July/August 2005

Science & Technology REVIEW

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

Mission Control for Laser Experiments

Also in this issue:

- A Random Walk with Einstein
- Pulsing the Earth for Methane
- The Physics of Nuclear Isomers

World Year of PHYSICS 2005

About the Cover

When the National Ignition Facility (NIF) is completed, scientists will use its 192 laser beams to compress fusion targets under the extreme conditions required for thermonuclear ignition and burn. Rarely featured in discussions of this national resource is NIF's integrated computer control system, a large-scale system as complex as any in government service or private industry. The article beginning on p. 4 describes this system, which was designed to coordinate the operation of the many electronic, optical, and mechanical devices used in NIF experiments. Every experimental shot requires the precise orchestration of more than 60,000 parts—such as motorized mirrors and lenses, energy and power sensors, video cameras, laser amplifiers, and diagnostic instruments. On the cover, operators in the main control room monitor their designated areas of operation. In the background, personnel service components inside the NIF target chamber.

Cover design: Dan Moore

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.

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.

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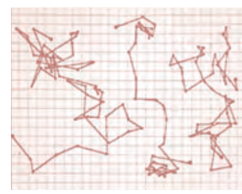

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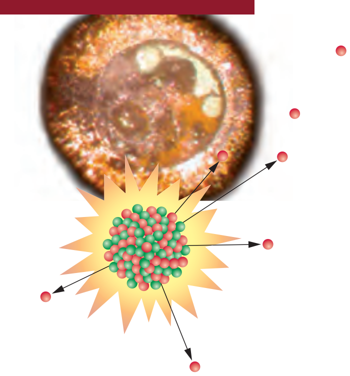

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Gene expression from extreme environments

In a collaboration involving Lawrence Livermore and Oak Ridge national laboratories, the University of California (UC) at Berkeley, and Xavier University in New Orleans, researchers are finding that communities of microorganisms are assembled from several disparate organisms that function together to survive. That is, microorganisms will adapt to extreme conditions, such as high temperature and toxicity, by evolving to specialize and cooperate with each other. The research team, led by UC Berkeley professor Jill Banfield, examined more than 2,000 proteins produced by five species in a community that thrives in the hot, highly acidic conditions of an abandoned mine at Iron Mountain, California.

"We found large numbers of proteins that don't resemble any other proteins we know about," says team member Michael Thelen, a protein biochemist in Livermore's Biosciences Directorate. "Also, many of these proteins are enzymes whose main function is to maintain the correct structure of other proteins exposed to this harsh environment."

The complex interaction of microbes, water, and exposed ore at the mine has generated dangerously high levels of sulfuric acid and toxic heavy metals. The microorganisms found there—called extremophiles for their affinity to harsh environments—grow as densely packed pink biofilm that floats on the mine water's surface. The millimeter-thick biofilm is a self-sustaining system, using carbon and nitrogen from the atmosphere within the mine and deriving energy from the iron that has leached from the iron sulfide rock.

The team's results, published in the June 24, 2005, issue of *Science*, indicate that many functions, such as nitrogen fixation, are handled by specialized microbes. Thelen adds that studies such as this one will help researchers learn how biofilm functions in different environments, what mechanisms are involved in assembling microbial communities, and how metabolic tasks and resources are partitioned.

Contact: Michael Thelen (925) 422-6547 (mthelen@llnl.gov).

Measuring the composition of Titan's atmosphere

Livermore is collaborating with the National Aeronautics and Space Administration (NASA), the University of British Columbia (UBC), and NASA's Jet Propulsion Laboratory (JPL) to measure the temperature, winds, and chemical composition of Titan's atmosphere. Led by principal investigator F. Michael Flasar of NASA's Goddard Space Flight Center, the team is using the Cassini Composite Infrared Spectrometer (CIRS) on the Cassini-Huygens spacecraft to record data from Titan's atmosphere.

CIRS measures the intensity of far-infrared radiation, light with wavelengths between those of radar and near-infrared light. The abundance of methane in Titan's atmosphere is determined by comparing the intensity of spectral emission lines from the atmosphere with laboratory measurements. Livermore physicist Edward Wishnow measured the spectrum of methane at temperatures and densities similar to Titan's—about 113 kelvins and about 1 atmosphere of pressure. Because the laboratory absorption spectra correspond well with the Titan spectral lines, the laboratory results can be used to determine the amount of methane in Titan's upper atmosphere. UBC scientists Herbert Gush, Irving Ozier, and Mark Halpern collaborated on the laboratory work, and JPL scientist Glenn Orton helped interpret the data.

Titan is the only moon in the solar system with a substantial atmosphere, and that atmosphere is primarily composed of nitrogen, making it similar to Earth's. Scientists want to study Titan's atmosphere because the organic chemistry occurring there is analogous to the processes that may have occurred in the early terrestrial atmosphere. CIRS observations of Titan's stratosphere also indicate that its winter (northern) pole has many properties in common with Earth's. Titan's cold temperatures, strong circumpolar winds, and concentrations of several compounds are analogs to the polar winds and ozone hole on Earth. Both also have strong winds that isolate the polar air and inhibit mixing with air at lower latitudes.

Cassini-Huygens is an international collaboration between NASA and the European and Italian space agencies. Cassini is the first spacecraft to explore the Saturn system of rings and moons from orbit. Results from the team's research appeared in the May 13, 2005, issue of *Science*.

Contact: Edward H. Wishnow (925) 422-7208 (wishnow@llnl.gov).

New approach to the study of microbes

Scientists from the Department of Energy's Joint Genome Institute have developed an approach that uses information-rich snippets of DNA from Minnesota farm soil and whalebones recovered from a mile underwater to analyze terrestrial and aquatic habitats. Called environmental genomic tags (EGTs), these indicators capture a DNA profile of a particular niche and reflect the presence and levels of light, nutrients, pollutants, and other features. Led by JGI scientist Susannah Green Tringe, the researchers compared the DNA pieces to determine site-specific motifs. Then they used this information to detect environments under stress and evaluate the progress of remediation efforts.

The abundances of genes in the EGT data reflect the demands of a particular setting. For example, genes involved in breaking down plant material are overrepresented in soil and absent in seawater. In seawater, genes involved in the passage of sodium, a major chemical component of salt water, are particularly abundant. By evaluating the EGT data, scientists can determine what is happening in an environment without identifying the microbes that live there.

A report on the team's research appeared in the April 22, 2005, issue of *Science*.

Contact: Art Kobayashi (925) 296-5765 (akobayashi@llnl.gov).

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The Grand Challenge of Thermonuclear Ignition

SCIENTISTS often refer to formidable scientific and technological hurdles with far-reaching consequences as grand challenges. One of the enduring grand challenges is achieving nuclear fusion—the power source of the Sun and stars and the physical process at the core of Livermore's national security mission—in a laboratory environment.

Since our founding, Lawrence Livermore National Laboratory has been one of the world's centers for fusion research. Immediately after the laser was invented in 1960, Laboratory scientists understood the possibility of using coherent light to ignite a fusion microexplosion. Since then, Livermore researchers have led the world in the goal of achieving controlled thermonuclear burn in the laboratory using laser light.

Ignition and thermonuclear burn will release more energy than is required to initiate the reaction and may offer an environmentally sound method to supply energy. Ignition in the laboratory will be a key capability for stockpile stewards to help ensure the safety and reliability of the nation's nuclear weapons. It will also provide new insights into the world of high-energy-density physics, recently dubbed by the National Academy of Sciences as the "X-Games of Contemporary Science."

An overarching goal of the National Ignition Facility (NIF) is to attempt to achieve thermonuclear burn in 2010. NIF is the most recent in a long line of increasingly more powerful solid-state lasers constructed at Livermore. It is nearly 100,000 times more energetic than the first system. In working to make NIF a success, our scientific and engineering team has achieved breakthroughs in laser architecture, developed new optical materials and target designs, and devised innovative diagnostic systems. In many ways, these technological and scientific advances have received all the glory.

However, no breakthrough has been more important, no undertaking more challenging than finding a way to control the more than 60,000 components that make up NIF. This integrated computer control system (ICCS) is the linchpin that makes NIF operations and experiments possible. It is the most complex real-time control system ever designed for a scientific machine. Described in the article beginning on p. 4, ICCS will ensure that all of NIF's 192 laser beams arrive at a tiny target within a few tens of microseconds of each other and that a host of diagnostic instruments record data in a few billionths of a second.

We've designed an extremely complex system whose pieces operate individually but, at the time directed, work in unison. The NIF control system uses an innovative architecture that allows 24 bundles of eight laser beams to be aligned and prepared for a shot independently. With this modular approach, scientists can design experiments so that individual bundles have different energy and waveform characteristics. In response to an input command, ICCS software calculates the required configuration of the laser beams, aligns them on target, fires the laser, and collects the data. NIF is thus an unusually flexible user facility that will provide scientists the wide experimental regime they need in the decades ahead.

ICCS demonstrated its effectiveness during the 18-month-long experimental campaign called NIF Early Light, which was completed in October 2004. This campaign used the first four lasers beams to conduct more than 400 shots. It validated the modular architecture while performing unique experiments in high-energy-density physics supporting stockpile stewardship.

As we continue to complete NIF, we will be refining and replicating the software that controls each bundle. We are now turning from a build-and-test mode to one of activating equipment and planning for a full-scale shot schedule for ignition in 2010.

NIF is a grand-challenge machine. We are confident that it will allow us to meet the goal of thermonuclear burn—a goal that scientists at Livermore and throughout the world set nearly a half-century ago. Experiments conducted on NIF will make significant contributions to national security, could lead to practical fusion energy, and will help the nation maintain its leadership in basic science and technology. This goal is a grand challenge that only a national laboratory such as Livermore can accomplish.

■ Edward I. Moses is acting associate director of National Ignition Facility Programs.

Orchestrating the World's Most Powerful Laser

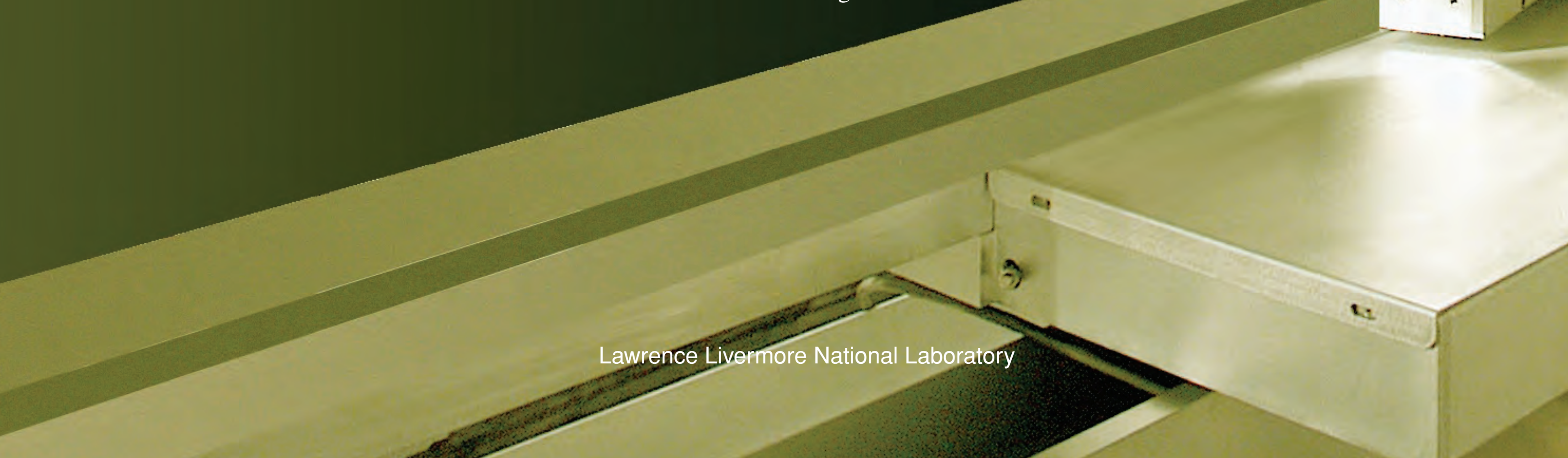
The integrated computer control system for the National Ignition Facility monitors and controls the devices comprising the giant laser on the path to ignition.

WHEN completed, the National Ignition Facility (NIF) will be, by far, the world's largest and most energetic laser and a major international scientific resource. Designed to study the physics of matter at extreme densities, pressures, and temperatures, NIF will use 192 laser beams to compress fusion targets to conditions required for thermonuclear ignition and burn. In the process, more energy will be liberated than is used to initiate the fusion reactions. (See the box on p. 6.)

Every NIF experimental shot requires the coordination of complex laser equipment. In the process, 60,000 control points of electronic, optical, and mechanical devices such as motorized mirrors and lenses, energy and power sensors, video cameras, laser amplifiers, pulse power, and diagnostic instruments must be monitored and controlled. The precise orchestration of these parts will result in the propagation of 192 separate nanosecond long bursts of light over a 1 kilometer path length. These 192 beams must arrive within 30 picoseconds of each other at the center of a target chamber 10 meters in diameter, and they must strike within 50 micrometers of their assigned spot on a target measuring less than 1 centimeter long.

Indeed, fulfilling NIF's promise requires a large-scale computer control system as sophisticated as any in government service or private industry. Conceived and built by a team of 100 software developers, engineers, and quality control experts, NIF's integrated computer control system (ICCS) software, now nearly 80 percent complete, will soon have about 1.4-million lines of code running on more than 750 computers. ICCS, which is operated from a main control room, fires the laser and conducts these experiments automatically.

ICCS proved itself over the past two years during the NIF Early Light campaign, which used beams from the first four completed lasers, or quad, to conduct more than 400 shots. With the first quad in operation, at least



The control system for the National Ignition Facility (NIF) monitors thousands of components, such as this calorimeter, which measures the energy of the laser.

one of every type of hardware device was successfully monitored and controlled by ICCS. Among its many accomplishments, the control system demonstrated that it can use deformable mirrors to maintain the optical quality in laser beams, synchronize the beams' arrival at their targets, and align the laser's optical elements to ensure that beams hit their targets precisely. "NIF Early Light served as the ultimate test bed for the control system software and was crucial to our development efforts," says Paul VanArsdall, associate project manager for ICCS.

Ralph Patterson, NIF deputy project manager for controls and information systems, says, "NIF Early Light was a challenge we placed on ourselves to acquire as much information as possible about the performance of the hardware and software." Perhaps more importantly, physicists from both Lawrence Livermore and Los Alamos national laboratories, with collaborators from Sandia National Laboratories and the University of Rochester's Laboratory for Laser Energetics, were able to

A Closer Look at the National Ignition Facility

The National Ignition Facility is a stadium sized complex. When complete, it will contain a 192 beam, 1.8 megajoule, 700 terawatt laser system adjoining a 10 meter diameter target chamber with room for nearly 100 experimental diagnostics. NIF's beams will compress and heat small capsules containing a mixture of hydrogen isotopes of deuterium and tritium. These fusion targets will ignite and burn, liberating more energy than is required to initiate the fusion reactions. NIF experiments will allow scientists to study physical processes at temperatures approaching 100 million kelvins and 100 billion times atmospheric pressure. These conditions exist naturally only in the interior of stars and in nuclear weapon detonations.

A cornerstone of the National Nuclear Security Administration's Stockpile Stewardship Program, NIF will help ensure the reliability of the U.S. nuclear weapons stockpile by allowing scientists to validate computer models that predict age-related effects on the stockpile. Access to these regimes will also make possible new areas of basic science and applied physics research.

NIF's 192 beams are organized in quads, bundles, and clusters. Quads are four beams with the same pulse shape. Each NIF bundle an upper and lower quad is controlled independently from the others.

In July 2001, the NIF Project began working on an accelerated set of milestones leading to NIF Early Light, a campaign to demonstrate NIF's capability to deliver high quality laser beams to the target chamber in support of early experiments. The first quad was activated in December 2002. On May 30, 2003, NIF produced 10.4 kilojoules of ultraviolet laser light in a single laser beamline, setting a world record for laser performance. By the end of the Early Light campaign, in October 2004, more than 400 shots had been performed. During that time, NIF met performance criteria for beam energy and power output, beam to beam uniformity and timing, and delivery of shaped pulses for ignition and nonignition experiments.

When all beams are operating, NIF will deliver more than 60 times the energy of Livermore's Nova laser, which was decommissioned in 1999, or the OMEGA laser at the University of Rochester's Laboratory for Laser Energetics. NIF will make significant contributions to astrophysics, hydrodynamics, materials science, and plasma physics. Experiments will create physical regimes never before seen in any laboratory setting—to benefit maintenance of the U.S. nuclear weapons stockpile, spur advances in fusion energy, and open new vistas in basic science.

The stadium-sized National Ignition Facility.

conduct experiments on NIF, including studies of laser beam propagation in plasmas, energy delivery into targets of importance to the National Ignition Program, and the hydrodynamics of materials subjected to laser-driven shocks. ICCS managers obtained valuable feedback from the physicists to better fulfill the physicists' experimental needs and increase NIF's operational efficiency.

Over the next few years, as laser "bundles" of eight beams—the basic modular unit of NIF—are completed, computers and software that were fielded for the first bundle will be replicated. NIF's independent bundle architecture simplifies the task of controlling the laser because each bundle is prepared for the upcoming shot independently. The bundles are synchronized just before shot time so that even the most complex experiments can be carried out efficiently with a short turnaround time.

VanArsdall emphasizes the importance of this concept. "With the bundle approach, we have a highly manageable way to bring additional lasers on line. We designed each bundle to be controlled by its own software segment. As a result, performance remains constant regardless of the number of bundles installed." A more traditional approach would have resulted in a control system of overwhelming complexity because software would have to be scaled up to control all 192 laser beams simultaneously.

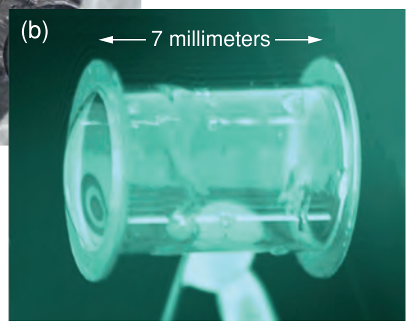
"Instead, we just have to deploy 24 copies of the control system," says VanArsdall. "We've demonstrated the architecture during extensive commissioning shots and user experiments. Once we control one bundle, it is a straightforward task to extend controls to all. In this way, we've simplified our design and dramatically improved the performance of ICCS."

The modular control system concept dovetails well with plans for NIF experiments. For example, although achieving ignition will require all 192 beams, many experiments will require fewer laser beams.

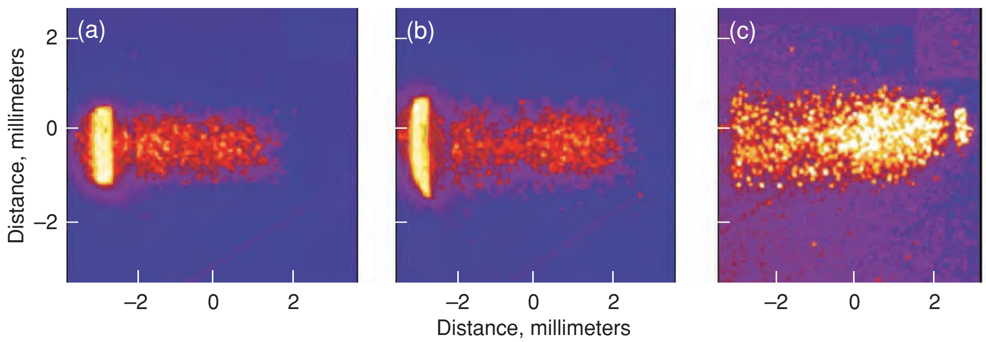
Control System's Stiff Requirements

ICCS was designed to fire and diagnose laser shots every four hours. This requirement includes software for setting up the shot and countdown sequence; performing automatic alignment, laser beam diagnosis, and control of power conditioning and electro-optic subsystems; monitoring the status of all subsystems and components; and providing operators with graphics interfaces to display those data. ICCS also must maintain records of system performance and archive the experimental data recorded by NIF's advanced diagnostic instruments.

"We started building the first software prototypes for NIF in 1997 with a team of about eight people," recalls Bob Carey, lead software architect and one of the original eight developers. From that modest group,



(a) Livermore personnel service hardware inside the NIF target chamber. (b) This target was designed for use in laser–plasma experiments on NIF.



These x-ray images from a NIF experiment show beam transport through a target at (a) 1.5, (b) 2.5, and (c) 3.5 nanoseconds. The integrated computer control system (ICCS) records and archives all experimental data. Operators use the ICCS's graphics interfaces to display the results.

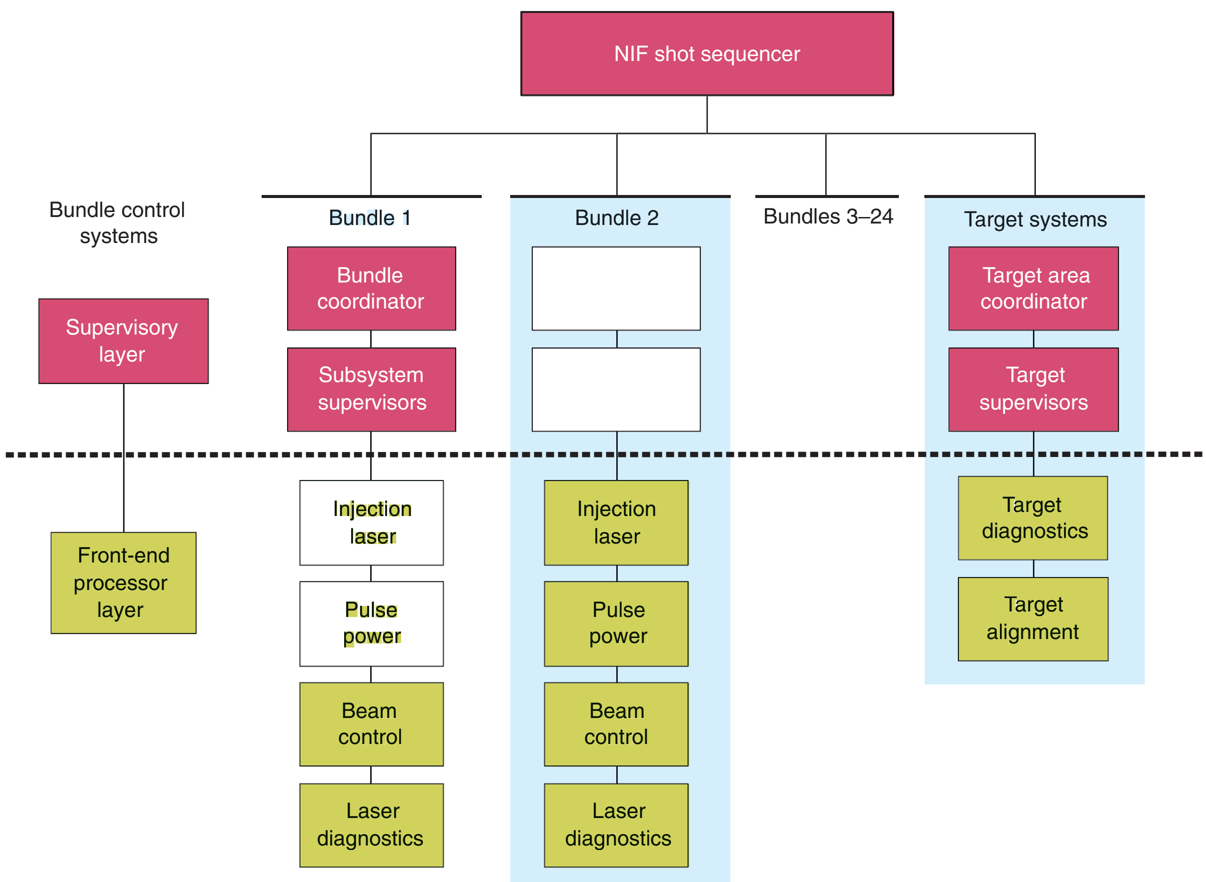
the organization grew to include many additional software developers, information technologists, systems engineers, quality control managers, and an independent testing group. Computer scientists and engineers on the team average 20 years of experience in such fields as database design, real-time controls, test engineering, graphics user interfaces, and object-oriented programming.

"Our staff is very talented and experienced," says Larry Lagin, associate project manager for software engineering and a division leader in the Computation Directorate. Lagin points out that many of the people on the ICCS team helped develop control systems for past Livermore projects including the Atomic Vapor Laser Isotope Separation Program and the Shiva and Nova lasers. "The experience gained from previous large laser systems has been invaluable in developing an integrated, scalable, and robust system with the flexibility and automation required," says Jerry Krammen, a computer scientist who has worked on many laser projects at the Laboratory. "We were also successful at building up the team with specialists who had appropriate skills from working at other research laboratories and industry," says Lagin, who worked previously for a major aerospace firm and on Princeton University's fusion energy program.

NIF was designed to be operational over a 30-year lifetime. Therefore, control software must be flexible and easy to update. "We wanted an architecture that provided an integrated control system we could maintain for the foreseeable future," says Lagin.

ICCS's architecture is hierarchical in nature. The two main layers are a front-end or bottom layer consisting of about 700 front-end processors (FEPs) and a supervisory or top layer of 50 powerful computers—all managed in the main NIF control room from an ensemble of 14 operator consoles. The supervisory layer includes operator-controlled graphics displays and automated controls that work with the FEPs to coordinate components in all 192 beams. Databases and common services incorporated into the supervisory layer support control system operation.

A high-performance network, with a throughput of 1 gigabit per second, interconnects these computers for passing commands, assessing bundle status, and retrieving diagnostics data. The network also carries video images of the laser



The architecture of NIF's integrated computer control system is divided into layers. A front-end or bottom layer consists of about 700 front-end processors, and a supervisory or top layer has 50 powerful computers. Each bundle of eight beams has its own independent control system, which is replicated for the others.

beams generated by over 300 high-resolution digital cameras that serve as the eyes of the control system for monitoring and adjusting the laser alignment automatically.

Microprocessors and Supervisors

The FEPs, which attach to the laser hardware, operate as real-time applications running on industrial-grade microprocessors. They are organized to support hardware in NIF's functional systems: injection laser, beam controls, laser diagnostics, pulse power, and target diagnostics.

Different types of FEPs optimize the control of similar devices, such as beam motion or the main power supplies. Installed in racks, the FEPs interface to devices such as stepping motors, transient digitizers, calorimeters, and photodiodes. For example, a single beam control FEP drives as many as 100 motors to precisely adjust the laser beam so that the laser is kept on course within 50 micrometers (about half the width of a human hair). In keeping with the independent bundle concept, these FEPs are wired to control devices associated with a single bundle.

Supervisor systems run on servers and workstations located near the main NIF control room and provide operators with system status and other data from the FEPs. Operators access supervisor-system data through a hierarchy of on-screen graphics interfaces. Operators can also view video images of the laser beams from any of the hundreds of sensor cameras located throughout the complex.

Daily operation of NIF is managed by the on-duty shot director, who oversees control room activities and operates the laser and target systems for conducting shot experiments. The ICCS team developed shot-supervisor software that assists the shot director and the control room staff to prepare and fire each shot by automatically sequencing the system's many functions. "The software puts everything within each bundle in a specific time sequence and makes sure all the components play together to achieve the required laser performance," says Dave Mathisen, lead designer of the shot-supervisor software. The shot director interacts with this software to ensure that experiments run successfully.

In designing the NIF central control room, VanArsdall studied the layout of the National Aeronautics and Space Administration's (NASA's) mission control room in Houston, Texas. NIF laser physicist and former NASA astronaut Jeff Wisoff notes that both control rooms have operator stations corresponding to different hardware systems. In NIF's case, each console corresponds to a functional system on the laser. Similar to NASA operators in the Launch Center control room, operators located in the NIF control room continuously track data on their monitors.

Wisoff sees other similarities between executing a NIF shot and launching a Space Shuttle. "Launch of a Space Shuttle is controlled by software centered in the Launch Center control room until *T* minus 31 seconds—or 31 seconds before liftoff," says Wisoff. "Then computers onboard the shuttle take over." Similarly, countdown for a NIF shot includes computer checks

Electronics engineer Judy Liebman analyzes a video of a NIF laser beam produced by one of the 300 high-resolution cameras.

Livermore engineer Rob Hartley tests a beam-control front-end processor, which is used to position motors in the alignment system.

of every subsystem, and the control system will automatically stop events from proceeding unless all conditions are satisfactory. At *T* minus 2 seconds, the ICCS software turns over control to a high-precision integrated timing system designed to trigger thousands of laser modules and diagnostics at exactly the right instant.

Automation Does It All

Achieving the 4-hour shot turnaround time requires automating the numerous tasks involved in NIF shots. Efficient shot campaigns begin with careful advance planning. Information technology (IT) analysts evaluated the work processes needed for physicists and managers to plan, approve, and review experimental campaigns. IT developers then implemented campaign management tools that captured user requirements and prepared electronic shot plans for the control system.

A laser performance operations model (LPOM), which is an integral part of the supervisor software, translates user goals from the shot plan into the optimal operating parameters to be set by the control system at the start of each experiment. According to NIF physicist Mike Shaw, "Efficient operation of NIF experiments depends on obtaining precisely specified energy waveforms and producing energy balance among the beams." The energy of every beam could differ because of slight differences in amplifier gains and optical transmission losses in each beamline. By running a computational model of the facility before each experiment, the team determines in advance how to configure the system so that the total requested beam energy and power output are delivered.

Shot automation software, delivered in April 2005, computerizes the preparation of each NIF bundle independently from the others. When the 24 bundles are ready, the software then synchronizes the countdown of all 192 beams to fire the shot. "We always knew we would have to develop this layer, but we needed NIF Early Light to provide the exact requirements," says Carey. During the Early Light campaign, the ICCS and shot operations teams developed a 6,000-line checklist procedure showing how operators used the software during a busy shot schedule, which allowed the control system managers to improve the automation and reduce manual tasks.

"We want NIF operations to be as efficient and automated as possible," says VanArsdall. He notes the tremendous success developers achieved in aligning NIF's beams automatically. The alignment control system software determines the position of NIF's laser beams on the optics by analyzing sensor video images with a variety of computer-vision algorithms. Motor control robotics software uses the sensor information to remotely position more than 9,000 stepping motors and other actuators. These devices point the beams through pinholes, center them on mirrors and lenses, and focus them onto the target—achieving greater precision and effectively eliminating the need for personnel to adjust the beamlines manually. "The precision we have achieved

Software is tested offline in the ICCS Integration and Test Facility, which emulates hardware components.

is comparable to hitting the strike zone with a baseball thrown from 350 miles away," says Patterson.

At the same time, the system retains the facility's flexibility so that the beams can be configured in many different modes depending on the experiment. "Our experience during NIF Early Light demonstrated that we can efficiently perform shots," says Lagin. Thanks to the underlying control system architecture, adding the automation did not require rewriting other software layers.

Architecture Offers Flexibility

Control system software is written in two languages: Ada for the FEPs and the common services, such as timing; and Java for user interfaces and databases. Ada is often used in mission-critical applications such as real-time transportation and military systems to improve reliability and reduce maintenance. The mixed language environment offers support for engineering the core of the control system in Ada while providing tools to quickly develop graphics and other applications in Java.

The ICCS team developed a software framework of tools and patterns for building the large number of FEPs and supervisory systems. With this dynamic configuration framework, the team can replicate the software completed for one bundle simply by modifying parameters in the database and running another copy. ICCS software accesses the database during initialization to assign each process in the control system to prescribed bundles. "We wanted a plug-and-play capability for our system to make it simple to expand and service," says VanArsdall. "Rather than writing new software each time, the FEPs and supervisors are simply configured in the database to bring each new bundle online."

NIF managers adopted a strategy of incremental cycles of software development and formal testing to successfully deliver the large-scale system. Numerous software releases and updates have been delivered to date. "We plan and develop each release consistent with project goals," says Lagin. "Then we test and, if necessary, modify it to meet the system's requirements."

Quality control and assurance processes are part of the development effort. Before software releases are approved for deployment, they are tested extensively to verify their performance. "We've made a significant investment in testing prior to deployment," says Lagin. Quality control is performed independent from software development and constitutes 20 percent of the total software effort. "The ratio of software developers to testers is about four to one, which is consistent with the computer industry's best practices," says Lagin.

Offline Testing Followed by Online

Software testing begins with offline tests conducted in the ICCS Integration and Test Facility. "We have had tremendous success with our offline test program, finding the majority of software defects before deployment—when it is most cost effective," says Drew Casavant, Controls Verification and Validation manager. "Offline testing substantially decreases the time we need to validate a software release."

The Integration and Test Facility contains servers, workstations, network equipment, FEPs, embedded controllers, and example devices to be controlled

Software releases are tested online with NIF hardware before they are approved for deployment.

during testing. Because it is impractical to reproduce NIF in the test bed, simulation software and other test aids are often used. “Simulations can offer high fidelity in testing the behavior of NIF systems,” says Casavant, “but we also run tests with real hardware as the final confirmation that the systems operate correctly and meet the performance requirements.”

Software testing can range from controlling an individual motor to executing a full shot sequence. In addition, fault conditions can be introduced during offline tests to confirm expected system behavior without risk of misoperating equipment or adversely affecting the facility. NIF shot directors and control room console operators participate toward the end of offline test cycles to learn about the new software and prepare for online deployment.

Once fully integrated and qualified in the test bed, the software release is approved for deployment to NIF. The configuration management team installs the software and verifies the release is complete and starts correctly. Testers ensure that software continues to work as expected and that new functionality operates as designed. Test personnel receive extensive training in safety, site work controls, and operation of the laser equipment.

NIF Early Light Proved the System

During the next 4 years, as more laser equipment is installed, the ICCS software and controls proven on the first quad will be installed to activate the remaining bundles. Additional automation is being developed for the target area control system. The team wants to reduce the number of manual activities required to control the target positioner, diagnostic manipulators, target diagnostic instruments, and other equipment in and around the target chamber.

“We can keep building onto the control system because the right architecture was laid down early in the project,” says Patterson. Looking to the future when all 192 beams are firing regularly, he envisions a continual process for improving ICCS to make operations even more efficient and easier for experimenters.

“We’ve established disciplined software engineering to deliver a majority of the software, and we’ve proven the control system architecture,” says VanArsdall. The team is increasingly confident that NIF will be a vital resource for keeping the U.S. nuclear stockpile safe and reliable, advancing scientific knowledge of the physics of matter under extreme conditions, and taking the next steps in fusion energy toward achieving ignition. “Many of us have devoted most of our careers to achieving ignition in the laboratory,” says Lagin. “It’s a grand challenge, and it’s also a great privilege to be part of the team working to achieve it.”

—*Arnie Heller*

Key Words: front-end processor (FEP), integrated computer control system (ICCS), laser performance operations model (LPOM), National Ignition Facility (NIF), NIF Early Light, stockpile stewardship.

For further information contact Paul VanArsdall (925) 422-4489 (vanarsdall1@llnl.gov) or Larry Lagin (925) 424-3331 (lagin1@llnl.gov).

A Random Walk through Time and Space

Random motion rules from the smallest molecules to the largest meteorological events, with enormous results.

IN 1905, Albert Einstein published five papers that shook the world of physics. His elegant arguments and conclusions were marvels of physical intuition that addressed dilemmas raised by experimental evidence. Those papers have been so important to physics research that 1905 is known as Einstein's miraculous year.

One of the papers, "On the Movement of Small Particles Suspended in Stationary Liquids Required by the Molecular-Kinetic Theory of Heat," has profoundly affected how scientists view the makeup of physical matter. In that paper, Einstein combined kinetic theory and classical thermodynamics, laying the theoretical groundwork for measurements to confirm the existence of atoms. Later that year, he extended his mathematical development of the theory, writing "On the Theory of Brownian Motion," which was published in February 1906.

In addition, he submitted his doctoral dissertation on the size of molecules. One of Einstein's most frequently cited papers, it shows how to use fluid phenomena to determine Avogadro's number—the number of atoms in a defined mass of material.

The work underlying these three publications embraced a branch of physics known as statistical mechanics and helped confirm the atomic theory of matter. A century later, it continues to form the basis for much of the Laboratory's work in molecular dynamics, Monte Carlo statistical techniques, and physical chemistry.

The Molecular Dance

The story of Brownian motion begins long before Einstein's time. In the summer of 1827, the botanist Robert Brown noted that when pollen grains suspended in water were viewed through a microscope, they appeared to be dancing as if they were alive. Brown showed that this motion occurred whenever such small particles—living or nonliving—were suspended in water. The movement neither slowed nor stopped, but it was affected by the temperature of the liquid in which the particles were suspended.

At the time, many scientists suspected this random motion had to do with molecular movement, but no one could explain it quantitatively until Einstein published his 1905 paper. In so doing, he managed to reconcile the laws of thermodynamics—the mechanical actions of heat flow—with the kinetic theory of gases.

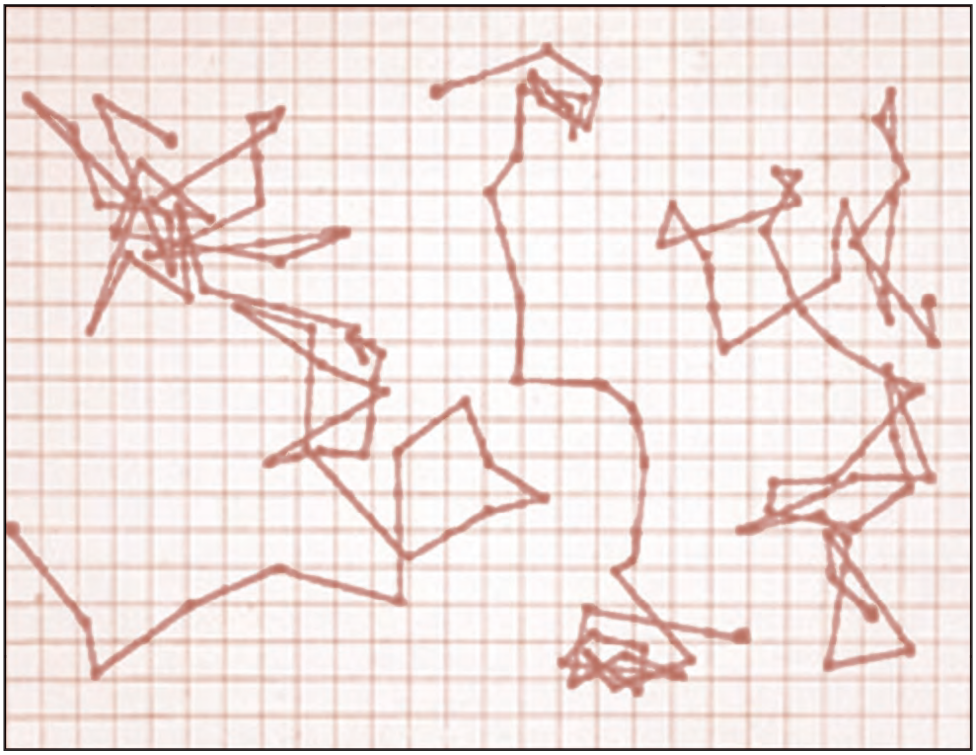
The first law of thermodynamics relates heat, energy, and useful work to each other in thermal processes. If all matter consists of atoms or molecules, then heat is the energy of motion—the kinetic energy—of these atoms. The first law, which is basically conservation of energy, states the reversibility of physics and could be understood in terms of the motions and collisions of Newtonian atoms. A movie showing collisions between simple atoms looks normal if run backward. The second law of thermodynamics defines the flow of heat in natural processes, such as the melting of ice. This law is irreversible: Ice that has melted at room temperature will not refreeze by itself.

Faced with the paradox that interactions are reversible and nature is irreversible, some scientists chose to deny the existence of atoms. Two physicists, James Clerk Maxwell and Ludwig Boltzmann, approached the issue by building on the 18th-century idea that matter, such as a volume of gas, is composed of many tiny particles. Boltzmann, in particular, resolved the contradiction between Newtonian mechanics and thermodynamics by interpreting the second law as a statistical law, not an absolute. Many results of thermodynamic experiments, he said, could be explained by calculating the average or statistical behavior of such a collection of particles.

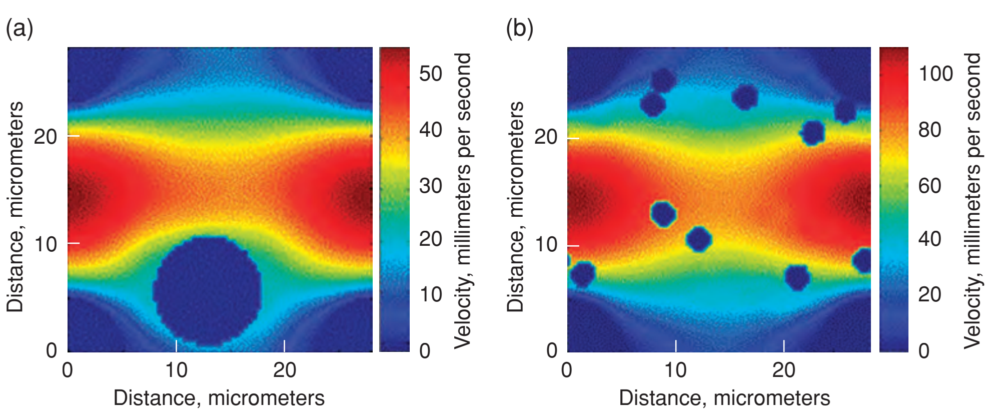
Of Random Walks and Statistics

Einstein's doctoral dissertation developed a statistical molecular theory of liquids. (See the box on p. 15.) In his subsequent 1905 paper, he predicted that randomly moving molecules in liquid impact larger suspended particles, causing them to move randomly. He derived a relation between how far these particles jiggled over time and the temperature, the liquid's viscosity, the number of molecules in the liquid, and their size. Knowing this mathematical relationship, Einstein reasoned, scientists could then measure the size and number of the molecules in a liquid using a microscope and a stopwatch. A few years later, French physicist Jean Perrin and his students conducted such an experiment, and by 1913, most physicists accepted the atomic theory of matter.

Einstein's work on Brownian motion also was the first practical application of random processes for understanding physical phenomena, because he related the random walk of a single particle to the diffusion of many particles. This randomness was the source of the irreversibility of many macroscopic



Albert Einstein's papers on Brownian motion led French scientist Jean Perrin to record the irregular motion of suspended particles in a solution.



The lattice Boltzmann code characterizes fluid flow and filtration, using the generalized Einstein equation to study hindered transport phenomena. These examples show results from the characterization of (a) hindered convection and (b) species capture in a regular array of cylinders.

processes and, hence, the second law of thermodynamics.

Studies of these processes were just beginning in 1905. Today, many projects at Lawrence Livermore reflect back to Einstein's seminal work on Brownian motion, random processes, and statistical mechanics. These projects all build on Einstein's legacy, from understanding biological functions and simulating the movement of molecules and individual atoms in plutonium, to using Monte Carlo techniques for atmospheric predictions and discovering the existence of a low-temperature quantum fluid in hydrogen.

Statistically Speaking of Fluids

In one project, Livermore engineer David Clague leads an effort to develop computational tools for statistically studying fluid behavior. These simulations do not track individual molecules; instead, they represent the collective behavior of fluid molecules in different regions. One of these models includes a generalized Einstein equation to study hindered transport phenomena. "Basically," says Clague, "we're simulating how very small particles—from nanometers to micrometers in diameter—move through fluids and filtrate or pass through a barrier."

Clague's team has modeled the process of kidneys filtering out contaminants and microfluidic systems designed to capture and analyze pathogenic particles. The three-dimensional (3D) transport model is based on the lattice Boltzmann (LB) equation. This equation statistically describes the fluid as a cubic lattice, where each lattice site represents up to several thousand individual fluid molecules. Developed with funding from Livermore's Laboratory Directed Research and Development (LDRD) Program, the LB model incorporates external forces and structures such as biological membranes or porous glass to study thermal diffusion and the dynamic behavior of a collection of particles.

Clague is working with Kevin Ness, a doctoral student from Stanford University, on a multiphysics version of the LB model. This code includes detailed descriptions of microstructures, the relevant surface forces that characterize microstructure capture and release of specific species such as types of DNA, and the temperature effects for both liquid- and gas-phase systems. The simulations use complicated 3D models of actual materials rather than idealized models of materials. Ness is using the multiphysics code to model hindered transport on a microfluidic chip that has small glass pillars designed to capture DNA for analysis.

The multiphysics code also contains modules that can create a complete picture of how particles flow in liquids or gases, and it works with both natural and manufactured materials. "It even works with physiological media," says Clague. "It's all about diffusion, which takes us right back to Einstein and his work."

Zeroing In on Atmospheric Releases

In another LDRD project, Livermore physicist Branko Kosovic and engineer Bill Hanley are developing a computational tool to help scientists at Livermore's National Atmospheric Release Advisory Center better predict the consequences of hazardous releases to the atmosphere, which is particularly challenging when the source of the release is unknown or poorly characterized.

Atmospheric dispersion is complex and difficult to reconstruct. For instance, an explosion releases contaminants instantaneously, but a forest fire spews them out continuously. Contaminants also may be static or moving, and they may be released near Earth's surface or at elevated altitudes. In addition, atmospheric conditions such as wind direction, velocity, and turbulence affect their movement.

The Livermore-developed reconstruction capability rests on Bayesian inference, a probabilistic approach that combines observed data, physical models, and prior knowledge. The result is a sample of likely dispersion scenarios given what is known thus far. When all of the observed data are available up front, the event reconstruction uses Markov chain Monte Carlo (MCMC) to sample the dispersion scenarios, including the possible location of the emitting source.

His Thesis Lives On

In his doctoral thesis, Albert Einstein used statistical mechanics (the study of the motion of objects using mathematical tools for dealing with large numbers of objects) to estimate the size of molecular radii and how many molecules would be found in a fixed amount of material.

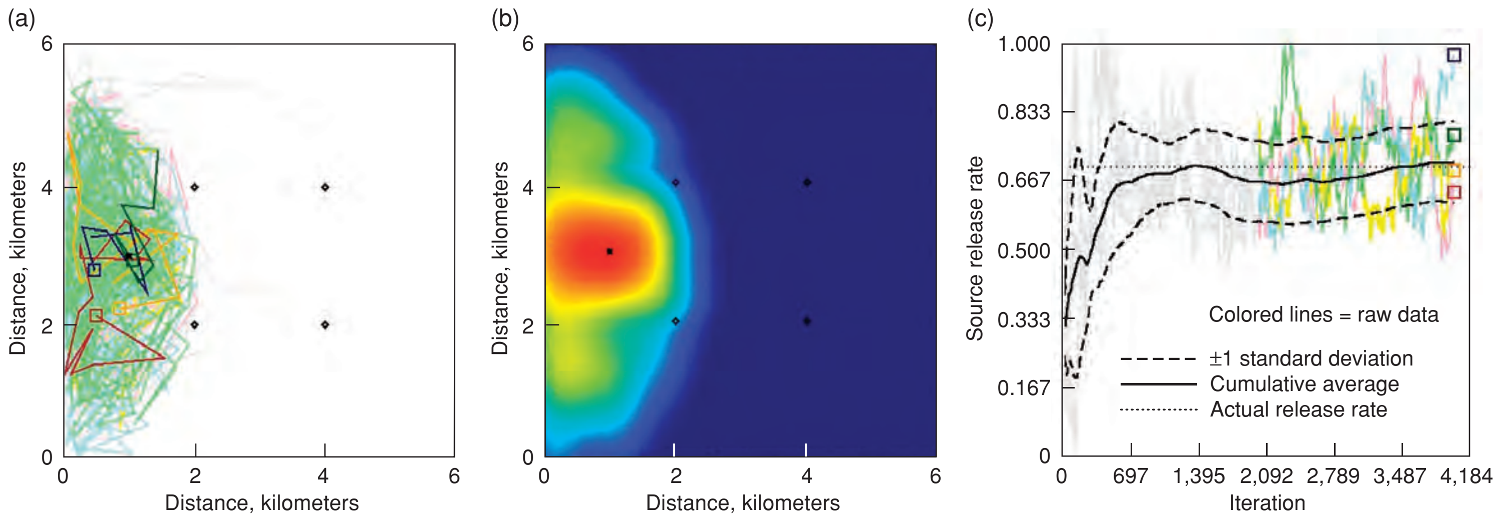
At that time, the existence of molecules and atoms had not been definitively established. In his thesis, Einstein used atomic theory to explain how substances such as sugar would dissolve into water. He related the diffusion coefficient (the measure of how quickly materials diffuse in a liquid) to the temperature, number of atoms, viscosity of the liquid, and the size of the atoms dissolving into the liquid. This fundamental relation is now known as the Einstein equation. Using values of the diffusion coefficient and viscosity obtained from experiments done at fixed temperatures, Einstein related the total number of atoms in the liquid to the size of the sugar molecules. Einstein also showed that the liquid's viscosity depended on how much volume was taken up by the dissolved material.

Of all Einstein's work in 1905, his thesis had the most practical applications. The techniques he employed have been used to explain the motion of sand particles in concrete mixes, protein blobs in milk, and aerosol particles in clouds.

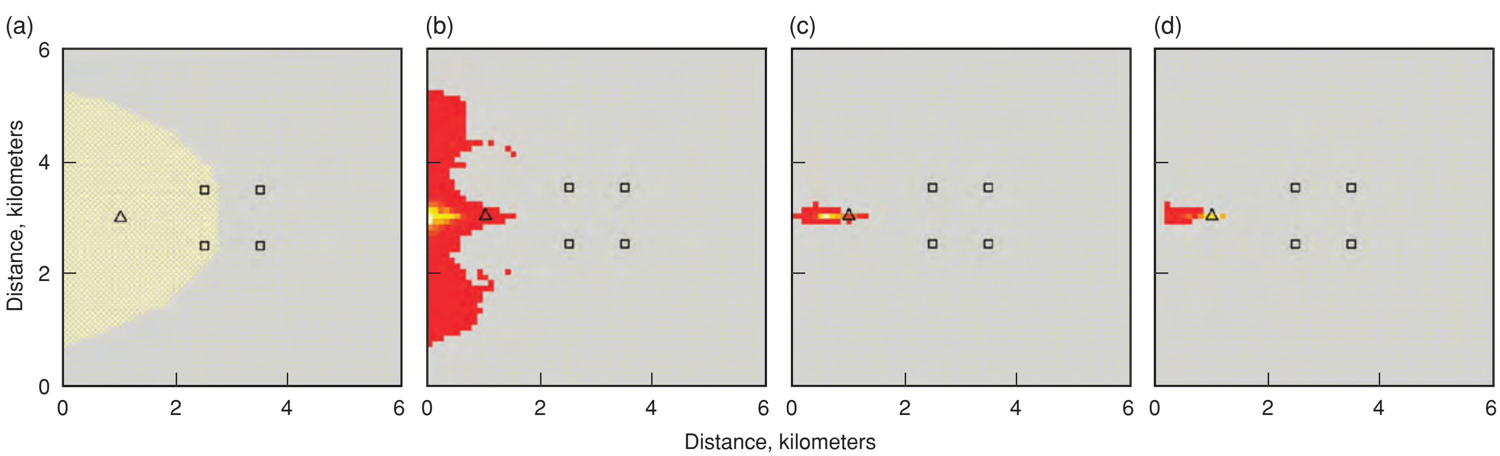
In a more dynamic setting, where the data are accumulated over time as the event unfolds, the reconstruction relies on a sequential Monte Carlo (SMC) sampling approach.

"MCMC is a proven technique that typically uses a random-walk-type procedure to sample possible outcomes when given all the available data up front," says Hanley. "However, MCMC is inefficient and costly when the goal is to dynamically update the pool of possible outcomes as more data become available. The SMC sampling approach was developed to handle those cases. It reweights and resamples the current pool of possible outcomes to reflect the newly available data in an efficient way."

Statistical theory and the related science-based application tools seem a long way from Einstein's original papers. Yet, in some ways, they are direct descendants from his work. "As the problems of event reconstruction get



(a) In a random walk reminiscent of Perrin's 1908 recordings of particles in a fluid, a two-dimensional code does a statistical dance to reconstruct the characteristics of a hypothetical atmospheric release based on concentrations measured by four sensors in a square array. This feasibility demonstration started with a square sensor array and uses Monte Carlo statistics to deliver a probabilistic determination of (b) the source location and (c) the release rate.



Using sequential Monte Carlo for atmospheric event reconstruction allows the code to dynamically update its calculations as more data are gathered over time. In this two-dimensional example, the release starts after a 10-minute interval, with an exponentially decaying release rate over the next 50 minutes. Data are gathered at 10-minute intervals. (a) The initial conditions, before stochastic sampling begins, are used to set the source term parameters (given the wind direction, we know the source is not located to the right of the sensors). The probability distribution for source location is shown after (b) 20 minutes, (c) 40 minutes, and (d) 60 minutes of data gathering and code calculations. Each color represents a 10-percent probability mass, where red is low probability and yellow is high.

increasingly complex and uncertain, we need proven computational models to handle uncertainties whether they stem from changing meteorological conditions or unknown variables in the data we've collected," says Kosovic. "The stochastic methodologies introduced by Einstein and others are adaptable to many dynamic systems. It's just the beginning for us."

Seeing Atoms

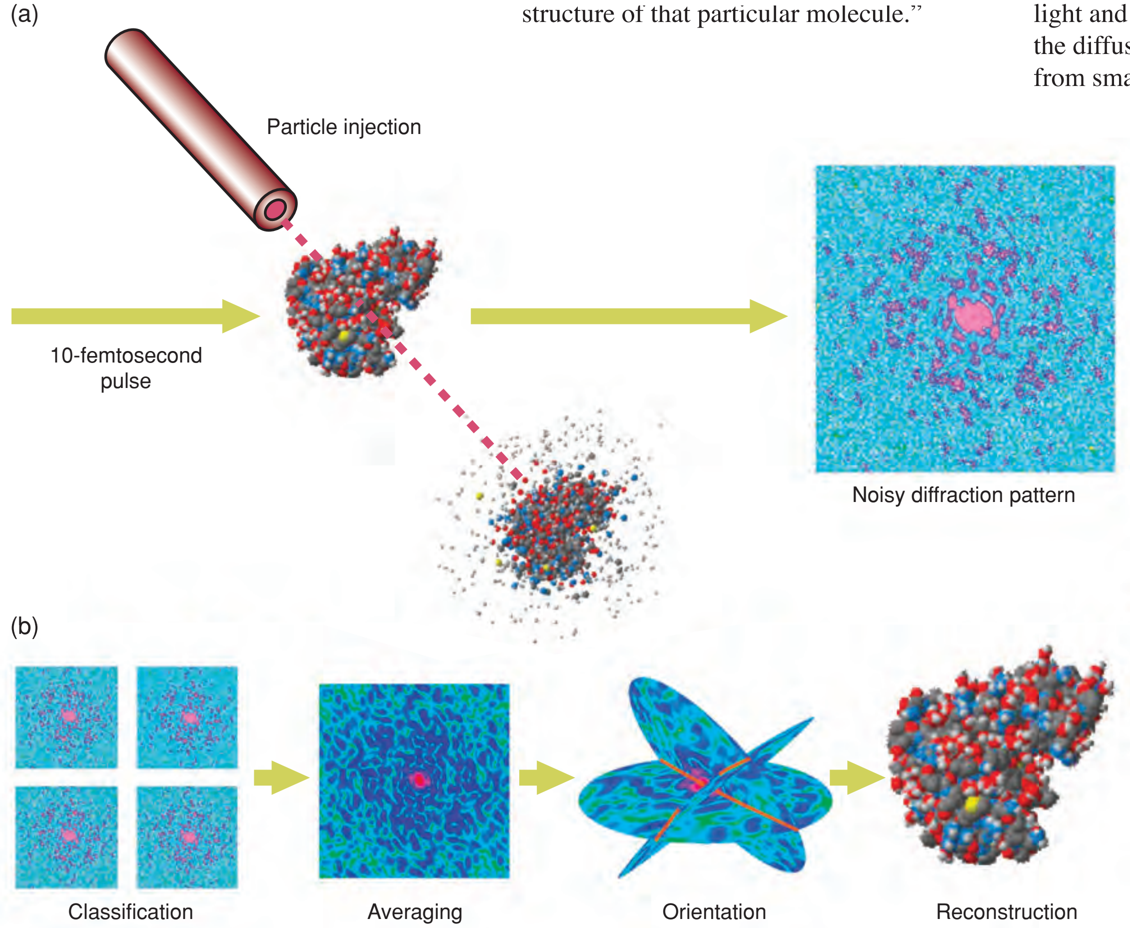
The scientists of Einstein's day had no hope of seeing atoms, but a century later, new technologies are making that a reality. Livermore physicists Henry Chapman and Stefan Hau-Riege received LDRD funding for their work on a project that will use the Linac Coherent Light Source at the Stanford Linear Accelerator Center to image complex biological molecules composed of 10,000 to 100,000 atoms. (See *S&TR*, September 2000, pp. 23–25; December 2003, pp. 4–10.) "We've moved in the space of a century from discussing whether atoms exist to actually being able to image atoms in crystals," says Chapman, "and we're on the threshold of imaging them in noncrystalline biological macromolecules, protein complexes, or viruses."

The basic technique for constructing these images is to inject a single molecule into the path of an incoming x-ray pulse and then measure the resulting diffraction pattern—the pattern of scattered x rays just before the molecule explodes from energy absorbed. "One image doesn't give us a full 3D picture of the molecule, so we repeat the process many times," says Hau-Riege. "We combine data from all of the images to build a 3D model of the molecule, which gives us an average structure of that particular molecule."

Although the same type of molecule is being imaged each time, the diffraction patterns differ. "Brownian motion is partly to blame," says Chapman. "The molecules are jiggling and so are the atoms. Atoms also have thermal vibration, and even though they're bonded to each other, they're moving about. Some even swing at the end of their bonds, like a tether ball." To resolve this problem, the team is developing methods to align the molecules so they will always have the same orientation when imaged.

Looping the DNA Loop

In 1908, Perrin's team used microscopes to view particles one-thousandth of a millimeter in diameter and timed the diffusion over a given distance. Today, Livermore chemist Chris Hollars and physicist Ted Laurence are using laser light and fluorescing dyes to determine the diffusion of single molecules, ranging from small organic molecules less



(a) To image biological molecules with atomic resolution, Livermore physicist Henry Chapman and his team will inject single molecules into the beam of the x-ray free electron laser, irradiate each molecule with a blast of x-ray laser light, and record the resulting two-dimensional diffraction pattern before the molecule disintegrates. (b) A single three-dimensional image of a representative molecule will be constructed from terabyte data sets consisting of millions of diffraction patterns.

than a nanometer in diameter to large biomolecules 10 nanometers in diameter.

This LDRD project, led by Livermore physicist Daniel Barsky, combines molecular dynamics simulations with experiments to track the random walk of a protein "sliding clamp" as it scoots around a ring-shaped DNA molecule. Sliding clamps work much like a carabiner on a climbing rope and can "ride" more than 10,000 bases along a DNA double helix in less than a second. Interpreting the details of their zigzagging motions will help scientists understand the processes of DNA replication, recombination, and repair.

Hollars and Laurence are using single-molecule fluorescent resonance energy transfer (FRET) measurements to infer the speed and diffusional characteristics of an individual clamp protein as it moves. For the FRET measurements, scientists label a molecule with a photoluminescent "tag." Then they illuminate the molecule with laser light tuned to a specific wavelength, which causes the tag to fluoresce and give off light of a different wavelength. The laser beam is focused down to a volume of about 1 cubic micrometer, and the scientists watch for a DNA ring and clamp to diffuse into the volume. "We have a low concentration of DNA molecules in the mix, so we can view one molecule at a time," says Laurence.

Once a molecular complex arrives in the focus, the clamp fluoresces. If the clamp slides within 5 nanometers of the ring's labeled area while in the focus, the label absorbs the clamp's green photons and fluoresces red.

"The experiment," notes Hollars, "involves Brownian motion on two scales: the motion of the DNA ring as it dances through the volume, and the motion of the clamp as it slides around the ring."

Eventually, the team hopes to label multiple areas of the DNA loop with other fluorescent tags to provide an even more detailed picture of how the clamp moves around the DNA ring.

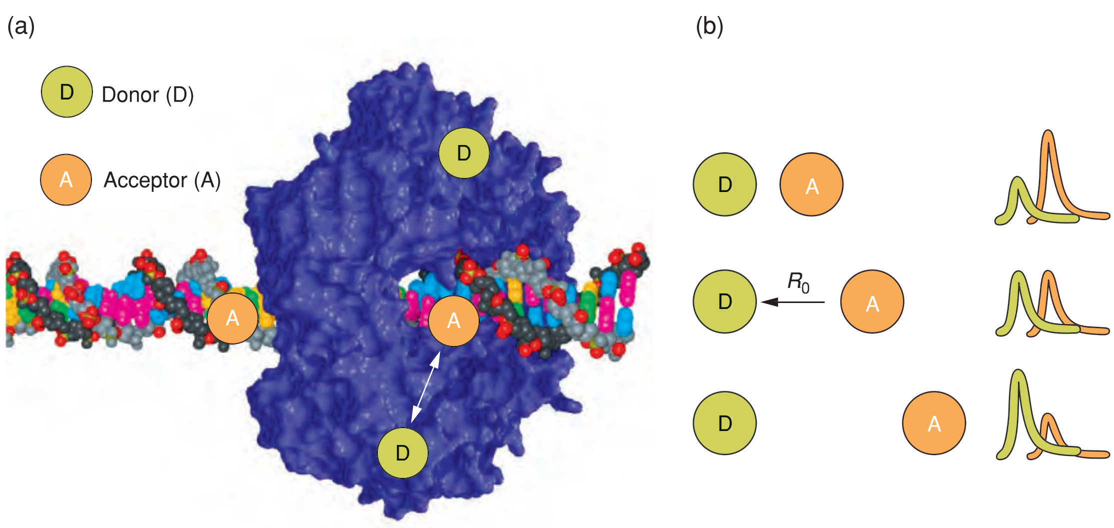
Bubble, Bubble, Toil, and Trouble

"Brownian motion is a beautiful example of Einstein's insight," says Livermore physicist Bill Wolfer. "He showed that by examining a particle moving in a gas or fluid, we can extract information on a physical aspect of that particle—the diffusion coefficient."

As it turns out, this property is of great importance in stockpile stewardship research, particularly for plutonium aging. When plutonium—or any radioactive material— decays, it generates helium atoms, which diffuse into small bubbles about 1.5 nanometers in diameter. These bubbles can affect the material's properties such as its strength.

To measure how much helium has been formed, scientists usually melt a material and extract the trapped helium, but this technique is too volatile for plutonium studies. "When we heat a material with bubbles of gas in it, the bubbles expand and eventually burst, sending material splattering everywhere," says Wolfer. "That is not an experiment we can conduct with plutonium."

Instead, to determine how the helium behaves when plutonium is heated to melting and beyond, Wolfer and chemical engineer Alison Kubota simulated the discrete motions of individual plutonium atoms and their interactions over time and at varying temperatures. Using the molecular dynamics code MDCASK, Kubota modeled the behavior of helium atoms in a block of aluminum as it was heated to the melting point. The simulations correctly yielded the diffusion coefficient and showed that a bubble will coalesce in about 1 nanosecond; two bubbles will diffuse and



Fluorescence resonance energy transfer (FRET) can be used to measure the distance between two labeled biomolecules. (a) When the two molecules are close together, the donor molecule in the proton clamp emits a photon of a given wavelength, which is absorbed by the second molecule in the DNA ring. (b) The strength of the two signals depends on the distance (R_0) between the donor and the acceptor. When the two are farther apart, only the donor wavelength is observed. When they are close together, the acceptor wavelength dominates.

touch in 680 nanoseconds and then fuse in 30 picoseconds. Says Kubota, "Brownian motion turns out to be the deciding factor in the process."

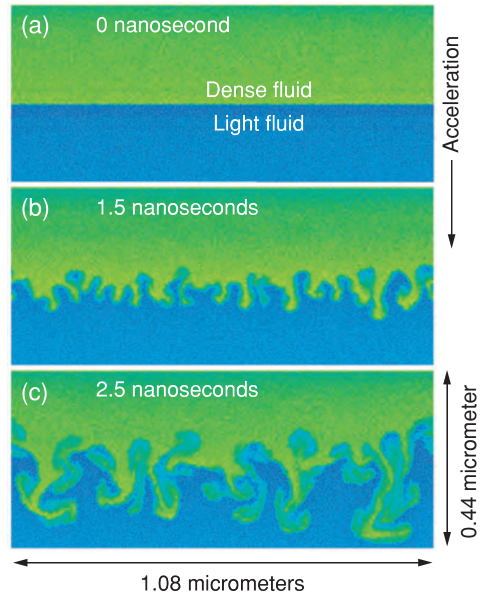
Yet, a bubble is not a solid pollen particle suspended in a liquid. Thus, Einstein's papers on Brownian motion turn out to be far more profound and transcend the explanation of the original experiments that inspired them. Brownian motion applies to any observable feature in a gaseous or fluid medium, such as interfaces between proteins and water, between a gas and a fluid in a bubble, or between two different fluids. In fact, bubbles diffuse because the bubble surface is subject to Brownian motion. The random motion of atoms along an interface between two different liquids also seeds hydrodynamic instabilities. This connection has long been accepted by scientists, but it had not been demonstrated until the recent work of Kubota in her LDRD project to model hydrodynamic instabilities at the atomic level.

Hydrodynamic instabilities are fluid phenomena involving the mixing between two fluids of different densities at the fluid interface, due to some external acceleration such as gravity. By simulating these instabilities in 3D, Kubota and her collaborators hope to obtain an atomic-scale view of phenomena and include those data in continuum-type fluid codes. "For instance, when we look at two fluids mixing, we often see bubbles," says Kubota, "but we have no idea how those bubbles affect the instabilities. Now, with these powerful codes and supercomputers, we can work it out from the most basic of Newton's laws."

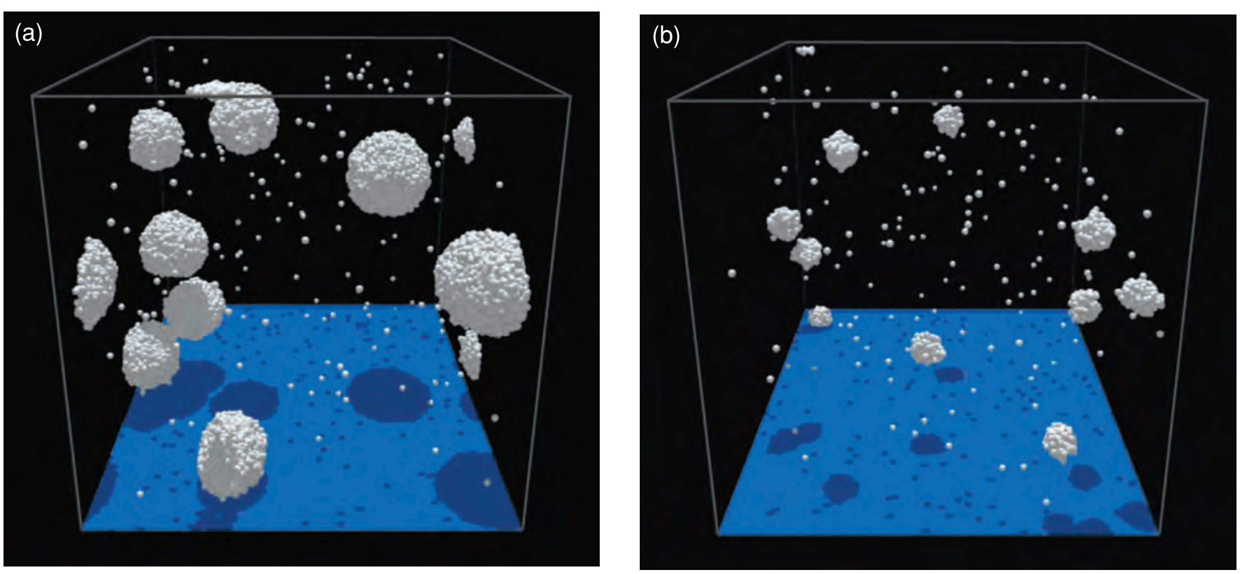
From First Principles

Another group at Lawrence Livermore is simulating the motion of atoms from first principles using the laws of quantum mechanics as their only input. The Quantum Simulations Group investigates material behavior at high temperatures and pressures, at the nanoscale, and in solution. Livermore physicist Giulia Galli, who leads the group, says, "Two of these areas in particular involve Brownian motion: materials in extreme conditions and materials in fluids."

Members of the group use first-principles molecular dynamics and quantum Monte Carlo codes to examine the motion of liquids at the microscopic level. Their projects, many of which are LDRD funded, include solving quantum mechanical



Hydrodynamic simulations of systems with millions of atoms are now possible at the atomic scale, given the increased power of supercomputer systems such as BlueGene/L and codes such as MDCASK. Sample results from a two-dimensional atomistic simulation of a Rayleigh–Taylor instability.



Models of helium atoms show how the atoms behave when a material is heated to the melting point: (a) 3,000 atoms forming bubbles at 4 nanometers, and (b) 200 atoms forming bubbles at 1.5 nanometers.

calculations for large numbers of atoms in a variety of physical conditions.

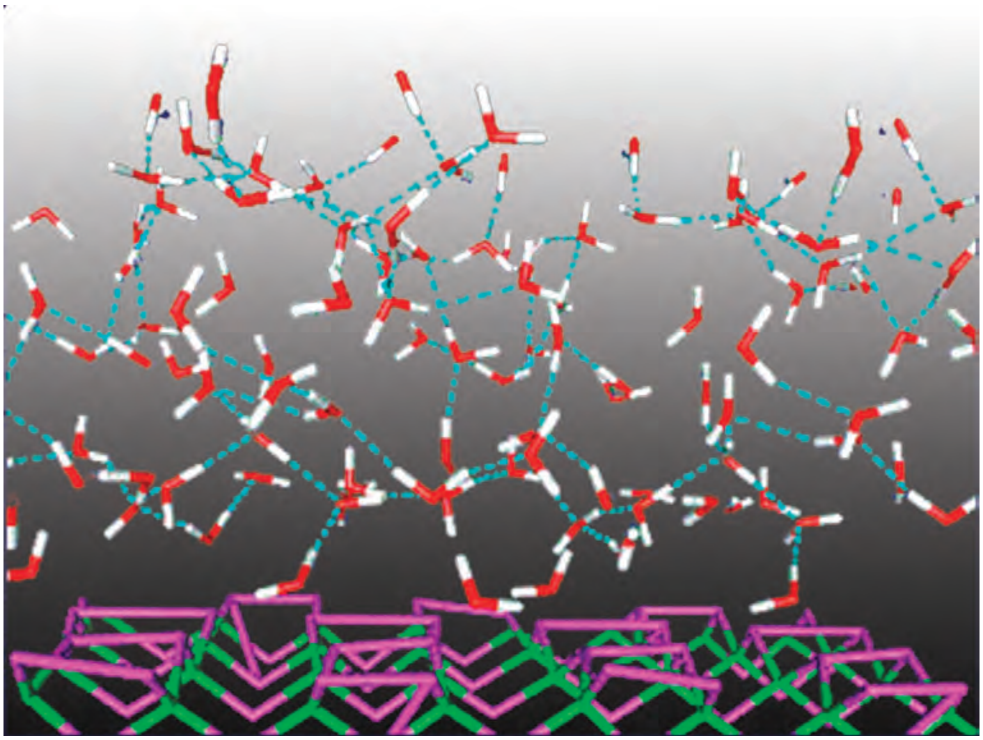
A recent success is the discovery of a new melt curve of hydrogen at extremely high pressures. (See *S&TR*, January/February 2005, pp. 4–13.) Results from these simulations provided strong evidence that a low-temperature quantum fluid may exist in hydrogen. The team is developing experimental measurements to help verify the existence of a maximum melting temperature and the transformation of solid molecular hydrogen to a metallic liquid at enormous pressures.

Molecular dynamics codes are also used to examine the behavior of water and its structural, dynamic, and electronic properties at the molecular level. "It may sound strange that now, at the beginning of the 21st century, scientists still don't completely understand the bonding of water both theoretically and experimentally," says Galli. The group is studying water under ambient conditions, under pressure, and in confined geometries to determine how its structure and electronic properties change as thermodynamic conditions vary.

The group's calculations point out the challenges that remain in understanding this abundant material. "At the nanoscale, predicting the behavior of water and aqueous solutions is extraordinarily challenging, and experimental data are still sparse," says Galli. "In this regime, classical simulations can become unreliable. Quantum simulations, in contrast, require no experimental input, so they can make accurate predictions."

One example of the group's work involves simulations of liquid–solid interfaces, particularly the diffusion of water on surfaces. Recent simulations show that water does not uniformly wet the surface of silicon carbide, a leading candidate semiconductor for biocompatible devices. Rather, water molecules prefer to bind along directions parallel to silicon atoms forming pairs (dimers) on the surface.

"We're following in Einstein's footsteps," says Galli. "In our calculations and simulations, we're using his concepts of Brownian motion at the atomic level, combined with computers now powerful enough to predict the motion of individual atoms, to build a greater understanding of our world as a whole."



Giancarlo Cicero, a postdoctoral researcher at Livermore, and his colleagues conducted quantum simulations of water on silicon carbide, allowing scientists to better understand the electronic, structural, and dynamic properties of the liquid–solid interface at the microscopic level.

It's Totally Random

Later in his life, Einstein became immersed in searching for a "theory of everything" and dismissed his work on Brownian motion as unimportant. However, random fluctuations and statistical mechanics are fundamental to the most elemental building blocks of the physical world and are called on to explain the mysterious processes of protein folding, cell-membrane function, evolution, and even stock market behavior. In demystifying Brownian motion, Einstein linked statistical mechanics to observable reality. At Lawrence Livermore, scientists continue to reap the rewards of his discovery and intuition.

—*Ann Parker*

Key Words: Albert Einstein, Brownian motion, fluid behavior, fluorescent resonance energy transfer (FRET), helium bubbles, hindered transport, hydrodynamic instabilities, lattice Boltzmann (LB) model, Markov chain Monte Carlo (MCMC) technique, molecular dynamics, quantum simulations, random walk, sequential Monte Carlo (SMC) technique, statistical mechanics, thermodynamics.

For information on Lawrence Livermore's activities for the World Year of Physics, see www.llnl.gov/pao/WYOP.

The Search for Methane in Earth's Mantle

PETROLEUM geologists have long searched beneath Earth's surface for oil and gas, knowing that hydrocarbons form from the decomposition of plants and animals buried over time. However, methane, the most plentiful hydrocarbon in Earth's crust, is also found where biological deposits seem inadequate or improbable—for example, in great ocean rifts, in igneous and metamorphic rocks, and around active volcanoes. Some scientists thus wonder whether untapped reserves of natural gas may exist in Earth's mantle.

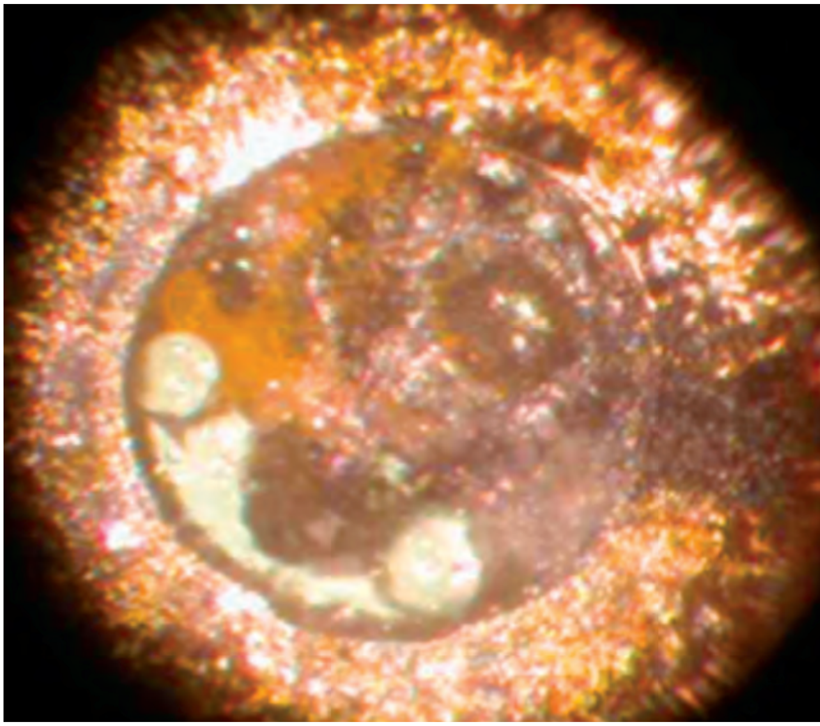
A collaboration of researchers from Lawrence Livermore and Argonne national laboratories, Carnegie Institution's Geophysical Laboratory, Harvard University, and Indiana University at South Bend is finding that methane may also be formed from nonbiological processes. Experiments and calculations conducted by the team indicate that Earth's mantle may provide the temperature and pressure conditions necessary to produce methane.

The idea that methane could be formed nonbiogenically came from observing the solar system. In the 1970s, astronomer Thomas Gold proposed that methane must form from nonbiogenic materials as well as from biological decomposition because large amounts of methane and other hydrocarbons could be detected in the atmospheres of Jupiter, Saturn, Uranus, and Neptune. In fact, in studying Titan, Saturn's largest moon, researchers found seven different hydrocarbons.

At the time Gold proposed this theory, conventional geochemists argued that hydrocarbons could not possibly reside in Earth's mantle. They reasoned that at the mantle's depth—which begins between 7 and 70 kilometers below Earth's surface and extends down to 2,850 kilometers deep—hydrocarbons would react with other elements and oxidize into carbon dioxide. (Oil and gas wells are drilled between 5 and 10 kilometers deep.) However, more recent research using advanced high-pressure thermodynamics has shown that the pressure and temperature conditions of the mantle would allow hydrocarbon molecules to form and survive at depths of 100 to 300 kilometers. Because of the mantle's vast size, its hydrocarbon reserves could be much larger than those in Earth's crust.

Simulating Thermochemical Conditions

Livermore's work on the methane research, led by chemist Larry Fried, uses a thermodynamics code called CHEETAH to



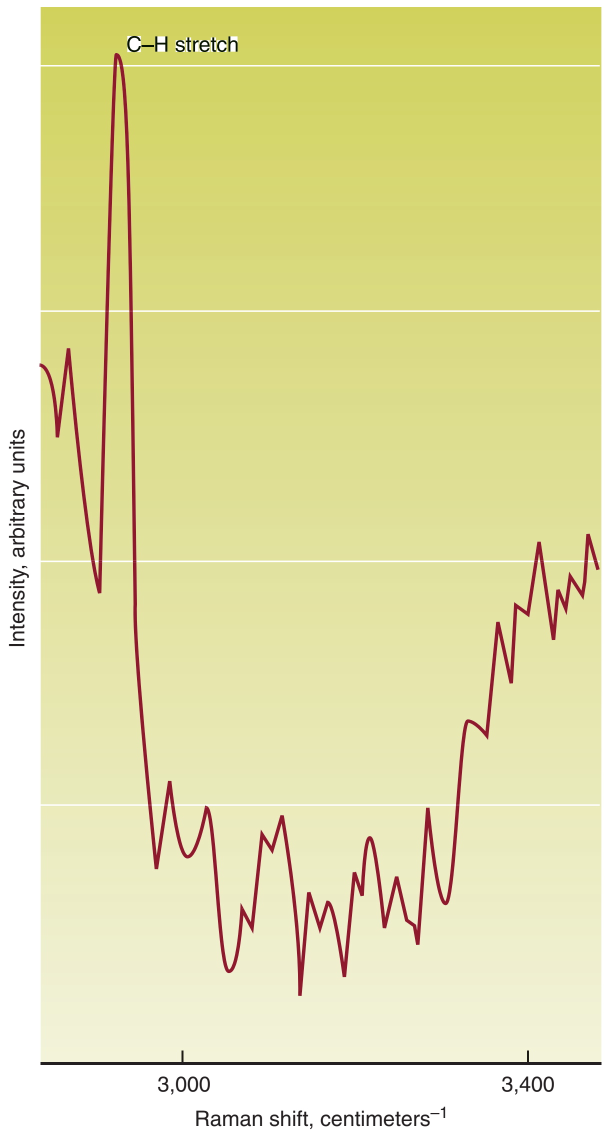
Research indicates that methane bubbles form when iron oxide, calcite, and water are heated to about 1,500°C at a pressure of 5.7 gigapascals and then decompressed at room temperature to 0.5 gigapascal.

simulate chemical reactions using data from the collaboration's experiments. Fried developed CHEETAH in 1993 for the Department of Defense (DoD) to predict the performance of different explosives formulations. Since then, Fried and his colleagues have continued to improve the code. (See *S&TR,* May 1999, pp. 4–11; June 1999, pp. 12–18; July/August 2003, pp. 20–22; July/August 2004, pp. 14–19.)

One improvement was to include intermolecular interaction potentials. As a result, CHEETAH can model accurate equations of state, describing the relationship of a material's pressure, volume, and temperature at the molecular level, for a broad range of thermodynamic conditions. Because materials behave differently under extreme pressures than they do at normal atmospheric pressure, the equation-of-state data produced with CHEETAH help improve the precision of other computer codes used to model materials for stockpile stewardship.

With funding from the Laboratory Directed Research and Development Program, Fried's team is using CHEETAH to analyze the data from experiments conducted at the Geophysical Laboratory and at Argonne. "CHEETAH was designed for defense-related efforts," says Fried. "Our current studies for the methane collaboration are validating the code for work in high-pressure chemistry. These results will in turn help us better understand the processes occurring in a high-explosive detonation."

For the methane experiments, researchers at the Geophysical Laboratory used Argonne's diamond anvil cell (DAC)—a small mechanical press that forces together the tips of two diamond anvils and creates extremely high pressures on a sample of a material held within a metal gasket. DACs allow researchers to measure material properties under static pressure and at varying pressures and temperatures over many hours. (See *S&TR*, December 2004, pp. 4–11.) Diamonds are used because they can withstand these ultrahigh pressures. Also, their transparency permits diagnostic radiation, such as x rays and visible light, to pass unhampered through their crystalline structure.



In one experiment, a sample of iron oxide, calcite, and water is heated to 600°C at a pressure of about 2 gigapascals. Raman spectra of the sample show a carbon–hydrogen (C–H) stretching vibration at 2,932 centimeters^{-1}, which is the industry-standard signature for methane.

Comparing Experimental Results with Calculations

To determine the chemical reactions that might occur at the pressures and temperatures of Earth's upper mantle, the researchers used the DAC to squeeze a microgram sample of iron oxide, calcite, and water to pressures up to 11 gigapascals at temperatures of more than 1300°C. Then they analyzed the results using Raman spectroscopy, synchrotron x-ray diffraction, and optical microscopy.

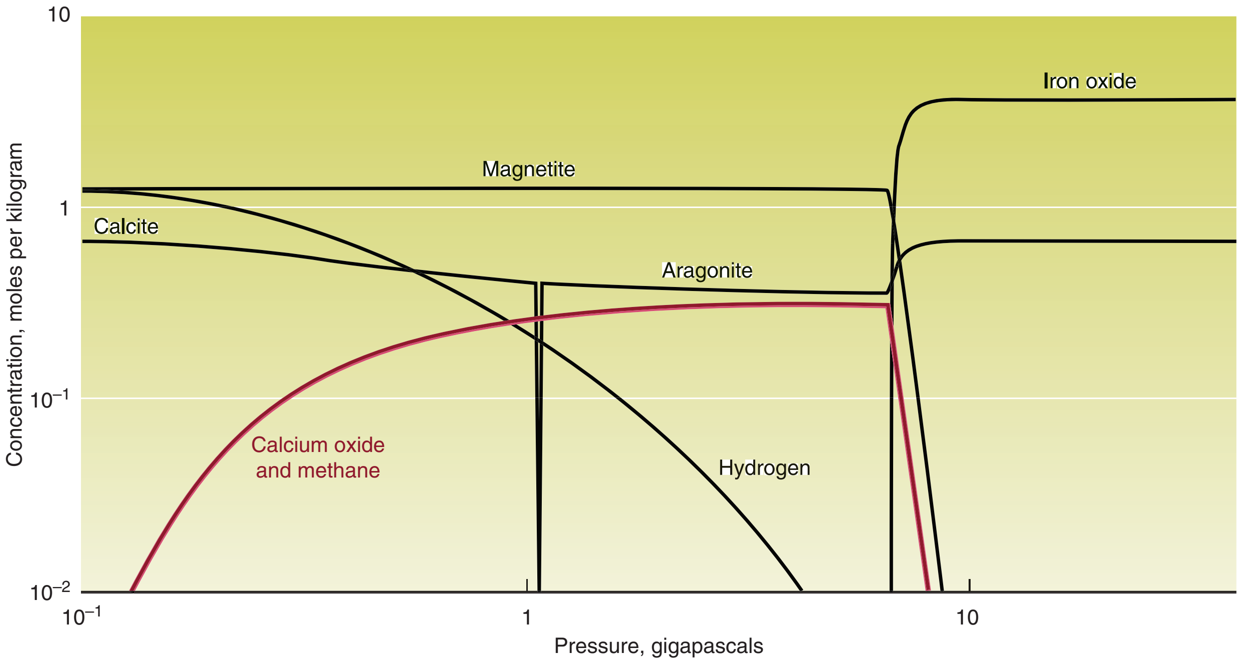
Raman spectroscopy measures the wavelength and intensity of scattered light from molecules as they vibrate about their bonds. These vibrations occur at certain frequencies. At normal pressures, electrons are tightly held within an atom's inner electron bands or shells. Squeezing a material under extreme pressures forces its atoms into a different orientation, which causes the delocalization of electrons and changes a material's properties and molecular structures.

By observing the frequency created when the electrons move or vibrate, scientists can tell how the elements are bonding to each other. Raman spectroscopy is highly sensitive to the stretching vibrations between carbon and hydrogen. The Raman spectra for the DAC samples showed hydrocarbon-rich regions. The bond vibration between carbon and hydrogen becomes apparent in the spectra when the sample temperature reaches 500°C and is very strong by 600°C.

The researchers used synchrotron x-ray diffraction to determine the principal reaction products that occur as the DAC squeezes the samples. With synchrotron x-ray diffraction, a beam of x rays passes through the sample, and the resulting diffraction pattern is recorded on an x-ray film or detector. Changes in the pattern reveal how much of each element is involved in the chemical reaction at different temperatures and pressures. Diffraction results on the team's samples showed the presence of calcium oxide and magnetite—a chemically reduced form of iron oxide. When researchers examined the samples using optical microscopy, they again found changes indicating the presence of methane. Most notable were bubbles, which Raman measurements confirmed to be methane.

The Potential for Unlimited Energy Reserves

The DAC experiments provided the researchers with accurate data on the chemical reactions occurring at the temperature and pressure conditions of Earth's mantle. Fried's team then



Thermochemical calculations for a mixture of iron oxide, calcite, and water heated to 500°C show that methane is produced at pressures up to almost 7 gigapascals.

simulated these reactions using CHEETAH. "Our goal," says Fried, "is to perform thermochemical calculations to determine which temperatures, heating mechanisms, and pressures are most favorable for methane formation." The CHEETAH calculations indicated that methane production is most likely to occur at temperatures near 500°C when pressure is less than 7 gigapascals. These conditions correspond to depths between 100 and 200 kilometers.

"According to our calculations, methane is thermodynamically stable at 500°C and at pressures up to 7 gigapascals," says Fried. "Those results indicate that methane reserves could possibly exist below Earth's surface with a half-life of millions of years." Although methane continued to form up to 1,500°C, the simulations showed that at higher temperatures, the carbon in calcite formed carbon dioxide rather than methane. The calculations also confirmed experimental results indicating the presence of magnetite.

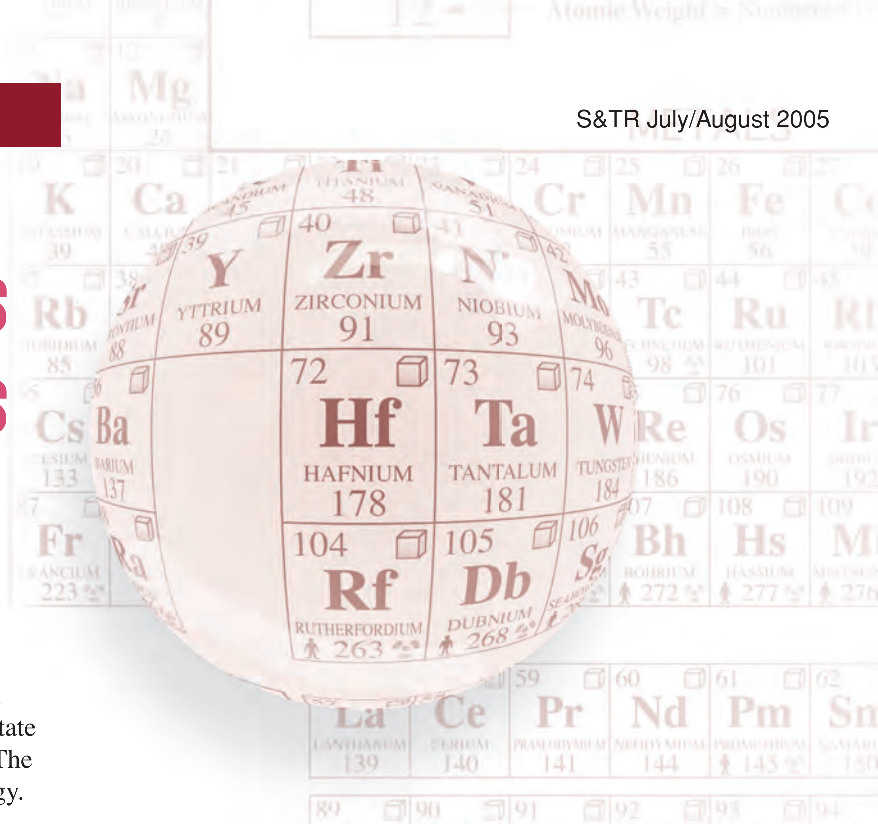
Fried cautions that these findings are preliminary, and more research is needed to determine whether hydrocarbon reserves are indeed available in Earth's mantle. Nevertheless, the Livermore team is pleased with the results. "This work is a good example of collaborative success with groups outside the Laboratory, and it shows a successful dual-use of defense-related technologies," says Fried.

Livermore researchers plan to examine other simple molecular compounds under high pressure, for example, water under conditions that exist in the interiors of giant planets. They will use molecular dynamics and Raman spectroscopy to investigate the existence of a superionic phase of water. In this phase, oxygen atoms are fixed while hydrogen atoms diffuse freely. For Livermore researchers, the ability to study materials under extreme temperatures and pressures means that even the simplest substances may yield many surprises.

—Gabriele Rennie

Key Words: CHEETAH code, diamond anvil cell (DAC), hydrocarbon, methane, Raman spectroscopy, thermodynamics, x-ray diffraction.

For further information contact Larry Fried (925) 422-7796 (fried1@llnl.gov).



Testing the Physics of Nuclear Isomers

FOR much of the past century, physicists have searched for methods to control the release of energy stored in an atom's nucleus. Nuclear fission reactors have been one successful approach, but finding other methods to capitalize on this potential energy source have been elusive.

One possible source being explored is nuclear isomers. An isomer is a long-lived excited state of an atom's nucleus—a state in which decay back to the nuclear ground state is inhibited. The nucleus of an isomer thus holds an enormous amount of energy. If scientists could develop a method to release that energy instantaneously in a gamma-ray burst, rather than slowly over time, they could use it in a nuclear battery.

Research in the late 1990s indicated that scientists were closer to developing such a method—using x rays to trigger the release of energy from the nuclear isomer hafnium-178m (^{178m}Hf). To further investigate these claims, the Department of Energy (DOE) funded a collaborative project involving Lawrence Livermore, Los Alamos, and Argonne national laboratories that was designed to reproduce those earlier results.

A Concern for National Defense

DOE was interested in the hafnium claims because, if verified, they presented new national security issues as well as potential scientific and energy applications. Nuclear isomers with a long lifetime and a high energy release offer the potential to be a stand-alone energy source. However, if scientists could accelerate an isomer's decay so that gamma rays are emitted in an instantaneous burst, they could also use these isomers to develop propellants and explosives.

"Many applications might be possible if we could duplicate the gamma-ray burst reported in the original research," says Livermore physicist John Becker, who led the tri-laboratory effort. "For example, we might consider developing a gamma-ray laser or a nuclear battery that could power a spacecraft. But we did a textbook nuclear physics experiment, and our results did not match the original claim."

A Nucleus with Energy to Burn?

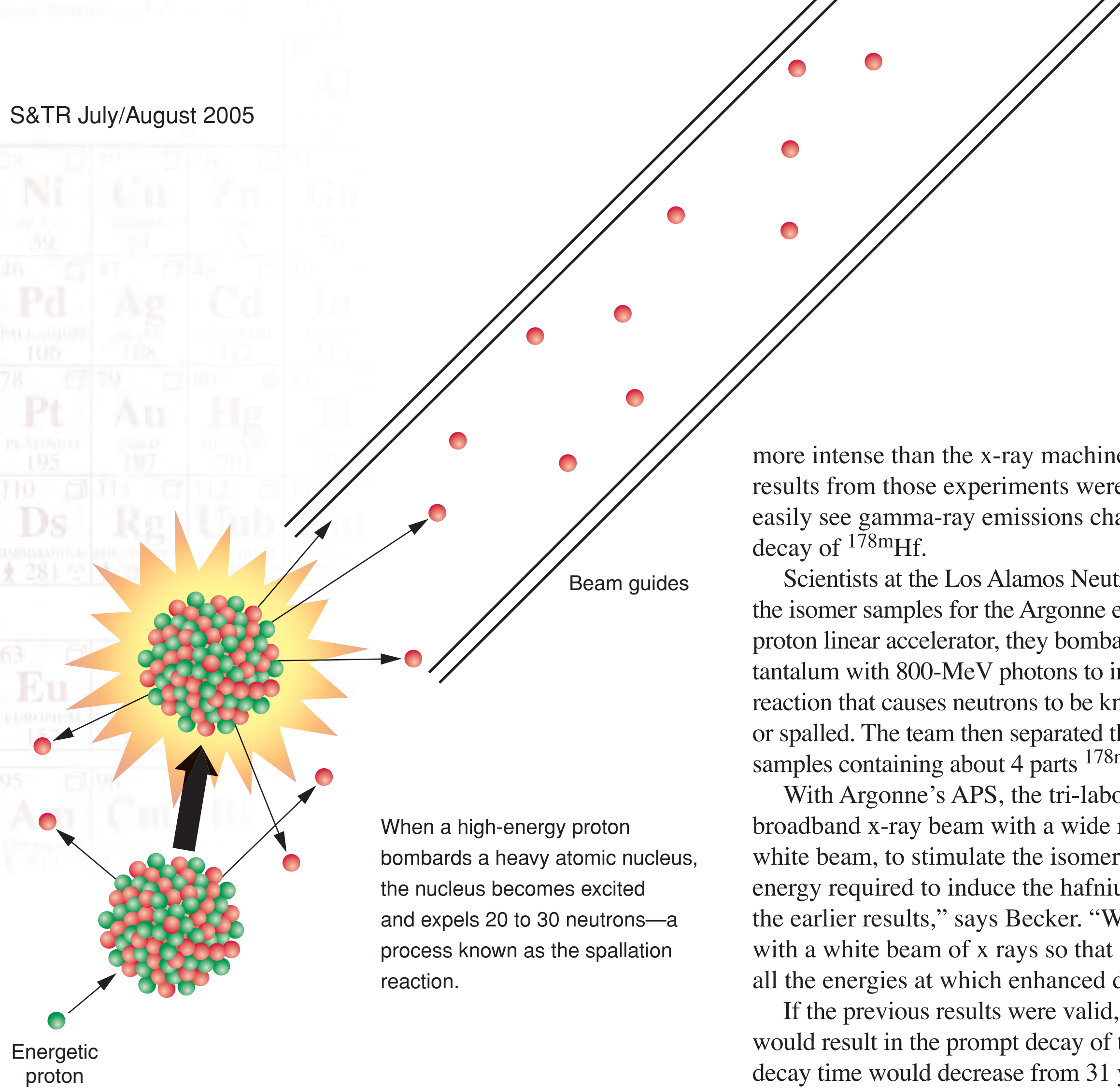
A nuclear isomer is an atom whose nucleus is in a higher energy state than its ground state. This excited state is very long-lived compared with the usual lifetimes of excited nuclear states. The long lifetime results because transition to the ground state would require a large change either in the spatial structure of the atom's nucleus (for a shape isomer) or in the angular momentum (a measure of the spin of the nucleus) between the isomer and the nuclear ground state (for a spin isomer). Both types of isomers release energy, usually as electromagnetic radiation, when the nuclei transition from a high energy state to a lower one.

Nuclear isomers have a wide range of lifetimes, radiating away the extra energy anywhere from about a picosecond (one-trillionth of a second) to years. A common nuclear isomer is tantalum-180m (^{180m}Ta), whose half-life is about 10^{15} years (a quadrillion years). In its ground state, tantalum-180 (^{180}Ta) is very unstable and decays to other nuclei in about 8 hours. Tantalum-180 is never found in natural samples, which are billions of years old, but its isomeric state, ^{180m}Ta, is found in natural samples. This metastable excited state has an excitation energy 75 kiloelectronvolts (keV) higher than ^{180}Ta, and its decay is inhibited because the angular momentum of the isomer's nucleus is so different from that of the ground state's nucleus.

Hafnium-178m, the isomer studied by Becker's team, has a long half-life of 31 years and a high excitation energy of 2.4 megaelectronvolts (MeV). As a result, 1 kilogram of pure ^{178m}Hf contains approximately 1 million megajoules (10^{12} joules) of energy. Some estimates suggest that, with accelerated decay, 1 gram of 100-percent isomeric ^{178m}Hf could release more energy than the detonation of 200 kilograms of TNT.

Reality Check

To verify the results of the earlier experiments, the tri-laboratory collaboration used Argonne's Advanced Photon Source (APS) as the x-ray trigger for the energy release. This light source is 100,000 times



When a high-energy proton bombards a heavy atomic nucleus, the nucleus becomes excited and expels 20 to 30 neutrons—a process known as the spallation reaction.

The Advanced Photon Source at Argonne National Laboratory.

more intense than the x-ray machine used in the 1990s. Thus, if results from those experiments were valid, Becker's team would easily see gamma-ray emissions characteristic of the accelerated decay of ^{178m}Hf.

Scientists at the Los Alamos Neutron Science Center fabricated the isomer samples for the Argonne experiments. Using the center's proton linear accelerator, they bombarded the atomic nucleus of tantalum with 800-MeV photons to induce spallation—a nuclear reaction that causes neutrons to be knocked out of the atom's nucleus, or spalled. The team then separated this material to produce hafnium samples containing about 4 parts ^{178m}Hf to 10,000 parts ^{178}Hf.

With Argonne's APS, the tri-laboratory team generated a broadband x-ray beam with a wide range of wavelengths, called a white beam, to stimulate the isomer samples. "The precise x-ray energy required to induce the hafnium decay had not been cited in the earlier results," says Becker. "We chose to bombard the sample with a white beam of x rays so that our experiments would include all the energies at which enhanced decay had been reported."

If the previous results were valid, the tri-laboratory experiments would result in the prompt decay of the isomer samples—that is, decay time would decrease from 31 years to less than seconds. Instead, the collaboration's results were consistent with expected prediction of nuclear physics. In fact, the team's cross-section limits, which represent the probability of an interaction event between the x rays and ^{178m}Hf, were more than 100,000 times lower in the relevant energy regions than those previously reported. Says Becker, "We conducted a classic experiment, but we saw no evidence of triggered decay."

These findings can allay DOE's concern about potential applications of the purported isomer energy source. X-ray induced decay of the hafnium isomer does not present a new concern for national security. It also is not a viable alternative as a stand-alone energy source. Nuclear physicists at Livermore and throughout the world continue to investigate such unusual nuclear processes.

—Maurina S. Sherman

Key Words: Advanced Photon Source (APS), gamma rays, gamma-ray lasers, hafnium, Los Alamos Neutron Science Center, nuclear battery, nuclear isomers, radioactive decay, stimulated emission.

For further information contact John Becker (925) 422-9676 (becker3@llnl.gov).

Continued from p. 2

Human effects on global climate

A joint study by scientists in the Laboratory's Program for Climate Model Diagnosis and Intercomparison (PCMDI) and at the Scripps Institution of Oceanography concluded that the warming of the world's oceans is a clear signal of human effects on global climate. The recent study—which also involved scientists at the University of Reading and the National Center for Atmospheric Research—compared climate model simulations with observed estimates of how ocean temperatures changed over the second half of the 20th century. Previous research had linked recent ocean warming to human activities, and the new work significantly strengthens this conclusion.

The study focuses on the complex vertical structure of ocean warming and shows that computer models capture this structure if they are run with natural external forcings (solar irradiance and volcanic aerosols) combined with changes in human-induced forcings (well-mixed greenhouse gases, ozone, and sulfate aerosols). Models run with natural forcings alone do not explain the observed ocean warming. Results from this project appeared in the June 2, 2005, issue of *Science Express*.

The researchers used fingerprinting, a technique for determining how different climate forcings affect temperature. A climate model provides the physically based estimates of the shape, size, and evolution of the fingerprint. Researchers then compare the model fingerprint to past records of observed climate. In the PCMDI–Scripps study, the models depicted a warming signal in the upper 700 meters of the major ocean basins, which correlates well with past measurements of observed climate. Because the simulations reproduce the structure in such fine detail, the researchers concluded that the models are capturing the physical mechanisms involved in the penetration of the ocean warming signal.

Contact: Benjamin Santer (925) 422-2486 (santer1@llnl.gov).

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

Absolute Calibration of Optical Flats

Gary E. Sommargren
U.S. Patent 6,876,456 B2
April 5, 2005
The invention uses the phase-shifting diffraction interferometer (PSDI) to provide a true point-by-point measurement of absolute flatness over the surface of optical flats. Beams exiting the fiber optics in a PSDI have perfect spherical wavefronts. The measurement beam is reflected from the optical flat and passed through an auxiliary optic and then combined with the reference beam on a charge-coupled device. The combined beams include phase errors due to both the optic under test and the auxiliary optic. Standard phase extraction algorithms are used to calculate these combined phase errors. The optical flat is then removed from the system, and the measurement fiber is moved to recombine the two beams. The newly combined beams include only the phase errors due to the auxiliary optic. When the second phase measurement is subtracted from the first phase measurement, the absolute phase error of the optical flat is obtained.

Tilted Fuel Cell Apparatus

John F. Copper, Nerine Cherepy, Roger L. Krueger
U.S. Patent 6,878,479 B2
April 12, 2005
Bipolar, tilted embodiments of high temperature, molten electrolyte electrochemical cells capable of directly converting carbon fuel to electrical energy are disclosed herein. The bipolar, tilted configurations minimize the electrical resistance between one cell and others connected in electrical series. The tilted configuration also allows continuous refueling of carbon fuel.

Electronic Unit Integrated into a Flexible Polymer Body

Peter A. Krulevitch, Mariam N. Maghribi, William J. Benett, Julie K. Hamilton, Klint A. Rose, James Courtney Davidson, Mark S. Strauch
U.S. Patent 6,878,643 B2
April 12, 2005
A peel-and-stick electronic system is composed of a silicone body and at least one electronic unit connected to the silicone body. The electronic system is produced by providing a silicone layer on a substrate, a metal layer on the silicone layer, and at least one electronic unit connected to the metal layer.

Differential Optical Synthetic Aperture Radar

Eddy A. Stappaerts
U.S. Patent 6,879,279 B2
April 12, 2005
A new differential technique for forming optical images using a synthetic aperture is introduced. This differential technique uses a single aperture to obtain unique (N) phases that can be processed to produce a synthetic aperture image at points along a trajectory. The aperture is divided into two equal subapertures, each having a width that is less than the actual aperture, along the direction of flight. As the platform flies along a given trajectory, a source illuminates objects and the two subapertures are configured to collect return signals. The techniques of the invention are designed to cancel common-mode errors, trajectory deviations from a straight line, and laser phase noise to provide the set of resultant (N) phases that can produce an image having a spatial resolution corresponding to a synthetic aperture.

Parallel Object-Oriented, Denoising System Using Wavelet Multiresolution Analysis

Chandrika Kamath, Chuck H. Baldwin, Imola K. Fodor, Nu A. Tang
U.S. Patent 6,879,729 B2
April 12, 2005
The present invention provides a data denoising system using processors and wavelet denoising techniques. Data are read and displayed in different formats. The data are partitioned into regions, and the regions are distributed onto the processors. Communication requirements are determined among the processors according to the wavelet denoising technique and the partitioning of the data. The data are transformed onto different multiresolution levels with the wavelet transform according to the wavelet denoising technique, the communication requirements, and the transformed data containing wavelet coefficients. The denoised data are then transformed into its original read-and-display data format.

Limited-Life Cartridge Primers

Daniel M. Makowiecki, Robert S. Rosen
U.S. Patent 6,881,284 B2
April 19, 2005
This cartridge primer, called a limited-life primer, uses an explosive that can be designed to become inactive in a predetermined period of time. The explosive or combustible material of the primer is an inorganic reactive multilayer (RML). The reaction products of the RML are submicrometer-size grains of noncorrosive inorganic compounds that would have no harmful effects on firearms or cartridge cases. Unlike primers containing lead components, primers using RMLs would not present a hazard to the environment. The sensitivity of an RML is determined by the physical structure and the stored interfacial energy. The sensitivity lowers with time due to a decrease in interfacial energy resulting from interdiffusion of the elemental layers. Time-dependent interdiffusion is predictable, thereby enabling the functional lifetime of an RML primer to be predetermined by the thickness and materials of the reacting layers.

Chemical Micro-Sensor

Anthony J. Ruggiero
U.S. Patent 6,887,359 B2
May 3, 2005
An integrated optical capillary electrophoresis system is used for analyzing an analyte. A modulated optical pump beam impinges on an capillary containing the analyte–buffer solution, which is separated by electrophoresis. The thermally induced change in the light's index of refraction in the electrophoresis capillary is monitored using an integrated microinterferometer. The interferometer includes a first interferometer arm intersecting the electrophoresis capillary proximate the excitation beam and a second, reference interferometer arm. Changes in index of refraction in the analyte are measured by interrogating the interferometer state using white-light interferometry and a phase-generated carrier demodulation technique. Background thermo-optical activity in the buffer solution is cancelled by splitting the pump beam and exciting pure buffer solution in a second section of capillary where it crosses the reference arm of the interferometer.

High Resistivity Aluminum Antimonide Radiation Detector
John W. Sherohman, Arthur W. Coombs, III, Jick H. Yee
U.S. Patent 6,887,441 B2
May 3, 2005
Bulk aluminum antimonide–based, single-crystal materials have been prepared for use as room-temperature x- and gamma-ray radiation detectors.

Sol-Gel Manufactured Energetic Materials
Randall L. Simpson, Ronald S. Lee, Thomas M. Tillotson, Lawrence W. Hrubesh, Rosalind W. Swansiger, Glenn A. Fox
U.S. Patent 6,893,518 B1
May 17, 2005
Solgel chemistry is used to prepare energetic materials, such as explosives, propellants, and pyrotechnics, that have improved homogeneity or that can be cast to near-net shape or made into precision-molding powders. The solgel method is a synthetic chemical process in which reactive monomers are mixed in a solution. Polymerization then leads to a highly cross-linked, three-dimensional solid network, resulting in a gel. The energetic materials can be incorporated when the solution is formed or during the gel stage. The material's composition, pore and primary particle sizes, gel time, surface areas, and density may be controlled by the solution chemistry. The gel is then dried using supercritical extraction to produce a highly porous, low-density aerogel or by controlled slow evaporation to produce a xerogel. Applying stress during the extraction phase can result in high-density materials. Thus, the solgel method can be used to manufacture precision detonator explosives, propellants, pyrotechnics, and high-power composite energetic materials.

PCR Thermocycler
William J. Benett, James B. Richards
U.S. Patent 6,893,863 B2
May 17, 2005
Features etched into this sleeve-type silicon polymerase chain reaction (PCR) chamber or thermocycler improves thermal performance by reducing the sleeve's thermal mass and increasing its surface area for cooling. These improvements increase the speed and efficiency of the reaction chamber. Grooves etched in the faces of the sleeve are connected with a series of grooves on the chamber's interior surface. These grooves can be anisotropically etched in the silicon sleeve when the chamber is formed.

Awards

Siegfried Glenzer, a physicist in Livermore's National Ignition Facility Programs Directorate, received the **Alexander von Humboldt Foundation Research Award**. The foundation promotes international scientific cooperation by annually selecting 100 scientists from around the world to conduct research projects of their choice in cooperation with specialist colleagues in Germany. Glenzer was invited by Ronald Redmer to spend an academic year at the Universität Rostock and at the Deutsches Elektronen-Synchrotron (DESY) facility in Hamburg. At Rostock, Glenzer will collaborate with Redmer on planning and interpreting x-ray Compton scattering experiments, and he will teach a lecture series in plasma diagnostics to advanced students. At DESY, he will participate in the first short-wavelength free-electron laser experiments, which will begin this year.

The **American Nuclear Society** (**ANS**) awarded a 2005 **Edward Teller Medal** to Livermore physicist **Max Tabak**, who works in the Laboratory's Defense and Nuclear Technologies Directorate. Tabak is best known as the lead inventor of fast ignition, a technique that uses powerful short-pulse lasers to directly ignite precompressed fusion fuel. ANS honored Tabak for being "an effective mentor and group leader, whose team has made major contributions to a broad range of topics in Inertial Confinement Fusion (ICF) and high-energy-density physics and has stimulated advanced research all over the world."

Also receiving an Edward Teller Medal is former Laboratory employee **Joseph Kilkenny**, who now serves as vice president for Inertial Fusion Technology at General Atomics in San Diego, and associate director for Science and Technology at the Laboratory for Laser Energetics of the University of Rochester in Rochester, New York. Kilkenny led Livermore's ICF program in 1995. Experiments he initiated were the basis for recommendations issued by the National Academy of Sciences in support of the National Ignition Facility.

ANS presents two Edward Teller Medals biennially to recognize pioneering research and leadership in inertial fusion sciences and applications. The award is named in honor of Lawrence Livermore's cofounder and former director, the late Edward Teller. He is recognized worldwide as a pioneer in inertial fusion sciences.

Abstracts

Orchestrating the World's Most Powerful Laser

The integrated computer control system (ICCS) for the National Ignition Facility (NIF), which will have about 1.4-million lines of code running on hundreds of computers, is designed to operate laser shots automatically. ICCS proved itself over the past two years during the NIF Early Light campaign, which used the first four completed lasers, called a quad, to successfully conduct more than 400 shots. With the first quad in operation, at least one of every hardware device was operated and successfully monitored and controlled by ICCS. During the next four years, as more hardware is installed, control system software proven on the first quad will be replicated to activate the remaining quads. The ICCS architecture has independent control systems for each of the 24 bundles of 8 beams and includes a front-end or bottom layer consisting of about 700 front-end processors and a supervisory or top layer of 50 powerful computers. Shot supervisor software is designed to automate the operation of components in all 192 beams.

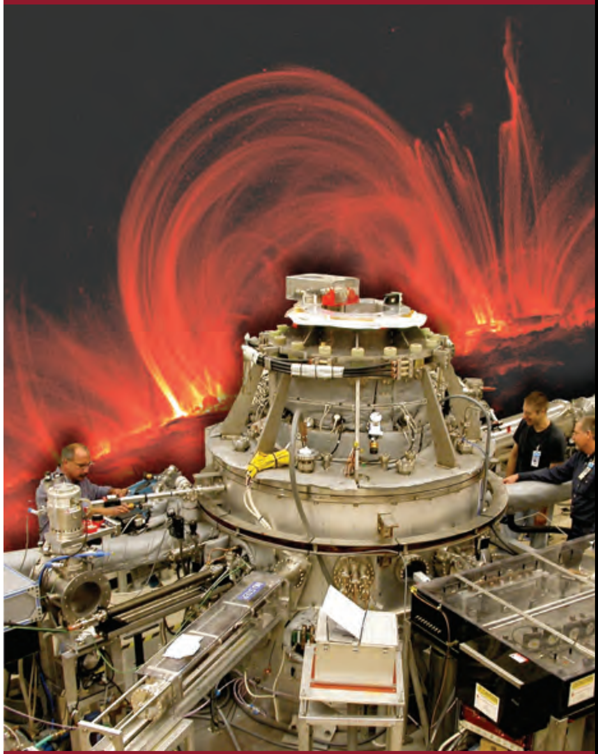
Contacts:
Paul VanArsdall (925) 422-4489 (vanarsdall1@llnl.gov) or
Larry Lagin (925) 424-3331 (lagin1@llnl.gov).

A Random Walk through Time and Space

In 1905, Albert Einstein shook the world of physics with five important papers that led to a century of spectacular advances in physics research. In three of these papers, he demystified Brownian motion and random fluctuations by linking statistical mechanics to observable reality and thus helped confirm the atomic theory of matter. Today, the work underlying these papers continues to form the basis for much of the Laboratory's work in molecular dynamics, Monte Carlo statistical techniques, and physical chemistry. Random fluctuations and statistical mechanics are fundamental to the most elemental building blocks of the physical world and are called on to explain such processes as protein folding, cell-membrane function, and evolution. Livermore scientists also apply advances in statistical mechanics in developing codes to model fluid behavior, predict the consequences of hazardous releases to the atmosphere, and simulate the diffusion of helium atoms in plutonium. A century ago, Einstein transformed physics research, and scientists continue to reap the rewards of his discoveries and intuition.

World Year of Physics events at Livermore: www.llnl.gov/pao/WYOP.

A Dynamo of a Plasma



The self-organizing magnetized plasmas in a Livermore fusion energy experiment are akin to solar flares and galactic jets.

Also in September

• Einstein's E mc^2 *is the equation that changed physics and the world.*

• New analytic solutions for imploding spherical shells give scientists additional tools for verifying codes.

• Scientists solve the mystery of what causes the strongest astronomical feature in stardust.

Coming Next Month

U.S. Government Printing Office: 2005/783-059-10009

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