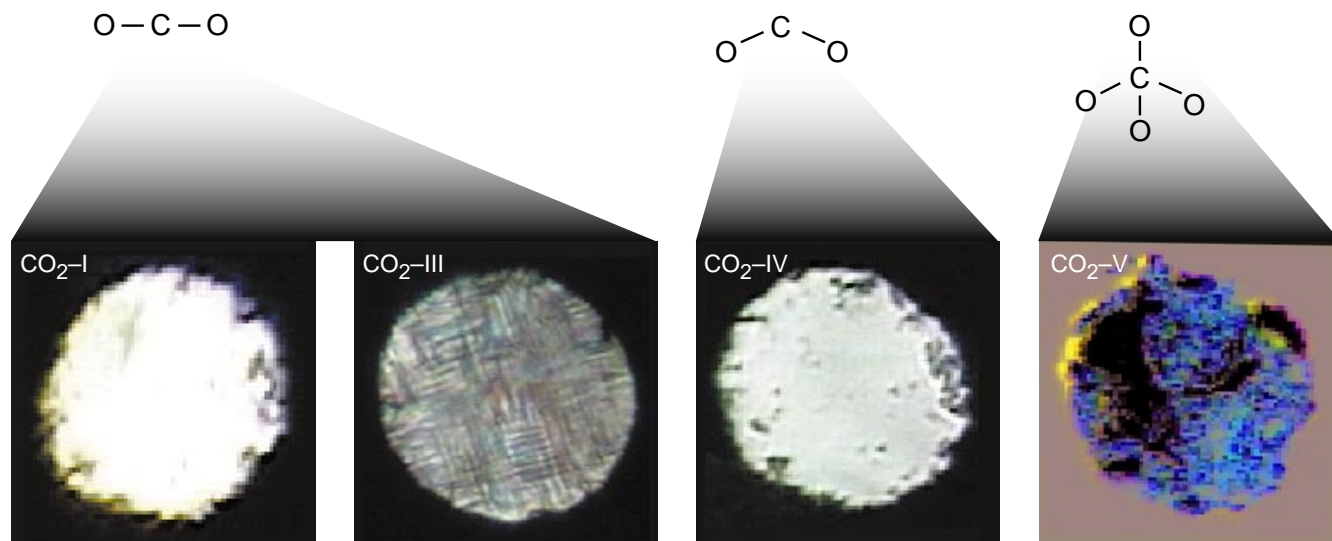
Phase changes in carbon dioxide result in changes in its molecular configuration. Phases I and III are linear structures, phase IV is a bent molecule, and phase V has covalent bonds. (Phase II was recently discovered and is still under study.)
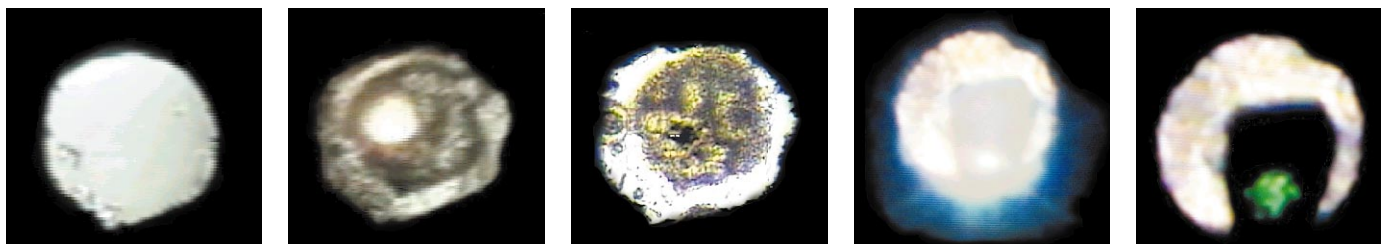
Heated CO_2-V emits green light, which is the second harmonic of the laser light used to heat the sample.

and quenching the sample to 300 kelvins. They found that with increasing pressure, the interactions weakened. At about 80 gigapascals, the quenched sample collapsed into an amorphous solid. If laser heating was continued with increasing pressure, the CO_2-IV transformed into polymeric CO_2-V above 30 gigapascals.

Stabilizing CO_2-V

If this new, very hard CO_2-V can be stabilized at ambient temperatures and pressures, it will have many uses. New classes of high explosives, nonlinear optical materials with high thermal and mechanical stability, high-strength glass, and superhard materials for tools are all candidates. Crystals that can double the frequency of laser light from infrared to green would be valuable for Livermore's inertial confinement fusion energy program.

So far, once CO_2-V has been created at high pressures and temperatures, it retains its structure at room temperature but only at pressures above 1 gigapascal. Below that pressure it collapses and is no longer a polymer. Nearly half a century ago, when scientists were trying to produce the first synthetic diamonds, the same problem arose. Diamond could be synthesized only at high temperatures and pressures until

scientists learned its growth mechanism. Then they were able to synthesize it at lower pressures and temperatures using catalysis. Now diamond is routinely manufactured at ambient pressure with very little heat. Says Yoo, "We'll be looking for something like that with this new carbon dioxide."

Other applications of the team's research are truly out of this world: the experimental temperatures and pressures used to create CO_2-V are comparable to those inside giant gas planets like Uranus and Neptune. Who knows what lurks in their interiors?

—*Katie Walter*

Key Words: carbon dioxide, diamond anvil cell.

Award-Winning System Assays Radioactive Waste with Radiation

MORE than half a million drums of radioactive waste are stored at 30 Department of Energy sites across the nation, with thousands more to come as additional facilities at weapons complex sites are dismantled. All of these drums must be assayed to determine and verify their contents and levels of radioactivity before they can be transported for permanent storage or disposal.

A system that assays containers of radioactive waste safely, accurately, and nonintrusively has garnered a prestigious R&D 100 Award for Lawrence Livermore National Laboratory and its commercial partner, Bio-Imaging Research, Inc. (BIR) of Lincolnshire, Illinois. This award is presented annually by *R&D Magazine* to "the 100 most technologically significant new products and processes of the year."

The award-winning Waste Inspection Tomography for Non-Destructive Assay (WIT-NDA) system was developed by a team of engineers and physicists headed by Livermore's Patrick Roberson and Harry Martz. The system combines active and passive computed tomography and nuclear spectroscopy to accurately quantify all detectable gamma rays emitted from waste containers. The WIT-NDA is part of BIR's Waste Inspection Tomography system, which provides nondestructive examination and assay of radioactive waste and has been commercially available since August 1999. "The WIT-NDA is an excellent example of successful technology transfer between a DOE national laboratory and a small private business," says Richard Bernardi, WIT program manager for BIR.

Bio-Imaging Research, Inc. of Lincolnshire, Illinois, is collaborating with Livermore researchers in developing nondestructive evaluation technology. Here, BIR's trailer is the site of an experiment using active and passive computed tomography to identify and quantify materials inside nuclear waste drums.

Lawrence Livermore National Laboratory

Safe and Accurate

As recently as 10 years ago, researchers could accurately assay the contents of a waste drum only by sampling, and for that they had to break the container seals. Opening containers meant workers—and possibly the public—risked exposure to radiation and other hazardous materials. Beginning in 1990, physicists Harry Martz and David Camp headed a Livermore team to research ways to estimate the radioactivity of drum contents from the outside. Over the years, the team received funding for research and development from Livermore's Engineering Directorate, the Laboratory Directed Research and Development program, and DOE's Environmental Management program, as well as from BIR.

The Livermore team developed a process that pinpoints where radioactive materials rest inside the drum and accurately quantifies and identifies these isotopes, whether they are plutonium, uranium, or some other gamma-ray-emitting radioactive waste. "This system is unique in that to use it, we don't need to open the container, we don't need any prior knowledge of the radioactive waste inside, and we don't have to calibrate the system to a specific waste stream," explains Roberson.

Determining the exact amount of radioactivity in each drum is essential to DOE's waste disposal efforts, Roberson notes. "DOE needs to characterize its radioactive wastes to verify that the waste drums meet criticality constraints and to differentiate transuranic from low-level wastes." Transuranic waste drums contain isotopes with atomic numbers greater than 92 (such as plutonium and uranium), radioactive decay half-lives greater than 20 years, and radioactivity levels greater than 100 nanocuries per gram of net waste weight.

Each class of waste is sent to a different disposal site. For example, the DOE Waste Isolation Pilot Plant (WIPP) in New Mexico accepts only transuranic wastes and, furthermore, has a limit on the total amount of radioactivity that can be placed within its underground repository. So waste drums must be nondestructively assayed to determine if they contain transuranic waste, and all radioisotopes in each drum must be inventoried to ensure that the WIPP limit is not exceeded. With NDA systems of lesser accuracy, waste regulators must err on the side of safety and designate waste disposal based on higher-end estimates of radioactivity.

Two-Step Process

The WIT-NDA has a unique two-step process that provides an assay of greater accuracy than previously possible. It collects two tomographic measurements—one active and one passive—using six external radioactive sources collimated to shine through the waste drum into six opposing, high-purity germanium detectors.

The first step is active computed tomography, which, like radiographic techniques that produce medical x rays, measures the attenuation of radiation intensity that travels from an external source through an object to a detector. In this active measurement, the external radiation sources are aimed at the sealed drum. The sources emit gamma rays at discrete energy levels. As the rays pass through the drum and the various densities of material within, they are attenuated to varying degrees. On the other side of the drum, the gamma-ray spectrometer measures the resulting attenuated gamma radiation. Measurements are taken for 2.25-cubic-inch volumes

(a)
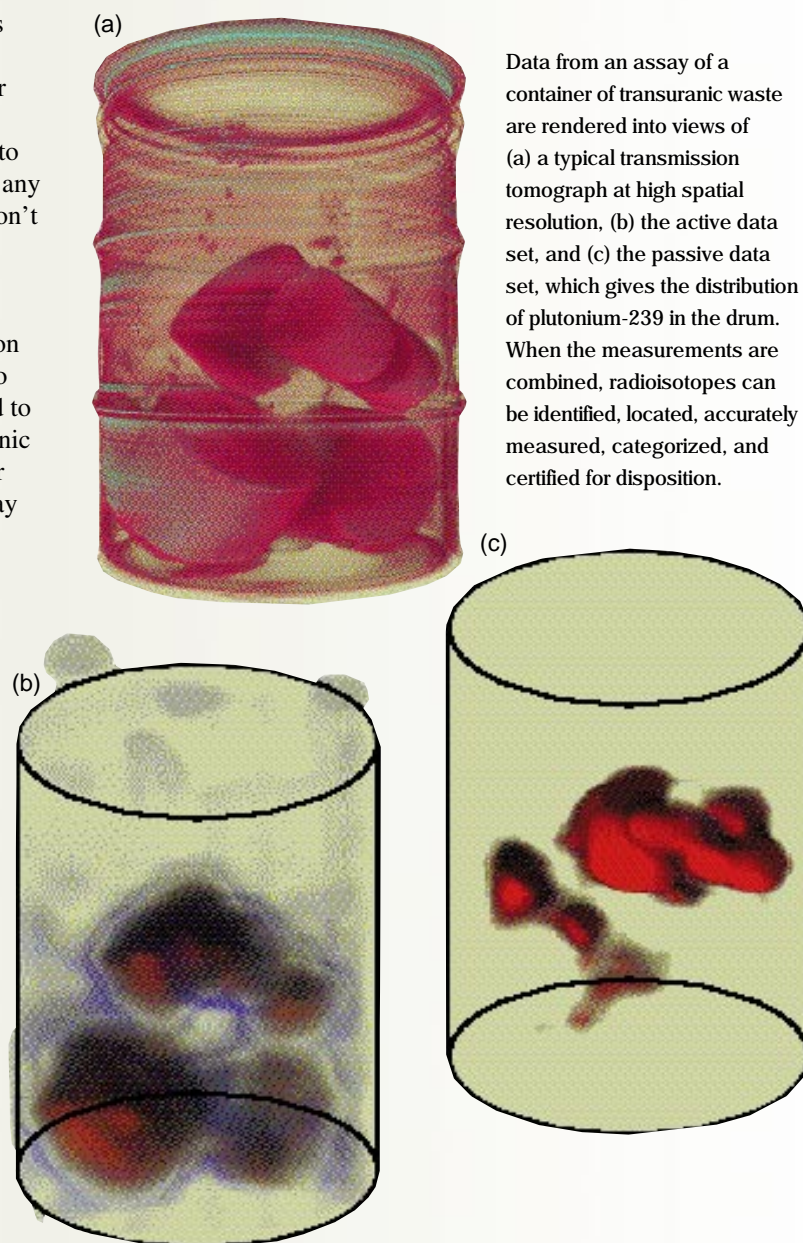
Data from an assay of a container of transuranic waste are rendered into views of (a) a typical transmission tomograph at high spatial resolution, (b) the active data set, and (c) the passive data set, which gives the distribution of plutonium-239 in the drum. When the measurements are combined, radioisotopes can be identified, located, accurately measured, categorized, and certified for disposition.

(c)

(b)

over the entire drum (a total of 2,304 volume elements for a standard 55-gallon drum). By detecting and measuring the attenuated gamma-ray intensity levels at specific energies, one can determine a map of the linear attenuation coefficient (a function of material density and atomic number) of the waste drum and its contents. These maps can be reconstructed to depict a drum's waste matrix attenuation per volume element and energy.

In the second step, called the passive measurement, the six transmission sources are shuttered. The six detectors measure the gamma-ray spectra emitted from inside the drum. Measurements are taken of all the volume elements. During the passive computed tomography reconstruction, the attenuation in these emission measurements, caused by material between the isotope and the detector, is corrected by using the active attenuation map. This correction leads to a far more accurate assay of radioactivity within the drum. The spectra

are also used to automatically identify the isotopes within the drum, because each isotope emits a unique signature within the energy spectrum.

Unparalleled Accuracy

Other systems and techniques do not approach the accuracy of the WIT-NDA system. This was demonstrated by a DOE test that compared the performance of the WIT-NDA and fifteen other NDA systems. It was a blind test using a drum containing a simulated sludge with low levels of transuranic waste, one of the most challenging things to assay but typical of the types of wastes and drums the DOE must assay and dispose of. The WIT-NDA performed the best of all the systems by detecting the radioactivity within the sludge drum to within 1 percent of the known value. The nearest competing system detected only about 80 percent of the known radioactivity.

In the combined series of required DOE-sponsored tests for all NDA techniques that are proposed for certifying waste for disposal at WIPP, the WIT-NDA had a mean accuracy of 97.6 percent, with a precision within 4.1 percent. As Steven Cooke of DOE's Federal Energy Technology Center (now the National Energy Technology Laboratory in Morgantown, West Virginia) notes, "These results are truly exceptional in a difficult arena where par for the course is often plus or minus 50-percent accuracy."

Other Applications

Roberson notes that since the WIT-NDA operates independently of whatever wastes are in the drum, it could also be used to measure the radioactivity in waste products from nuclear power plants or from industries that use radioactive tracers, such as the medical industry. "The system could also be used to quantify special nuclear materials in efforts to safeguard them and prevent their proliferation," he adds.

—Ann Parker

The WIT-NDA team (from left): DeLynn Clark, David Camp, Dennis Goodman, Harry Martz, Jr., Jessie Jackson, Dan Decman, Pat Roberson, Erik Johansson, Steve Azevedo, and BIR members (inset) Dave Nisius, Dick Bernardi, and Dave Entwistle.

Key Words: active and passive computed tomography, nondestructive assay (NDA), nondestructive evaluation, R&D 100 Awards, waste disposal, waste inspection tomography, Waste Isolation Pilot Plant (WIPP).

For further information contact Patrick Roberson (925) 422-8693 (roberson1@llnl.gov).

Nanoscale Chemistry Yields Better Explosives

ONE thousand years ago, black powder was prepared by grinding saltpeter, charcoal, and sulfur together into a coarse powder using a mortar and pestle. Since then, the equipment for making energetic materials—explosives, propellants, and pyrotechnics—has evolved considerably, but the basic process for making these materials has remained the same. That, however, is changing, thanks to an explosive combination of sol-gel chemistry and modern-day energetic materials research.

At Livermore Laboratory, sol-gel chemistry—the same process used to make aerogels or "frozen smoke" (see *S&TR*, November/December 1995)—has been the key to creating energetic materials with improved, exceptional, or entirely new properties. This energetic materials breakthrough was engineered by Randy Simpson, director of the Energetic Materials Center; synthetic chemists Tom Tillotson, Alex Gash, and Joe Satcher; and physicist Lawrence Hrubesh.
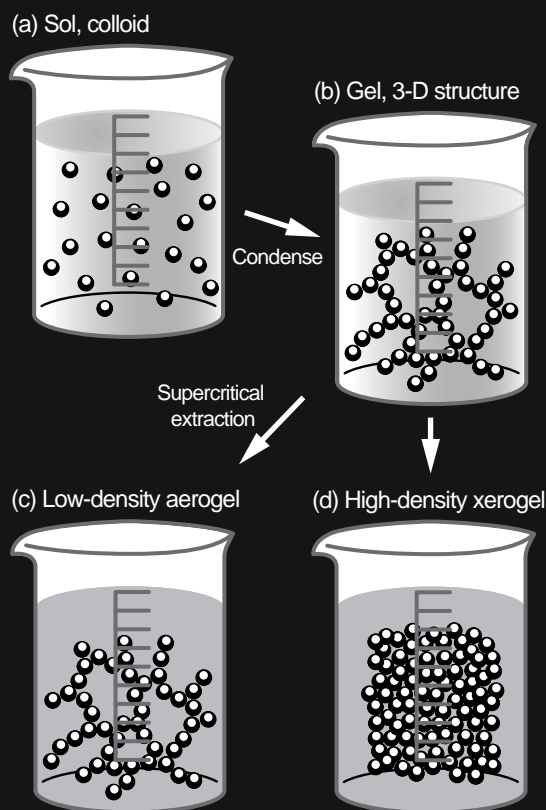
These new materials have structures that can be controlled on the nanometer (billionth-of-a-meter) scale. Simpson explains, "In general, the smaller the size of the materials being combined, the better the properties of energetic materials. Since these 'nanostructures' are formed with particles on the nanometer scale, the performance can be improved over materials with particles the size of grains of sand or of powdered sugar. In addition, these 'nanocomposite' materials can be easier and much safer to make than those made with traditional methods."

Energy Density vs Power, the Traditional Tradeoffs

Energetic materials are substances that store energy chemically. For instance, oxygen, by itself, is not an energetic material, and neither is fuel such as gasoline. But a combination of oxygen and fuel is.

Energetic materials are made in two ways. The first is by physically mixing solid oxidizers and fuels, a process that, in its basics, has remained virtually unchanged for centuries. Such a process results in a composite energetic material such as black powder. The second process involves creating a monomolecular energetic material, such as TNT, in which each molecule contains an oxidizing component and a fuel component. For the composites, the total energy can be much greater than that of monomolecular materials. However, the rate at which this energy is released is relatively slow when compared to the release rate of monomolecular materials. Monomolecular materials such as TNT work fast and thus have greater power than composites, but they have only moderate energy densities—commonly half those of composites. "Greater energy densities versus greater power—that's been the traditional trade-off," says Simpson. "With our new process, however, we're mixing at molecular scales, using grains the size of tens to hundreds of molecules. That can give us the best of both worlds—higher energy densities and high power as well."

(a) Sol, colloid

(b) Gel, 3-D structure

Condense

Supercritical extraction

(c) Low-density aerogel

(d) High-density xerogel

In sol-gel methodology, (a) chemicals in solution produce nanometer-size particles called sols. (b) These sols are linked into a three-dimensional solid network called a gel. (c) The solution can be supercritically extracted to produce aerogels, or (d) evaporated to create xerogels.

Energetic Nanostructures in a Beaker

To control the mix of oxidizer and fuel in a given material at the nanometer scale, Livermore researchers turned to sol-gel methodologies. Sol-gel chemistry involves the reactions of chemicals in solution to produce nanometer-size particles called sols. These sols are linked together to form a three-dimensional solid network or skeleton called a gel, with the remaining solution residing in the open pores of the gel. The solution can then be supercritically extracted to produce aerogels (highly porous, lightweight solids) or evaporated to create xerogels (denser porous solids).

"A typical gel structure is extremely uniform because the particles and the pores between them are so small," notes Tillotson. "Such homogeneity means that the material's properties are also uniform. Our main interest in the sol-gel approach is that it will allow us to precisely control the composition and morphology of the solid at the nanometer scale so that the material's properties stay uniform throughout—something that can't be achieved with conventional techniques."
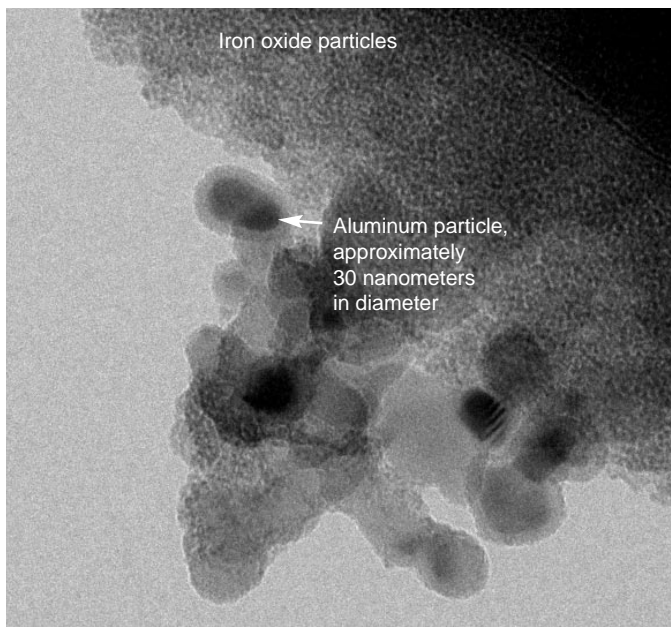
Transmission electron micrograph of a thermitic nanocomposite energetic material. The material is made up of an extremely fine iron oxide xerogel (approximately 2-nanometer particles) that has approximately 30-nanometer-diameter aluminum metal spheres (the larger globules) embedded in it.

Using these sol-gel-processing methods, the team derived four classes of energetic materials: energetic nanocomposites, energetic nanocrystalline materials, energetic powder-entrained materials, and energetic skeletal materials.

Energetic nanocomposites have a fuel component and an oxidizer component mixed together. One example is a gel made of an oxidizer with a fuel embedded in the pores of the gel. In one such material (termed a thermite pyrotechnic), iron oxide gel reacts with metallic aluminum particles to release an enormous amount of heat. "These reactions typically produce temperatures in excess of 3,500°C," says Simpson. Thermites are used for many applications ranging from igniters in automobile airbags to welding. Such thermites have traditionally been produced by mixing fine powders of metal oxides and metal fuels. "Conventionally, mixing these fine powders can result in an extreme fire hazard. Sol-gel methods can reduce that hazard while dispersing extremely small particles in a uniform way not possible through normal processing methods," adds Simpson. The Livermore team has successfully synthesized metal oxide gels from a myriad elements. At least in the case of metal oxides, sol-gel chemistry can be applied to a majority of elements in the periodic table.

In energetic nanocrystalline composites, the energetic material is grown within the pores of an inert gel rather than mixed into it. One way to initiate the growth is to dissolve the energetic material in the solvent used to control the density of the resulting gel. After the gel is formed, the energetic material in the pore fluid is induced to crystallize within the pores. The Livermore team synthesized nanocrystalline composites in a silica matrix with pores containing the high explosive RDX or PETN. The resulting structures contain crystals so small that they do not scatter visible light and are semitransparent.

In the powder-entraining method, a high concentration of energetic powders (90 percent by weight) is loaded within a support matrix (for example, silica) that takes up a correspondingly small mass. Highly loaded energetic materials are used in a variety of applications, including initiators and detonators. Manufacturing this type of energetic material using current processing technologies is often difficult. Producing detonators with pressed powders is a slow manufacturing process, mixing two or more powders homogeneously is difficult, and precise geometric shapes are not easy to produce. Also, pressing powders is a hazardous process.

Many of these problems may be overcome with the sol-gel process. One result is that the sol-gel explosives formed by adding energetic powders are much less sensitive than those

produced by conventional methods. "These results were surprising because conventionally mixed powders generally exhibit increased sensitivity when silica powders are added," says Simpson. "We're still exploring the reasons for this decreased sensitivity, but it appears to be generally true with sol-gel-derived energetic materials."

The final class of energetic material produced by sol-gel methods is energetic skeletal materials. Basically, the sol-gel chemistry is used to create a skeletal matrix, which is itself energetic. Satcher thinks that it might also be possible to form a nanostructure made up of a fuel–oxidizer skeleton with precise stoichiometry (the numerical relationship of elements and compounds as reactants and products in a chemical reaction). "This is something we are still looking into," he adds. In addition to providing materials that have high energy density and are extremely powerful, sol-gel methodologies offer more safe and stable processing. For instance, the materials can be cast to shape or do not require the hazardous machining techniques required by materials that cannot be cast.

Future Looks Bright

Right now, making energetic materials using the sol-gel technique is in the basic research stage, but results look promising. "Many compositions depend on a simple, inexpensive procedure that we can basically do in an ordinary chemistry beaker," says Tillotson. He notes that the practical advantages of these materials are encouraging. Some of the pluses are less sensitivity, safe mixing, low-temperature synthesis, safe handling, safe processing, and homogeneity leading to better performance.

"We've just begun to explore the possibilities for these new materials and the methodologies that produced them," adds Simpson. "This approach is like a new baby—it has lots of potential. The ramifications are still largely unknown."
—*Ann Parker*

In the laboratory, Alex Gash mixes a sol-gel to create an energetic material.

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Ronald B. Musket John D. Porter James M. Yoshiyama Robert J. Contolini	**Vapor Etching of Nuclear Tracks in Dielectric Materials** U.S. Patent 6,033,583 March 7, 2000	A process involving vapor etching of nuclear tracks in dielectric materials for creating high-aspect-ratio (length much greater than diameter) isolated cylindrical holes in dielectric materials that have been exposed to high-energy atomic particles. The process includes cleaning the surface of the tracked materials and exposing the cleaned surface to a vapor of a suitable etchant. Independent control of the temperatures of the vapor and the tracked materials provides the means to vary separately the etch rates for the latent track region and the nontracked material. As a rule, the tracked regions etch at a greater rate than the nontracked regions. In addition, the vapor-etched holes can be enlarged and smoothed by subsequent dipping in a liquid etchant. The 20- to 1,000-nanometer-diameter holes resulting from the vapor etching process can be useful as molds for electroplating nanometer-size filaments, etching gate cavities for deposition of nanocones, developing high-aspect-ratio holes in trackable resists, and filters for a variety of molecular-size particles in virtually any liquid or gas by selecting the dielectric material that is compatible with the liquid or gas of interest.
Robert W. Petersen	**L-Connect Routing of Die Surface Pads to the Die Edge for Stacking in a 3-D Array** U.S. Patent 6,034,438 March 7, 2000	Integrated circuit chips and method of routing the interface pads from the face of the chip or die to one or more sidewall surfaces of the die. The interconnection is routed from the face of the die to one or more edges of the die, then routed over the edge of the die and onto the side surface. A new pad is then formed on the sidewall surface, which allows multiple dies or chips to be stacked in a three-dimensional array, while enabling follow-on signal routing from the sidewall pads. The routing of the interconnects and formations of the sidewall pads can be carried out in an L-connect or L-shaped routing configuration, using a metallization process such as laser pantography.
M. Leslie Carman Robert T. Taylor	**System for Enhanced Longevity of In Situ Microbial Filter Used for Bioremediation** U.S. Patent 6,036,852 March 14, 2000	An improved method for in situ microbial filter bioremediation in which the filter emplaced in an aquifer has increasing operational longevity. A method for generating a microbial filter of sufficient catalytic density and thickness, which has a longer interval before replenishment, improved bacteria attachment and detachment characteristics, and endogenous stability under in situ conditions. A system for in situ field water remediation.
Lloyd A. Hackel C. Brent Dane Shamasundar N. Dixit Matthew Everett John Honig	**Laser Illuminator and Optical System for Disk Patterning** U.S. Patent 6,037,565 March 14, 2000	Magnetic recording media are textured over areas designated for contact in order to minimize friction with data-transducing heads. In fabricating a hard disk, an aluminum–nickel–phosphorous substrate is polished to a specular finish. A mechanical means is then used to roughen an annular area intended to be the head contact band. An optical and mechanical system allows thousands of spots to be generated with each laser pulse, and then the textured pattern is rapidly generated with a low-repetition-rate laser and an uncomplicated mechanical system. The system uses a low-power laser, a beam expander, a specially designed phase plate, a prism to deflect the beam, a lens to transmit the diffraction pattern to the far field, a mechanical means to rotate the pattern, and a trigger system to fire the laser when sections of the pattern are precisely aligned. The system generates an annular segment of the desired pattern with which the total pattern is generated by rotating the optical system about its optic axis, sensing the rotational position, and firing the laser as the annular segment rotates into the next appropriate position. This marking system can be integrated into a disk-sputtering system for manufacturing magnetic disks, streamlining the manufacturing process.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Robert S. Strait Peter K. Pearson Sailes K. Sengupta	**Method and System for Normalizing Biometric Variations to Authenticate Users from a Public Database and Ensure Individual Biometric Data Privacy** U.S. Patent 6,038,315 March 14, 2000	A password system comprising a set of code words spaced apart from one another by a hamming distance (HD) that exceeds twice the variability that can be projected for a series of biometric measurements for a particular individual but is less than the HD that can be encountered between two individuals. To enroll an individual, a biometric measurement is taken and exclusive-OR-functioned with a random code word to produce a reference value. To verify the individual later, a biometric measurement is taken and exclusive-OR-functioned with the reference value to reproduce the original random code word or its approximation. If the reproduced value is not a code word, the nearest code word to it is found, and the bits that were corrected to produce the code word are also toggled in the biometric measurement taken and the code word generated during enrollment. The correction scheme can be implemented by any conventional error correction code, such as Reed-Muller code R(m,n). In the implementation using a hand geometry device, an R(2.5) code has been used in this invention. The code word and biometric measurement can then be used to see if the individual is an authorized user. Conventional Diffie-Hellman public key encryption schemes and hashing procedures can then be used to secure the communication lines carrying the biometric information and to secure the database of authorized users.
Bernardino M. Penetrante George E. Vogtlin Bernard T. Merritt Raymond M. Brusasco	**Plasma-Assisted Catalytic Storage Reduction System** U.S. Patent 6,038,853 March 21, 2000	A two-stage method for NO_x reduction in an oxygen-rich engine exhaust comprises a plasma oxidative stage and a storage reduction stage. The first stage employs a nonthermal plasma treatment of NO_x gases in an oxygen-rich exhaust and is intended to convert nitrous oxide (NO) to nitrogen dioxide (NO_2) in the presence of oxygen and hydrocarbons. The second stage employs a lean NO_x trap to convert such NO_2 to environmentally benign gases that include NO_2, carbon dioxide, and water. By preconverting NO to NO_2 in the first stage with a plasma, the efficiency of the second stage for NO_x reduction is enhanced. The method allows for enhanced NO_x reduction in vehicular engine exhausts, particularly those having relatively high sulfur content.
Bernardino M. Penetrante George E. Vogtlin Bernard T. Merritt Raymond M. Brusasco	**Plasma Regenerated Particulate Trap and NO_x Reduction System** U.S. Patent 6,038,854 March 21, 2000	A noncatalytic two-stage process for removal of NO_x and particulates from engine exhaust comprising a first stage where plasma converts nitrous oxide (NO) to nitrogen dioxide (NO_2) in the presence of oxygen and hydrocarbons and a second stage—which preferably occurs simultaneously with the first stage—that converts NO_2 and carbon soot particles to environmentally benign gases that include N_2 and carbon dioxide (CO_2). By preconverting NO to NO_2 in the first stage, the efficiency of the second stage for NO_x reduction is enhanced, in that carbon soot from trapped particulates is simultaneously converted to CO_2 when reacting with the NO_2 (that converts to diatomic nitrogen, or N_2). The nitrogen exhaust components remain in the gas phase throughout the process, with no accompanying adsorption.
Joe N. Lucas	**Rapid Method for Measuring Clastogenic Fingerprints Using Fluorescence In Situ Hybridization** U.S. Patent 6,043,037 March 28, 2000	A method for determining a clastogenic signature of a sample of chromosomes by quantifying a frequency of a first type of chromosome aberration present in the sample; quantifying the frequency of a second, different type of chromosome aberration present in the sample; and comparing the frequencies of the first type and second type of chromosome aberration. A method is also provided for using that clastogenic signature to identify a clastogenic agent or dosage to which the cells were exposed.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Jeffrey D. Morse Robert J. Contolini Ronald G. Musket Anthony F. Bernhardt	**Formation of Nanofilament Field Emission Devices** U.S. Patent 6,045,678 April 4, 2000	A process for fabricating high-aspect-ratio, electroplated nanofilament structure devices for field emission displays. In the process, a via, or channel, is formed in a dielectric layer and is self-aligned to a via in the gate metal structure located on top of the dielectric layer. The desired diameter of the via in the dielectric layer is on the order of 50 to 200 nanometers, with an aspect ratio of 5:10. In one embodiment, after the via in the dielectric layer is formed, the gate metal is passivated and a plating enhancement layer is deposited at the bottom of the via. The nanofilament is then electroplated in the via, after which the gate passification layer is removed, the dielectric etched back, and the nanofilament sharpened. A hard mask layer may be deposited on top of the gate metal and removed following electroplating of the nanofilament.

Awards

Charles Alcock, former head of Lawrence Livermore's Institute for Geophysics and Planetary Physics, has won the American Astronomical Society's **Beatrice Tinsley Prize**. Awarded once every two years since 1986, the Tinsley Prize recognizes "an outstanding research contribution to astronomy or astrophysics, of an exceptionally creative or innovative character."

Alcock was recognized for his research into the nature of dark matter in the universe, which is invisible but thought to comprise most of the universe's mass. He and an international research team have been searching the Milky Way, looking for occasional amplifications of starlight from outside the galaxy caused by the gravitational effects of dark matter. They are testing the hypothesis that a significant fraction of the dark matter in the halo of the Milky Way is made up of objects like brown dwarfs or planets, which have come to be known as massive compact halo objects, or MACHOs. The work, which began in 1996, ended its data-collection phase at the beginning this year. Up ahead, says Alcock, is the ". . . tremendous job to analyze the data."

Alcock says he knew Tinsley, a New Zealand–born astronomer, and is honored to receive the award bearing her name. "She was very original. She made stunning contributions in astronomy," he says. He also says he owes thanks to all his collaborators and to the Laboratory for allowing him to pursue the study.

Don Correll, director of the Laboratory's Science & Technology Education Program (STEP), has been awarded **Fusion Power Associates' Special Award for Education**.

He was one of three recipients of the special award during the association's annual symposium in July.

Steve Dean, president of Fusion Power Associates, cited Correll's ". . . dedication and efforts to explain the fusion message to students, teachers, and the general public [which] have been a great service to our program and to our country."

Correll received his Ph.D. in physics from the University of California at Irvine in 1976 and was named an American Physical Society fellow in 1993. He joined the Laboratory in 1976 and held a variety of positions in the laser fusion program before being named director of STEP. Recently, he was also named point-of-contact for Laboratory postdoctoral fellows.

In the area of education, Correll has served on the Laboratory's Lawrence Fellowship Committee, Undergraduate Scholarship Committee, Student Policy Committee, and Lawrence Livermore–University of California at Davis Summer Institute Committee.

Mark Herrmann, a postdoctoral fellow working in the Laboratory's Defense and Nuclear Technologies Directorate, has been selected by the American Physical Society as this year's recipient of its **Award for Outstanding Doctoral Dissertation in Plasma Physics**. Herrmann, whose Ph.D. is from Princeton University, will receive the award during the society's meeting this month in Quebec City, Canada.

The citation on the award will read, "With elegant use of analytical theory and computation, and insightful comparisons to experiment, this thesis lays the foundation for how radio frequency waves might cool fusion byproducts in a tokamak."

Herrmann joined the Laboratory as a postdoctoral fellow in 1998. In 1990, he attended the Laboratory's Summer Institute in Applied Physics.

Abstracts

A New World of Seeing

A team of Lawrence Livermore researchers is developing a new generation of visualization tools for handling the immense amounts of data produced by Department of Energy supercomputers running nuclear simulation codes. The group, called VIEWS (Visual Interactive Environment for Weapons Simulation), is producing novel ways to store, retrieve, search, view, and analyze data. The pioneering work includes both hardware and software solutions. One emphasis is on three-dimensional tools that take advantage of the human eye's ability to discern subtle changes in colors and patterns. The Assessment Theater is the most striking example of Lawrence Livermore's new visualization world. Scientists use the theater to watch computer-generated movies of unprecedented image quality on a 5-meter-wide by 2.5-meter-tall plastic projection screen.

Contact:
Terri Quinn (925) 423-2385 (quinn1@llnl.gov).

Modeling Our Environment in Action
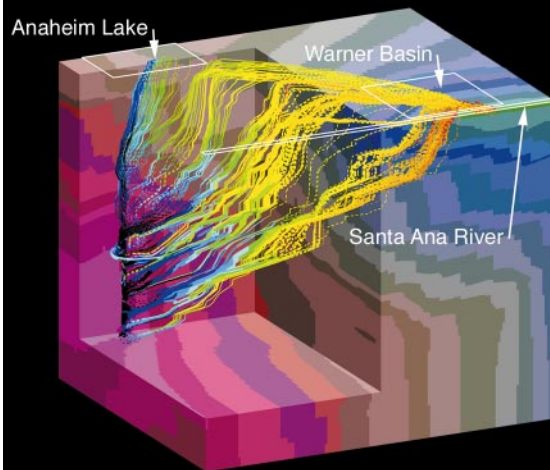
Terascale supercomputers are the springboard to a new level of environmental simulation that can provide multidimensional, time-scale models of natural events.

Also in November

• *The advantages of using protons instead of x rays as a radiographic probe into the performance and aging of weapon systems.*

• *A Laboratory–university collaboration produces a new, fundamentally simple tissue imaging technique to dramatically improve minimally invasive cancer detection.*

• *Livermore and Texas A&M University researchers have produced cold, thin matter that is the thermodynamic analog of the hot, dense matter found in white dwarf stars.*

Coming Next Month