Science and Technology in the Physics and Advanced Technologies Directorate

From January 2002 to October 2004

A compendium of LLNL Science and Technology Review articles involving scientist and engineers from the Physics and Advanced Technologies Directorate, from January 2002 to the present.
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Microturbulence, a long-time nemesis of magnetic fusion energy experiments, is being understood in unprecedented detail thanks to new three-dimensional simulations.

Since the 1950s, Lawrence Livermore has been one of the world’s leading centers of magnetic fusion energy research. Magnetic fusion uses intense magnetic fields to confine an extremely hot gas of electrons and positively charged ions called a plasma. Under the right conditions, the plasma ions undergo fusion reactions, the energy source of the Sun and other stars.

The long-standing goal of fusion researchers has been to duplicate the cosmos’s means of producing energy to provide a virtually inexhaustible source of reliable and environmentally benign energy on Earth. Despite the immense technical challenges involved in making magnetic fusion a source of commercial electrical power, important progress has been made in the past decade as researchers nationwide have collaborated on experiments and computer simulations.

Lawrence Livermore’s Fusion Energy Program carries out magnetic fusion energy research in two complementary thrusts. The first thrust is performing advanced fusion experiments. Livermore researchers are collaborators at the national DIII-D tokamak experiment at General Atomics in San Diego, California.

This Livermore simulation shows a magnetic field line (white) wrapping around a torus, or doughnut-shaped configuration of plasma. Magnetic field lines are embedded within the plasma, with individual particles traveling along each field line. The color contours indicate microturbulent fluctuations in the plasma density. Regions with similar density—microturbulent eddies indicated by regions of similar color—stretch along the field lines, while varying rapidly across the field lines. These microturbulent eddies transport heat from the plasma’s superhot core to the cold outer edge.
Laboratory scientists are also pursuing novel designs for magnetic fusion reactors, such as the spheromak experiment dedicated in 1998. (See S&TR, December 1999, pp. 18–20.)

Complementing the experimental work is an effort to accurately simulate the extraordinarily complex physics involved in magnetically confined plasmas. Lawrence Livermore scientists have developed a number of codes for simulating different aspects of magnetic fusion energy experiments. Its PG3EQ program, developed by physicists Andris Dimits, Dan Shumaker, and Timothy Williams, for example, is one of the most advanced programs available for simulating plasma turbulence. Another Livermore code, called CORSICA, goes a step further and links individual programs that model different aspects of magnetic fusion energy physics. (See S&TR, May 1999, pp. 20–22.)

Focus on Tokamak

A national team of researchers led by Laboratory physicist Bill Nevins is developing advanced simulation codes running on supercomputers to deepen scientific understanding of the plasma turbulence that occurs inside a tokamak, a magnetic confinement device. Tokamaks use powerful magnets to confine plasmas of fusion fuel on the toroidal, or doughnut-shaped, magnetic “surfaces” defined by individual magnetic field lines as they wind about within a vacuum chamber.

Plasma turbulence causes thermal energy to leak across the magnetic surfaces faster than it can be replaced by fusion reactions. This lost energy must be replaced by external sources to prevent the plasma from cooling below the 100-million-degree temperatures needed to optimize the rate of fusion reactions. However, current tokamak experiments are close to the major goal of breakeven, that is, the point at which the energy produced by the fusion reactions equals the energy applied from an external source to heat the fuel. A better understanding of plasma turbulence may allow researchers to reduce the rate of energy loss so that energy breakeven could be achieved in the current generation of tokamaks.

The national collaboration is called the Computational Center for the Study of Plasma Microturbulence. It is funded by the Department of Energy’s Office of Fusion Energy Sciences, a part of DOE’s Office of Science. The work is part of the Office of Science’s Scientific Discovery through Advanced Computing (SciDAC) program, which was launched in late 2000. SciDAC’s goal is to develop the scientific computing hardware and software needed for terascale (trillion-operations-per-second) supercomputing. The effort is similar to the National Nuclear Security Administration’s Accelerated Strategic Computing Initiative, which is making

![Cross section of a tokamak plasma. The color contours indicate microturbulent fluctuations in the plasma density. Livermore's PG3EQ code, which was used to produce this simulation, models a “tube” of magnetic flux as it wraps once around the tokamak poloidally, or the short way around. Toroidal symmetry was then used to displace this flux tube and fill the annulus.](attachment://tokamak.png)
available terascale computers for the nation’s Stockpile Stewardship Program.

The collaboration involves researchers from Lawrence Livermore, the Princeton Plasma Physics Laboratory, the University of California at Los Angeles, the University of Colorado, the University of Maryland, and General Atomics. These institutions were part of previous DOE magnetic fusion energy simulation efforts, including the Numerical Tokamak Turbulence Project (1993 to 1999), led by Livermore physicist Bruce Cohen, and the Plasma Microturbulence Project (2000 to 2001), led by Nevins.

The simulations are focused on microturbulence, a long-time nemesis of achieving breakeven conditions in magnetic fusion energy experiments. Microturbulence is one of two forms of plasma turbulence observed in magnetic confinement experiments. Macroturbulence, on the scale of centimeters to meters, has been largely tamed in advanced tokamak designs. Microturbulence, on the scale of tenths of millimeters to centimeters, has not.

**Fluctuating Plasma Soup**

Microturbulence is an irregular fluctuation in the plasma “soup” of electrons and ions. The fluctuations are caused by gradients of density and temperature. The fluctuations, a collective phenomenon, form unstable waves and eddies that transport heat from the superhot core across numerous magnetic field lines out to the much cooler plasma surface and, ultimately, to the tokamak’s walls. Energy researchers call this phenomenon energy transport.

Nevins notes that a tokamak’s plasma will undergo fusion reactions only if it is hot enough, dense enough, and kept away from the much colder reactor walls. By causing heat to be lost from the plasma core, microturbulence helps to degrade confinement and prevent breakeven conditions. “We want plasma at about 100,000,000°C in the center and below 1,000°C at the walls, so they don’t melt,” says Nevins. “We obviously need good thermal insulation, and that’s provided by the confining magnetic field. If we can minimize microturbulence, we can prevent heat leaking out faster than the fusion reactions can generate heat.”

Controlling microturbulence will be immensely important in determining whether an advanced experiment, currently in the early planning stages, will be a success. Nevins says that the largest tokamaks cost several hundred million dollars to build. Constructing an experimental device that would go beyond breakeven for a net production of energy would cost about $2 billion. If a way were found to control microturbulence, construction costs could decrease significantly.

Says Cohen, “If we had better energy confinement, we could build the next generation device at a much lower cost. To do that, we need to understand better the nature of plasma microturbulence.”

**Simulation Focus**

The collaboration’s current focus is on advanced codes, algorithms, and data analysis and visualization tools. Nevins says that simulating microturbulence has proved difficult because of the enormous range of time and space scales that occur in magnetic fusion plasmas. Indeed, scientists within the national magnetic fusion energy program have worked to model microturbulence for more than two decades.

Fortunately, massively parallel computers, which use thousands of microprocessors in tandem, are well-suited to this simulation task. These machines are ideal because the collective behavior of trillions of electrons and ions is complex, but the underlying physics—and the equations that describe it—are relatively straightforward.

Most computing is done remotely at the Department of Energy’s National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley

![Image (a)](image-a.png)

![Image (b)](image-b.png)

The UCAN code, developed by Livermore collaborators at the University of California at Los Angeles, produced these two images of tokamak plasmas. (a) Early in the development of the microturbulence, small-amplitude, radially elongated turbulent eddies form. (b) Fully developed microturbulence exhibits smaller, disordered structures.
Fusion combines the nuclei of light elements to form a heavier element. For example, two nuclei of hydrogen isotopes, deuterium and tritium, will overcome the natural repulsive forces that exist between such nuclei and combine under enormous temperature and pressure. The fusion reaction produces a single nucleus of helium, a neutron, and a significant amount of energy.

A device that creates electricity from fusion must heat the fuel to a sufficiently high temperature and then confine it for a long enough time so that more energy is released than must be supplied to keep the reaction going. To release energy at a level required for electricity production, the fusion fuel must be heated to about 100,000,000°C, more than 6 times hotter than the interior of the Sun. At this temperature, the fuel becomes a plasma, an ionized gas of negatively charged electrons and positively charged ions. Although rare on Earth, plasmas constitute most of the visible universe.

The challenge for scientists is how to confine the plasma under extreme temperatures and pressures. One solution is to use powerful magnetic forces. In the absence of a magnetic field, a plasma’s charged particles move in straight lines and random directions. Because nothing restricts their motion, the charged particles can strike the walls of a containing vessel, thereby cooling the plasma and inhibiting fusion reactions. In an appropriately designed magnetic field, the particles are forced to follow spiral paths about the magnetic field lines so they do not strike the vessel walls. The plasma is thus confined to a particular magnetic field line. The magnetic field line itself can be confined within a vacuum chamber if its path is restricted to a toroidal, or doughnut, shape.

A bundle of such magnetic field lines forms a doughnut-shaped magnetic “bottle” called a tokamak, an acronym derived from the Russian words meaning toroidal chamber and magnetic coil. In the tokamak, the stable magnetic bottle is generated both by a series of external coils, which are wrapped around the outside of the doughnut, and by a strong electrical current, up to several million amperes, that is induced in the plasma itself.

Half Century of Research

Magnetic fusion energy research has been under way for more than a half century and was one of Lawrence Livermore’s original programs. The idea was classified because the concept uses the energy released by the same reaction that takes place in a hydrogen or thermonuclear bomb. In the late 1950s, the research program, called Project Sherwood, was partially declassified because it was viewed as a long-term effort without immediate military application and one that would benefit greatly from international cooperation.

Considerable progress has been made in the last 20 years at Livermore and other research centers in meeting the scientific challenges of attaining the combination of temperature, density, and confinement time necessary to promote fusion reactions. At one point, several different types of devices, including Livermore’s magnetic “mirror” design, were pursued within the national program. Budget constraints, however, led to the adoption of the tokamak as the principal design for the U.S. program, with other approaches being explored at lower levels of resources.

The long-standing goal of magnetic fusion energy is to produce abundant, environmentally acceptable electric energy from a fusion-powered reactor. In fusion power plants, the heat from deuterium–tritium fusion reactions would be used to produce steam for generating electricity. Deuterium is abundant and easily extracted from ordinary water (about one water molecule out of every 6,000 contains deuterium). Tritium can be made from lithium, a plentiful element in Earth’s crust.

One kilogram of deuterium–tritium fusion fuel would produce the same energy as 30 million kilograms of coal. Other major advantages include no chemical combustion products and therefore no contribution to acid rain or global warming, radiological hazards that are thousands of times less than those from fission, and an estimated cost of electricity comparable to that of other long-term energy options.
National Laboratory. In fact, the collaboration is the biggest user of NERSC facilities. The current simulations typically require from 10 to 20 hours to complete using NERSC’s most powerful machines.

With the latest generation of supercomputers, says Cohen, “We can do bigger pieces of the simulation, with more physics.” Nevertheless, no computer yet built can perform simulations requiring six orders of magnitude in spatial size, eight to nine orders of magnitude in time scale, and three dimensions in space. As a result, “We have to be clever about reducing the scales and still obtaining accurate results,” says Cohen.

The hardware advances have been accompanied by the equally impressive development of efficient algorithms with which to solve the equations that form the basis of plasma simulation. The algorithms are of two kinds, particle-in-cell (PIC) models and continuum models, depending on how they track simulated electrons and ions in space and time. PIC models track individual electrons and ions; continuum models solve equations that do not involve individual particles.

The national effort is developing both kinds of algorithms because they offer a valuable means of verifying new codes. “Together, the two kinds of algorithms provide a balanced scientific approach to understanding microturbulence,” says Nevins. Each approach, however, pushes the limits of current supercomputer capability.

PIC and continuum algorithms can be used in two geometric representations: global and flux tube. Global simulations model the entire plasma core of a tokamak, whereas flux tube simulations represent a more limited area. Here again, says Nevins, the two geometric approaches serve as a useful cross-check on the results obtained from each other.

With the increased speed of microprocessors, additional memory, massively parallel supercomputers, and advanced algorithms, important progress has been made in the past few years in modeling microturbulence. Nevins points to significant improvements in the comparisons of simulations to experiment results, in the agreement of results from codes developed by collaborators from different centers of magnetic fusion energy research, and in the increasingly thorough and accurate physics content of the models.

An important aspect of the code work is developing new tools to analyze and visualize the simulation results. Data analysis and visualization provide the bridge between the microturbulence simulation and experimental research. Nevins has developed GKV, a program that allows the user to easily compute, analyze, and display results (in presentation-quality form) easily from microturbulence simulation data. The program is used by researchers nationwide.

A strong numerical model of microturbulence, combined with better

Livermore’s GKV program allows users to interactively compute, analyze, and display data from microturbulence simulations. This GKV image displays the Kubo number, or the number of times an ion circulates around a turbulent eddy before that eddy dissipates, versus the separation within a magnetic surface and the radial location of the magnetic surface. Distances are measured in ion gyro radii, that is, the radius of a typical ion’s orbit as it gyrates about a magnetic field line.
data analysis and visualization tools, is aiding the interpretation of experimental data and the testing of theoretical ideas about microturbulence and how to control it. The simulations are also helping scientists to plan future experiments. In addition, continued progress in code development may stimulate advances in the understanding of astrophysical plasmas and turbulence in fluids.

**Theorists Now Getting Respect**

Cohen recalls that five years ago, experimentalists paid much less attention to theorists regarding plasma turbulence. Today, however, simulations do such a good job in predicting experimental results that “experimentalists are really paying attention to the codes.” Simulations, he says, have achieved such a level of fidelity to the underlying plasma physics that they can often be used as a tool for experiments regarding plasma microturbulence.

Nevins points out that the cost of doing simulations is nearly negligible compared with the cost of building and running a new fusion ignition experiment (around $1 billion to $2 billion). “Inexpensive but increasingly realistic simulation capability will continue to have immense leverage on relatively expensive experiments,” he says.

He also points out that numerical simulation has a distinct advantage over experimental observations of microturbulence: The simulations give users access to virtually any portion of the plasma in time or space. Simulations use “synthetic” diagnostic tools, which mimic the signal that an experiment would be expected to produce on an experimental diagnostic.

Says Nevins, “We can put in better diagnostics on a computer code than we can during an experiment.” What’s more, the physics underlying observed microturbulence can often be ambiguous. “With a simulation, we can turn different physics on and off to isolate what is driving the microturbulence observed in the experiment.”

Not only have recent simulations produced a clearer understanding of microturbulence, but they have also provided a few surprises as well. For example, scientists have long puzzled over large but transient bursts of heat that are transported out of the core plasma by microturbulence eddies. “We would have expected the transfer of heat from the plasma core out to the walls to be homogeneous because of the small eddies caused by microturbulence. Instead, we’ve seen large, intermittent bursts 10 times the size of the eddies,” Nevins says.

**Learning from Sandpiles**

Nevins and others have noticed that these intermittent spikes are characteristic of “self-organized criticality,” a phenomenon that occurs in a system when certain key parameters reach critical values. Self-organized criticality is responsible, for example, for the occurrence of sudden avalanches as grains of sand are slowly added to the top of a sandpile. The Livermore simulation team is using the insights derived from self-organized criticality to account for these unexpected bursts of heat, which apparently are the combination of many turbulent eddies.

An important recent addition to the simulation codes is a phenomenon called flow shear that works to dampen microturbulence and thereby improve plasma confinement. The plasma rotates (flows) within each of the nested magnetic surfaces defined by individual magnetic field lines. The term flow shear describes spatially...
localized changes in the rate of plasma rotation. The flow shear sharply reduces the rate at which heat is transported out to the cold plasma edge by stretching and tearing apart the microturbulence eddies.

Nevins explains that heat must travel to the outer plasma edge across many nested magnetic surfaces. When the magnetic surfaces rotate relative to each other, the eddies transporting the heat tend to dissipate. He offers the analogy of a busy freeway, with each lane of cars (magnetic surface) at a different speed. If a driver must hand a rubber band (microturbulence eddy) to a driver in another lane passing by at a much faster rate, the rubber band will soon break and not be passed to the driver in the faster lane.

Flow shear can appear spontaneously during a magnetic fusion energy experiment. When that happens, says Cohen, “We get it for free.” Flow shear can also be created experimentally by applying a twisting force (torque) to the plasma using, for example, intense beams of neutral hydrogen atoms. The force pushes on the center of the plasma core to create barriers to heat transport.

“We want to understand much better how flow shear functions so we can know how much to apply to effectively control microturbulence,” says Cohen. Precisely applying flow shear could increase plasma confinement and significantly decrease the cost of new experimental facilities.

The national collaboration is working to provide a suite of modular, complementary computer programs, each with an identical user interface. Together, the modules will constitute a comprehensive code for microturbulence simulation, data analysis, and visualization. The modular architecture will enable physics simulations on diverse computer architectures with much less effort than current software approaches demand. Says Nevins, “We want to revolutionize the fusion community’s ability to interpret experimental data and test theoretical ideas. The result will be a much deeper understanding of microturbulence.”

As for the codes themselves, the collaborators are working on consolidating programs developed by individual research groups. Another area of activity is improving the physics simulated by the codes, for example, by refining the simulated diagnostic instruments and more accurately modeling the role of electrons involved in microturbulence.

Nevins is hopeful that by making the simulations easier to run and analyze, even more experimenters will choose to use them. “It was a heroic feat to make the codes work, but now we need to make them available to the experimental community,” he says. “We want these tools to be used more widely so that we expand the use of microturbulence simulation well beyond the existing small group of code developers. Our goal is to have experimentalists run the codes and understand the results much faster.”

Better simulation tools could bring dependable fusion energy much closer to reality. That would be welcome news for a nation recently reminded about the fragility of steady energy supplies and prices.

—Arnie Heller

Key Words: fusion, macroturbulence, magnetic fusion, microturbulence, National Energy Research Scientific Computing Center (NERSC), plasma, Scientific Discovery through Advanced Computing (SciDAC), tokamak, turbulence.

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FOR years, experts in terrorism have been warning that a terrorist attack with biological agents is not a question of “if” but “when.” As recent events have proved, when is now.

For almost a decade, researchers at Lawrence Livermore, working on the when-is-now premise, have been developing systems that can rapidly detect and identify biological agents, including pathogens such as anthrax and plague. (For more background on Livermore’s research against bioterrorism, see S&TR, June 1998, pp. 4–9, and May 2000, pp. 4–12.) Among such systems are the Handheld Advanced Nucleic Acid Analyzer (HANAA) and the Autonomous Pathogen Detection System (APDS).

Although HANAA and APDS are of different sizes and made for different situations, they have a common purpose: to get results, fast. Lawrence Livermore biological scientist Richard Langlois explains, “There are any number of laboratory tests available right now to analyze pathogens. They all require getting a sample and then transporting it to a laboratory for processing. Our systems use new instrumentation and methods that provide faster and more timely results, on the spot. Faster results mean the responders can act quickly and begin treatment earlier.”

HANAA in Hand

About the size of a brick, the HANAA biodetection system can be held in one hand and weighs less than a kilogram. The system was designed for emergency response groups, such as firefighters and police, who are often first on the scene at sites where bioterrorism may have occurred. Each handheld system can test four samples at once—either the same test on four different samples or four different tests on the same sample. HANAA can provide results in less than 30 minutes, compared with the hours to days that regular laboratory tests typically take.

The process of detecting and identifying what’s in a sample works like this. The operator prepares the samples by putting them in a liquid buffer and adding chemicals. A tiny disposable plastic tube holding about 0.02 milliliter of the prepared liquid is then inserted into the system. Many copies of a sample’s DNA are needed to analyze it and identify its makeup. HANAA uses a technique called the polymerase chain reaction (PCR), which amplifies agent-specific DNA fragments to a detectable level. In PCR, an aqueous sample is heated close to the boiling point and then cooled many times (40 times in HANAA). Every time the DNA is heated, the two intertwined strands of DNA unwind and come apart. As the sample cools down, the DNA makes a copy of itself. Thus, at the end of each cycle, the amount of DNA is doubled.

To detect the DNA in a sample, a synthesized DNA probe tagged with a fluorescent dye is introduced into the sample before it is inserted into the heater chamber. Each probe is designed to attach to a specific organism, such as anthrax or plague. Thus, the operator must have an idea of what substances might be involved. “The system doesn’t test for all unknowns,” says Langlois. “A responder has to decide what kinds of pathogens to test for ahead of time and set up the system accordingly.” If that organism is present in the sample, the probe attaches to its DNA, which is then amplified during the PCR process, releasing the fluorescent tag. HANAA
measures the sample’s fluorescence and the presence (or absence) of the targeted organism.

One of the big breakthroughs for the handheld system involved the design of a small silicon heater chamber for the heating and cooling cycle, a concept developed at Livermore by Allen Northrup, a former Laboratory scientist. “The commercial thermocyclers used for standard laboratory tests are pretty big, ranging from the size of a microwave oven to a large desk,” notes Langlois. “A typical large thermocycler takes about 3 minutes to cycle through one heating and cooling cycle, so a complete analysis requires 2 to 3 hours.”

In the HANAA system, the thermal cycling process occurs in tiny silicon heater chambers, micromachined by Livermore’s Center for Microtechnology. Each chamber has integrated heaters, cooling surfaces, and windows through which detection takes place. Because of the low thermal mass and integrated nature of the chambers, they require little power and can be heated and cooled more quickly than conventional units. The mini-chambers typically cycle from about 55°C to 95°C in about 30 seconds.

Using this technique, the HANAA system could, in principle, detect as few as 10 individual bacteria in one-hundredth of a milliliter in less than 30 minutes. The system has the potential of saving many lives by saving time—anthrax, for example, is highly treatable if detected early.

The Laboratory has a cooperative research and development agreement for HANAA with Environmental Technologies Group (ETG), a chemical and biological detector company and subsidiary of Smith’s Industries, based in Baltimore, Maryland. ETG expects to have a commercial version of HANAA available early this year. Ron Koopman, special projects manager for the Chemical and Biological National Security Program at Livermore, notes that HANAA is essentially ready to go at this critical juncture because of the forward-thinking efforts begun in the previous decade. “A number of people recognized the vulnerability of the country to bioterrorism a long time ago,” he says. “In 1996, although bioterrorism seemed far away and was something we hoped would never happen, the Laboratory and members of the defense community decided to invest in the research, just in case. Thanks to that investment, we now have something to put in the hands of people to protect us all, something that can help during the current crisis and in the long run.”

A Bio “Smoke Detector”

Whereas HANAA can be hand-carried to sites at which an attack is suspected to have happened, the APDS is stationed in one place for continuous monitoring and is designed to work much like a smoke detector, but for pathogens. When fully developed, the APDS could be placed in a large area such as an airport, a stadium, or a conference hall. The system will sample the air around the clock and sound an alarm if pathogens are detected.

“The important point here is that the system would be fully automated,” stresses Langlois. “The system will collect and prepare the samples, do the analysis, and interpret the results, all without human assistance.”

Livermore is testing the second APDS prototype, which is about the size and shape of a lectern or mailbox. The APDS-II consists of an aerosol collector, a sample preparation subsystem, and two subsystems for detecting and analyzing the samples: one based on PCR and the other based on flow cytometry, which uses antibodies to identify pathogens. “The final system will double-test each sample to decrease the likelihood of false positives and increase the reliability of identification,” explains Langlois.

The aerosol collector, which was designed by Vern Bergman and Don Masquelier at Livermore, gathers an air sample every 30 minutes—the length of time it takes to complete a sample analysis. A built-in fan pulls in the air, which passes through a glass tube containing water. The water traps any particles in the air, and the resulting fluid is pumped to the next stage for sample preparation and testing.

The flow-through PCR subsystem for the APDS includes a Livermore-designed thermocycler—much like the thermocycler in HANAA—along with a sequential injection analysis system. This analysis system performs all the necessary PCR sample preparation functions, such as mixing the sample with PCR measures the sample's fluorescence and the presence (or absence) of the targeted organism.
The Faster the Better

From handheld, immediate testing to autonomous and continuous testing, HANAA and APDS are two of many systems Livermore is developing to help the nation fight bioterrorism. With HANAA, emergency responders can get answers on the scene in less than half an hour. With APDS, no human direction will be necessary, and the system will perform on its own, completely self-contained, monitoring 24 hours a day, 7 days a week. “What ties these approaches together is the ability to analyze a sample quickly—within 30 minutes or less—and do it on site,” concludes Langlois. “Getting the answer quickly is important. In the case of a biological attack, the sooner we know what bioagent we’re dealing with, the sooner treatment can start for those affected. Systems such as these have the potential for saving many lives.”

—Ann Parker

Key Words: anthrax, Autonomous Pathogen Detection System (APDS), biodetectors, biological warfare agents, bioterrorism, DNA analysis, flow cytometry, Handheld Advanced Nucleic Acid Analyzer (HANAA), pathogens, polymerase chain reaction (PCR).

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Now, for the first time, using computer simulations, researchers can get an accurate look at what happens to individual atoms and molecules during those experiments.

Simulations based on quantum molecular dynamics make it possible to view experimental activity as it happens. Quantum molecular dynamics is quite different from classical molecular dynamics, which is primarily concerned with the classical motion of atoms interacting with a given potential. The interesting chemistry and physics of many molecules take place at the atomic and subatomic level. But Newton’s laws of classical mechanics no longer apply here. Physicists developed quantum mechanics early in the 20th century to appropriately describe the physics and chemistry of matter at the microscopic level. Quantum molecular dynamics focuses on all the interactions between atoms and electrons and does not involve fitting interactions to experimental data.

First-principles, or ab initio, molecular dynamics models use only the laws of quantum mechanics, the fundamental physics equations that describe electrons. (See the box on p. 8.) These models in combination with Livermore’s powerful computers allow scientists to create accurate, reliable simulations of complex physical phenomena.

Physicist Giulia Galli leads the Quantum Simulations Group at Livermore. In the four years since this group was established, it has explored entirely new territory. Early work included simulations of the mixing of water and hydrogen fluoride, DNA, and the elasticity of silicon carbide, a semiconductor material. (See S&TR, July/August 1999, pp. 20–22.) Their more recent simulations of shocked liquid hydrogen were the largest ab initio simulations to date on Livermore’s terascale computers, which are part of the National Nuclear Security Administration’s Advanced Simulation and Computing (ASCI) program. “Our hydrogen simulations were the first to look at an experiment in action,” says Galli. “We could actually see how a real experiment had gotten from ‘before’ to ‘after.’”
Quantum simulations are an excellent tool for predicting the properties of materials that cannot be measured directly. They provide accurate information about the properties of materials subjected to extreme conditions (for example, high temperature or high pressure) that are difficult to achieve experimentally. Simulations also help experimental physicists to interpret their results. “Simulation results neatly complement experimental results and may also guide the choice of new experiments,” says Galli.

**Codes Make It Work**

The computer code used to simulate dynamic processes is JEEP, which physicist Francois Gygi began developing about eight years ago when he was at the Swiss Federal Institute of Technology. Some physical properties of matter, such as optical properties, can be obtained more accurately using static calculations performed with quantum Monte Carlo codes, which are the specialty of physicists Andrew Williamson, Jeff Grossman, and Randy Hood.

JEEP and quantum Monte Carlo codes operate differently. Both have to make approximations in their equations, but quantum Monte Carlo codes make very few. JEEP operates faster and excels at deriving the location of atoms and molecules. The more accurate quantum Monte Carlo simulations cannot give dynamic properties but are a better tool for determining the optical properties of molecules. Quantum Monte Carlo calculations are also useful for testing the validity of approximations made in the JEEP code’s theory and for improving the accuracy of this theory.

**Simulations Resolve Differences**

Quantum simulations by Galli and Gygi may point out the differences found during two sets of high-pressure experiments on deuterium, an isotope of hydrogen with one proton and one neutron. One set of experiments was performed on Lawrence Livermore’s Nova laser. The other set was performed on Sandia National Laboratories’ Z accelerator, the world’s most energetic pulsed-power machine, in Albuquerque, New Mexico.

The Livermore experiments in 1997 and 1998 and the Sandia experiment in 2001 subjected a sample of liquid deuterium to a short, intense shock that caused the hydrogen to form a hot plasma and, very briefly, become a conducting metal. In the Nova experiments, a laser beam produced a steady shock wave aimed at the target cell holding the sample. The wave was smoothed to ensure a spatially planar and uniform shock front, critical for obtaining accurate measurements.

The experiment at Sandia used an entirely different technique for producing a shock wave. Pulsed-power machines have large banks of capacitors used to accumulate electrical charges over many hours. All of that stored energy is discharged in one enormous pulse that lasts for a fraction of a microsecond. The pulse creates a powerful electromagnetic field that slams a flyer plate into the deuterium sample capsule. Sandia’s magnetically driven plate is faster...

Experiments on (left) Livermore’s Nova laser and (right) Sandia National Laboratories’ Z accelerator shocked liquid deuterium, an isotope of hydrogen. In both experiments, a short, intense shock caused the hydrogen to form a hot plasma and, very briefly, become a conducting metal. The experiments found different compressibilities, which could affect the equation of state for hydrogen and its isotopes. Quantum simulations sought to point out physical reasons for the differences.
although smaller than the flyers used by Livermore’s two-stage gas guns for shock experiments. It thus results in higher shock pressures. The Z accelerator also sustains a shock for a longer time than the Nova laser.

The two sets of experiments on the Nova laser showed that the deuterium samples were compressed to a density much higher than anyone had expected. These data differed from those used to predict the then-current model of the equation of state (EOS) for hydrogen and its isotopes. An EOS is a mathematical representation of a material’s physical state as defined by its pressure, density, and either temperature or energy. It is a necessary constituent of all calculations involving material properties. Predictions concerning the formation and evolution of large planets, such as Jupiter, strongly depend on the EOS of hydrogen at pressures reached in the Nova experiments.

The Z flyer data reached pressures up to 70 gigapascals, which overlapped part of the pressure regime of the Nova laser experiments. The Nova experiments determined the EOS by using an x-ray probe and x-ray microscope to look into the deuterium as it was being shocked. The Sandia experiments simultaneously shocked a deuterium sample and a foil of aluminum. Researchers then found the EOS by comparing deuterium’s behavior with that of aluminum. Although the Sandia EOS data required the comparison with aluminum, the Z flyer produced a shock in the deuterium that held a constant pressure for much longer than did the experiments with the Nova laser.

At a pressure of 40 gigapascals, the Nova and Z data agree, showing that the hydrogen EOS is about 20 percent more compressible than it was earlier thought to be. In other words, at this pressure, hydrogen will squeeze into a smaller volume with a higher density than previous models had predicted. At a pressure of 70 gigapascals, the Nova data show an even larger compressibility compared with equilibrium theory—almost 50 percent higher—while the Z flyer data are about 7 percent higher than theory predicted. “This is a considerable and important discrepancy,” says Livermore physicist Robert Cauble, who oversaw the experiments on both the Nova laser and the Z accelerator.

Galli and Gygi performed two sets of simulations as they sought an explanation for the experimental results. The first simulations were of hydrogen under fixed pressure and temperature. The pressure values ranged from 20 to 120 gigapascals while temperatures ranged from 5,000 to 12,000 kelvins. Galli and Gygi then simulated the behavior of liquid deuterium during a shock experiment. Although the simulations of static conditions gave results that agreed with Sandia’s data,
the simulation of a shock in deuterium gave results that agreed with the Livermore Nova shocks.

Gygi notes that the conditions of the Nova and Z accelerator experiments differed. For one thing, the time scales of the pulse were different: 2 to 4 nanoseconds in Nova and about 30 nanoseconds in the Z machine. “Another variable may be that a laser beam is very different from a magnetic pulse,” says Gygi.

Although the simulations did not supply a full explanation for the difference between the two sets of experimental results, Galli and Gygi’s calculations did help to point out possible important differences. “In the past,” says Gygi, “experimentalists with different results just pointed fingers at each other. Now, we hope that simulations will help to explain the physical reasons causing disagreement between different experiments. Also, big experiments are often expensive to repeat. The Nova laser is gone completely, so reproducing part of the Nova results with simulations can be very useful.”

**Water, Water Everywhere**

Recent experiments also explored one of the most common liquids—water. “You would think that everybody knows everything about water,” says Galli, “but that is far from the truth. And water is in practically everything in our world.” Water is in many materials studied at Livermore: Biological systems are largely water, high explosives contain water, and water vapor may accumulate inside an aging nuclear weapon.

Physicist Eric Schwegler, Galli, and Gygi were interested in what happens to water under pressure, information important to Livermore’s U.S. nuclear weapons stockpile stewardship mission. In particular, they were interested in learning how the water molecule comes apart under high-pressure conditions.

First, they developed a model of liquid water at ambient conditions, which compared favorably with recent x-ray data gathered at the University of California at Berkeley and with neutron diffraction data gathered in England. Then they modeled water at moderate pressure and found structural data that agreed with recent diamond anvil cell experiments performed at Commissariat à l’Énergie Atomique (CEA) in France.

Scientists already knew that under ambient conditions, water molecules rarely dissociate (come apart)—just once every 11 hours. When dissociation does occur, two water (H₂O) molecules become hydroxide (OH⁻) and hydronium (H₃O⁺), with one proton hopping to the other H₂O molecule. How increased pressure affects dissociation has long been debated.

Experiments on water at extreme temperatures and pressures have been few. One pioneering 1985 experiment at Livermore used a two-stage gas gun to shock water with pressures up to 26 gigapascals and temperatures to 1,700 kelvins. This experiment did not find any evidence of H₃O⁺ under pressure. These data led to the suggestion that the dissociation mechanism at high pressures might be different from the one at ambient conditions, that perhaps a single H₂O molecule dissociates to H⁺ and OH⁻.

In quantum simulations of static pressure conditions ranging up to 30 gigapascals, Schwegler’s team found that the dissociation process begins in earnest at 14 gigapascals. By 30 gigapascals, dissociation is occurring once every billionth of a second. The team was surprised to discover the same dissociation process that occurs at ambient conditions in which a proton jumps across to another water molecule. The simulations also indicated why the 1985 experiment did not reveal this process. At very high pressures, the lifetime of a H₃O⁺ molecule is on average only 9.8 trillionths...
of a second, too short to be observed in the 1985 experiment with detection technologies available then.

**For Better Health**

Schwegler, Galli, and Gygi are also working with researchers in Livermore’s Biology and Biotechnology Research Program (BBRP) Directorate to simulate the dynamic behavior of DNA and other biomolecules. The goal is to combine Livermore’s expertise in biology, simulation methods, and high-performance computing to nurture a new Laboratory core competency in computational biology. (See S&TR, April 2001, pp. 4–11.)

The simulations of water at ambient conditions were a necessary jumping-off point since all biomolecules contain a high percentage of water. Such liquid-phase simulations are far more complicated than those of isolated molecules in the gas phase because of the increased number of atoms that must be modeled.

“Getting water right made our future work much easier,” says Schwegler. “And there are lots of experimental data to compare.”

Subsequently, the team developed first-principles simulations of the dissolution of sodium and magnesium ions in water. In each case, their simulations agreed with numerous experimental investigations by others, but they also found several interesting features that had not been seen before.

That work was preparation for quantum simulations of the DNA sugar–phosphate backbone connecting the millions of base pairs that make up our genetic code. The flexibility of DNA in solution is central to the formation of DNA–protein complexes, which in turn mediate the replication, transcription, and packaging of DNA. Part of this flexibility comes from rotations around the bonds found in the backbone.

To learn more about how these rotations work, the team modeled the...

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**Simulating Quantum Molecular Dynamics**

In the classical molecular dynamics approach, a model of interactions between atoms is supplied as input before a simulation can be carried out. Such models are based on a priori knowledge of the physical system being studied. “Those models work if you know the chemical bonds already,” says physicist Francois Gygi.

In contrast, first-principles, or ab initio, molecular dynamics does not require any a priori knowledge of interatomic interactions. These simulations use only the laws of quantum mechanics, the fundamental physics equations that describe electrons. The existence of chemical bonds is the result of electron interactions and the laws of quantum mechanics. Quantum simulations can describe the forming and breaking of chemical bonds, which cannot be done using classical molecular dynamics. Thus, classical molecular dynamics cannot explain complex states of matter such as hot, compressed fluids in which molecules come apart and regroup. Quantum molecular dynamics, however, is an ideal method for showing what happens to fluids under pressure.

The fundamental physics equations that must be solved in quantum simulations are extraordinarily complex. Until powerful computers such as Livermore’s ASCI White came along, ab initio quantum molecular dynamics simulations could handle only a few atoms. Even now, a model of a few hundred atoms over less than a millionth of a second takes days of computing time to complete on Livermore’s huge computers.

Modeling the behavior of molecules at the quantum level requires not only unprecedented computational power and speed but also specially designed simulation codes. One such code is JEEP, which Gygi began developing when he was at the Swiss Federal Institute of Technology.

JEEN is based on density functional theory, which describes the electronic density of a molecular or condensed system. Walter Kohn of the University of California at Santa Barbara won the Nobel Prize for Chemistry in 1998 for his development of density functional theory. In its original form, this theory was confined to ground-state properties of molecules. Since then, it has been expanded and made applicable to the study of atomic motion and complex dynamic effects of matter. Kohn’s work on density functional theory has revolutionized the way scientists approach the electronic structure of atoms, molecules, and solid materials in physics, chemistry, and materials science.

Since coming to Livermore, Gygi has adapted and optimized JEEP for use on the massively parallel computers of ASCI. Now, with ASCI computers, he can examine materials systems with hundreds of atoms and thousands of electrons extremely accurately.

Monte Carlo codes are more accurate but have been extremely demanding of computing time. Every increase in the number of particles (N) being modeled requires N^3 more computing time. Twice as many electrons requires 8 times more computing time, 3 times as many electrons requires 27 times more computing time, 4 times as many electrons requires 128 times more computing time, and so on. Modeling more than a few atoms requires prohibitively long periods of computing time. Recently, however, physicists Andrew Williamson, Jeff Grossman, and Randy Hood developed a technique that allows for linear scaling of computing time for quantum Monte Carlo calculations. In other words, doubling the number of electrons only increases computing time by a factor of two instead of a factor of eight. This important breakthrough is based on techniques also used in some quantum molecular dynamics codes.
smallest part of the DNA backbone, the dimethyl phosphate anion (DMP\(^-\)). They observed changes in the shape of DMP\(^-\) when it was exposed to a sodium cation, changes that had not been seen in any previous classical molecular dynamics simulation of DMP\(^-\) in water. In future simulations, they plan to examine the influence of magnesium and other cations on the shape and flexibility of DNA.

Schwegler’s team has also been collaborating on studies of cancer-fighting drugs known as phosphoramides being done by Mike Colvin and his associates in BBRP. These nitrogen-mustard-based drugs have been used to treat cancer for 50 years, so there is plenty of experimental data to compare with simulations. By examining how the phosphoramide molecules are activated, this team hopes to find ways to improve the drug and to make it more effective. (See S&T, April 2001, pp. 9–10.)

Mustard drugs are believed to work by forming cross-links between the two strands of a cancer cell’s DNA. Because the cell cannot easily eliminate the cross-links, the cell cannot replicate itself and dies. Before the drug can attach itself to the cancer cell’s DNA, it has to lose chlorine ions. With his quantum simulations, Schwegler is learning more about the activation process, examining how the drug loses the chlorine ions and how much energy is required.

Surface Chemistry Is Key

Livermore researchers used both density functional theory (on which the JEEP code is based) and quantum Monte Carlo codes to perform first-principles calculations of silicon nanoparticles, or quantum dots, which are tiny silicon molecules just a few nanometers in size, about 100,000 times smaller than the width of a human hair. These nanoclusters produce different colors of light depending on their diameter and are being considered as replacements for the fluorescent markers that researchers now use to tag proteins during experiments. With the markers, scientists can locate specific proteins and watch as they go about their business.

Existing fluorescent dyes work well as markers. But they are short-lived. Their fluorescence rapidly fades until they are no longer detectable. They also have to be excited by a specific wavelength of laser light that matches their absorption. If researchers are studying more than one protein at a time and use multiple fluorescent markers, they must also use as many lasers as there are different markers.

Silicon quantum dots have several advantages as biomarkers. They do not bleach out, and multiple markers can be excited by a single laser. “Given their small size, they would be a gnat on the side of a protein,” says Williamson, “and the protein should continue to act and react normally.”

The synthesis of silicon dots is still in its infancy. Livermore has several experimental efforts under way to synthesize them. A long-term goal is to use silicon nanoparticles in biosensors to detect biological and chemical warfare agents.

During the manufacture of the quantum dots, contamination is a
Oxygen, especially, can be a killer for silicon, notes Williamson. Recent Livermore simulations examined the effect of oxygen on silicon particles. A single oxygen atom, as well as many other contaminants, can make a big difference on a quantum dot because of the dot’s large ratio of surface area to volume. Surface chemistry plays a big role in the study of these tiny particles.

The effects of surface chemistry are illustrated in the figure above. The left portion of the figure shows a nanometer-size silicon quantum dot made up of 71 atoms. The white atoms on the surface are hydrogen atoms bonded to the dot in such a way as to “passivate” the surface. This means they attach themselves to the highly reactive surface silicon atoms (gray). The purple cloud shows the region where the electrons that will absorb light are most likely to be located in this silicon quantum dot. For a silicon dot completely passivated by hydrogen, the electrons are located in the center of the dot. The right portion of the figure shows how the situation changes when two of the hydrogen atoms are replaced by a more reactive oxygen atom. The electron charge cloud is drawn toward the oxygen atom, and this change in the electron density dramatically changes the optical properties of the silicon dot.

The team is currently broadening the scope of its nanostructure investigations to include other semiconductor materials such as germanium and cadmium–selenide.

Bigger and Better

One goal of Galli’s group for the next few years is to apply quantum simulations to a wider and broader set of problems and to use quantum simulations on a par with laboratory experiments as a tool for research in science and engineering. Quantum simulations are a fully predictive approach that will provide a new window through which scientists can observe the world at the atomistic level in exquisite detail, avoiding uncontrolled approximations. Galli’s group will focus on fluids under extreme conditions—for example, water under shocked conditions—and on building knowledge and expertise in the field of nanoscience, in particular, modeling artificial and biological nanostructures for labeling and sensing applications.

Because of the success of their quantum simulations, Galli and Gygi are working with IBM on the design of the next-generation ASCI computers. When these monster computers arrive, extremely complex simulations may be able to answer questions that cannot now be answered.

—Katie Walter

Key Words: hydrogen, JEEP, nanostructures, quantum dots, quantum molecular dynamics, quantum Monte Carlo calculations, quantum simulations, water.

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Once again, science fiction has predicted science fact. Remember those movies where the hero (or villain) uses a beam from a compact laser to blow a rocket out of the sky? Last December, that generic bit of sci-fi drama took a step closer to reality. In a demonstration at the White Sands Missile Range in New Mexico, the solid-state heat-capacity laser (SSHCL) burned a 1-centimeter-diameter hole straight through a 2-centimeter-thick stack of steel samples in 6 seconds. The electrical current to do so came from a wall outlet and cost no more than 30 cents. While large chemical lasers have successfully shot down tactical rockets, the SSHCL design supports the weight and size requirements for a future mobile deployment.

The SSHCL, designed and developed at Lawrence Livermore, is the prototype of a laser tactical weapon, which shows promise as the first high-energy laser compact enough in size and weight to be considered part of the Army’s future combat system (FCS) for short-range air defense. The FCS is a component of the Army’s vision of sensors, platforms, and weapons with a networked command and control system. The more advanced version of the laser weapon system, now under development, will be battery-powered and—at 2 meters long and less than a meter across—small enough to be mounted on a hybrid-electric high-mobility multipurpose wheeled vehicle (Humvee). In this configuration, the Humvee’s generator and batteries could power both the vehicle and the laser, requiring only diesel fuel to support full operation.

The SSHCL offers speed-of-light precision engagement and destruction of a variety of targets, including short-range artillery, rockets, and mortars. There is a current need for effective protection against these weapons on the battlefield. The project is sponsored by the U.S. Army Space and Missile Defense Command and has a number of commercial partners, including General Atomics, Raytheon Co., PEI Electronics Inc., Northrop Grumman Corp., Goodrich Corp., Armstrong Laser Technology Inc., and Saft America.

Meeting the Challenges

The SSHCL delivered to White Sands for testing last September has an amplifier composed of nine disks of neodymium-doped glass (Nd:glass). In this prototype, an electrical source powers flashlamps, which in turn pump the disks, which then release the energy in pulses of laser light. The average output power of the SSHCL is 10 kilowatts, and it can deliver 500-joule pulses at 20 hertz in 10-second bursts—essentially vaporizing metal. The prototype requires 1 megawatt of input power to produce a 13-kilowatt laser beam. Project manager Brent Dane, of Livermore’s Laser Science and Technology program, notes that the ultimate objective of the project is to build a next-generation system with enough electrical efficiency to
produce a 100-kilowatt laser beam from the same 1 megawatt of input power. The final version will be capable of firing 200 pulses per second.

The Livermore team is focusing on the technological challenges that remain to building the 100-kilowatt system. Dane enumerated the three areas of concentration: growing large crystals of neodymium-doped gadolinium–gallium–garnet (Nd:GGG) for amplifier disks; developing the technology needed to make diode arrays large, powerful, and cost-effective; and defining the laser architecture and technology that will allow high-quality beams to propagate precisely over long distances.

Although the prototype uses Nd:glass for its laser amplifier disks, the final version will use Nd:GGG. “There are many reasons for choosing Nd:GGG,” explains Mark Rotter, an electrical engineer who is leading the diode-pumped Nd:GGG effort. “Compared with Nd:glass, Nd:GGG boasts a higher mechanical strength and higher thermal conductivity, which, in combination, will allow us to rapidly cool the disks between runs and reduce the turnaround time between laser firings. The Nd:GGG is also twice as efficient in converting pump energy to output beam energy.” The challenge—to grow the crystals large enough to manufacture the nine 13-square-centimeter slabs needed for the 100-kilowatt laser—is well on its way to being met. Northrop/Grumman Poly-Scientific, the commercial partner responsible for growing the crystals, is now producing high-optical-quality Nd:GGG crystals up to 15 centimeters in diameter. The ultimate goal is to grow crystals approximately 20 centimeters in diameter.

To pump these Nd:GGG amplifier disks, the SSHCL will use arrays of laser diodes instead of flashlamps because diode arrays are more compact and efficient than flashlamps and, more importantly, diode radiation generates less heat in the Nd:GGG laser crystals. The challenge is to make the diode arrays large, powerful, and cost-effective and to come up with a cooling scheme that will work in the field.

Lawrence Livermore’s Ray Beach, who leads the diode array portion of the project, explains, “Cooling high-average-power laser diode arrays is a unique and challenging problem in the field of thermal engineering. Although laser diodes are extremely efficient devices by ordinary laser standards—they typically convert 50 percent of their electric input power into light output—the remaining 50 percent of the input power shows up as high-intensity heat from a very compact source.
Future Looks Bright

The solutions to these challenges are being incorporated into an SSHCL testbed—a module made up of a three-slab Nd:GGG amplifier pumped by laser diode arrays. This testbed will be configured as a laser system to demonstrate the pulse energy at a high repetition rate in 2003. The final version of the SSHCL, which would have an output power of 100 kilowatts under burst mode for several seconds, is expected to be ready to demonstrate to the Army by 2007.

Meanwhile, at the White Sands Missile Test Range, the Army, with Laboratory support, is putting the prototype through its paces, testing it on aluminum and steel to determine what types of power and pulse format will optimize the final weapon system. The Army will also use the prototype to address issues such as lethality, beam degradation due to atmospheric effects, and precision optical pointing and tracking.

The future for the solid-state laser looks promising, notes Dane. “The system we delivered to White Sands is just the starting point. The goal is to have a laser weapon system that is small, cost-effective, and mobile, which protects against tactical threats while meeting the sponsor’s other military requirements. We’re confident we’ll meet these goals.”

—Ann Parker


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In the Egyptian pantheon, Djehuty was the guide to heaven, earth, and the netherworld; lord of calculation, wisdom, and judgment; and protector of knowledge, mathematics, and science. It seemed appropriate, then, for Lawrence Livermore astrophysicists David Dearborn and Peter Eggleton to take his name for their breakthrough three-dimensional code that simulates the evolution and structure of stars.

The physical processes of stars have long been of interest to Livermore researchers because understanding the prime mechanism of stellar energy—thermonuclear fusion—is part of the Laboratory’s national security mission. “Stars are high-energy-density ovens,” says Dearborn. “Several Laboratory programs are interested in the properties of stars, and many Livermore physicists have backgrounds in astrophysics.”

Dearborn points out that stars provide the standards of reference for measuring the size, age, chemical composition, and evolution of the universe. Stars have also been used as physics laboratories for many hieroglyphic tablets.

A new three-dimensional code simulates for the first time the structure and evolution of stars.
that strengthen our understanding of complex physical processes. For example, they have been used to better understand the properties of hot plasmas as well as fundamental particles such as neutrinos. Stars have also been used to suggest the properties of exotic particles such as axions, which have been proposed to explain why the universe contains more matter than antimatter.

Eggleton notes that scientific knowledge of stars may appear to be mature, but in fact, much of what we know about stars—especially the way they generate energy and how they evolve from a dust cloud to a supernova or red giant—may well be significantly incomplete. “We need to improve our knowledge about stars,” he says.

The reason for the imperfect understanding is that many stellar processes are complex, three-dimensional phenomena that have been modeled only in coarse approximation using one-dimensional computer codes. For example, the transport of energy through a star by convection from its superhot core is a three-dimensional process, which limits the value of one-dimensional calculations, even for perfectly spherical stars. (See the box on pp. 6–7.) Although a one-dimensional convection simulation could be inaccurate by only 10 percent at any moment in time, such “small” errors can easily accumulate over time. The result might be a final discrepancy of 100 to 200 percent in some properties calculated for such stellar objects as Cepheids, which are large, pulsating stars often used to calculate the distance scale of the local universe.

**Need for 3D Codes**

Convection is only one of many stellar phenomena that require a three-dimensional simulation code for accurate modeling. Other complex phenomena that astrophysicists have long desired to simulate include the evolution of elements created in a star, the preexplosion structure of supernovas, and the physics of binary stars, which comprise nearly half of the visible mass of the universe.

Dearborn says that developing a three-dimensional code to realistically model stars is challenging for even the most accomplished teams of computer scientists and astrophysicists. Before Djehuty, three-dimensional stellar models were limited to about 1 million zones. (Computer simulations divide an object into numerous small cells, or zones, whose behavior is governed by sets of physics equations. The totality of the zones, or cells, is called a mesh.) The million zones represent only modest segments of a star. Moreover, the simplified models did not incorporate all the physics pertinent to a star’s core where nuclear energy is produced, and they did not simulate gravity in a realistic manner. “While the earlier codes are important starts toward improving our understanding, it is clear that the solutions to some problems necessitate whole-star modeling,” Eggleton says.

The advent of massively parallel computing, wherein computers have hundreds and even thousands of processors, and Livermore’s participation in the National Nuclear Security Administration’s Stockpile Stewardship Program—to assure the safety and reliability of the nation’s nuclear stockpile—led Livermore scientists to gain expertise in supercomputers and parallel codes. Along with astrophysicist Kem Cook, Dearborn and Eggleton saw that Livermore was becoming a uniquely qualified institution to move the calculation of stellar properties to a higher level of understanding. In particular, they saw that one element of stockpile stewardship, which uses massively parallel computing techniques to simulate the performance of nuclear warheads and bombs in a program called Advanced Simulation and Computing (ASCI), would be pertinent to their quest for a whole-star, three-dimensional model.

Dearborn and Eggleton’s vision was to take advantage of Livermore’s expertise in ASCI computations, code and algorithm development for massively parallel computers, astrophysics, high-energy-density physical data and processes, and experience in interdisciplinary coordination to attack the fundamental questions of stellar structure and evolution.

**A Laboratory-Wide Team**

In 1999, Dearborn and Eggleton assembled a team to develop Djehuty as a three-year Strategic Initiative under Laboratory Directed Research and Development funding. The collaboration has included John Castor, Steven Murray, and Grant Bazan from the Defense and Nuclear Technologies Directorate; Kem Cook from the Physics and Advanced Technologies Directorate; Don Dossa and Peter Eltgroth from the Computation Directorate’s Center for Applied Scientific Computing; and several other contributors. “Collaboration from throughout the Laboratory has been essential in this project,” says Dearborn.

The team designed Djehuty to operate on massively parallel machines with the best available physical data about stars and with algorithms tailored specifically for the massively parallel environment. Notes Dearborn, “There’s been tremendous work at the Laboratory in developing parallel codes and learning how to do calculations in a manner that won’t bog down the machines.” The code development process involved assembling and reconfiguring a number of Livermore codes that already existed, many of them parts of unclassified software belonging to the ASCI program, and optimizing them for astrophysical simulations.
Djehuty also takes advantage of the Laboratory’s significant knowledge about opacity (a measure of the distance photons at a particular frequency travel through a particular material) and equations of state (the relationship between a material’s pressure, temperature, and volume). Opacity and equation of state are two key pieces of data that are used in stockpile stewardship work for studying matter under extreme conditions. In that respect, says Dearborn, developing Djehuty is well aligned with Livermore’s programmatic interests that focus on understanding high-temperature physics and performing numerical simulations of complex physical reactions.

The code currently features accurate representations of different elements’ equations of state, opacities, radiative diffusion transport (how photons are absorbed and reemitted when they interact with atoms and electrons in a star’s interior), and nuclear reaction network (fusion reaction rates and abundance of species formed). Finally, Djehuty features a gravity package for spherical stars, a provision that is being improved significantly so it will be

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**Probing the Interiors of Stars**

Stars, unlike planets, produce their own energy and do so by thermonuclear fusion. Much of the complexity underlying the computer code Djehuty, Livermore’s three-dimensional code for star structure and evolution, is its realistic simulation of fusion, which converts hydrogen nuclei into helium ions. The process is often called hydrogen burning and is responsible for a star’s luminosity.

Fusion reactions occur in the core, the innermost part of the star. In a star about the size of our Sun, the hydrogen fuel is eventually consumed after billions of years. The core slowly starts to collapse to become a white dwarf while the envelope expands to become a red giant. Our Sun will reach this stage in about 5 billion years.

In contrast, the core of a star larger than the Sun is driven by a complex carbon–nitrogen–oxygen cycle that converts hydrogen to helium. In these massive stars’ cores, hot gases rise toward the surface, and cool gases fall back in a circulatory pattern known as convection. After depleting its hydrogen—and subsequently its helium, carbon, and oxygen—the contracting core of a massive star becomes unstable and implodes while the other layers explode as a supernova. The imploding core may first become a neutron star and, later, a pulsar or black hole.

The cores of stars are turbulent in a manner analogous to a boiling kettle, says Livermore astrophysicist Peter Eggleton. Driven by enormous heat, the material in a core takes about a month to completely circulate (our Sun accomplishes it in about two weeks). “One-dimensional simulations give you an average of what’s going on in the kettle instead of telling you what’s happening on a second-to-second basis, so we are forced to make some bold assumptions.”

Eggleton also says that one-dimensional codes cannot model time-dependent convection in such events as helium flashes, which occur in the late stages of a red giant star.

One of the long-standing issues of astrophysics has been determining the correct convective core size of stars. Astronomical observations have suggested that the convection region is larger than has been assumed since the 19th century. Astronomers call the situation convective-core overshoot, meaning that the core probably extends beyond the long-accepted boundary.

Determining the exact size of the convective core is of more than passing interest. If the core is indeed larger than has been assumed, then stars could be much older than has been believed, which has profound implications for how the universe evolved and its real age.

“The modeling of convection is one of the weakest points in our

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When low-mass stars such as our Sun become red giants, they grow a helium core. Eventually the helium core ignites and begins burning to carbon and oxygen. The ignition begins in a shell that initially expands and drives a weak shock into and out of the star. The image shows the velocity contours of the expanding shell in a cutaway segment of a star in which ignition is beginning. The red areas represent the highest velocity, corresponding to the rapidly expanding shell both in front and in back (barely visible).
possible to simulate a host of aspherical stellar objects.

The First Simulation

The team’s early strategy was to test the code’s accuracy and achieve some optimization of it. In September 2000, using the 680-gigaops (billion calculations per second) TeraCluster 2000 (TC2K) parallel supercomputer at Livermore, the team successfully executed a three-dimensional simulation of a star. This was the first three-dimensional simulation of an entire star, but it ran on just one of TC2K’s 512 processors, using only some of the code’s physics on a modest mesh containing approximately 400,000 cubic zones. “Our first models were too small to accurately represent a star’s structure, but they were sufficient to study different zone mesh structures and to optimize the physics equations we were using,” says Dearborn.

The issue over the size of the convection region is serving as a way to verify and validate the accuracy of Djehuty. The code development team made convective core overshoot a priority in part because the fusion process occurs during the earliest and simplest phase of stellar evolution—during what is called the main sequence. The main sequence is shown on a Hertzsprung–Russell diagram, which plots stars’ temperatures versus their brightness, thereby showing their evolution.

“Observations assure us that our best one-dimensional approximations of convection are flawed,” says Eggleton. “With Djehuty, we have a three-dimensional code with accurate physics to determine what exactly happens in the core. There are big rivers flowing in stars’ cores, and we want to follow them.”

One simulation modeled a star early in its evolution, prior to its joining the main sequence. As expected, it did not show any convection motions from thermonuclear fusion. Another simulation studied a massive star that had just reached the main sequence and so witnessed the onset of convective motion from fusion. A third simulation looked at a red giant, a very old star that possesses a large core of helium. The helium eventually ignites in what is called a helium flash.

The simulations suggested that a star’s convective core indeed exceeds its classical boundary. Additional computationally intense simulations, each requiring a month of supercomputer time, will be done this year to model a star’s convective core at key stages in its lifetime.
Satisfied with the early simulations on one processor, the team then modified the code to run in a massively parallel computing environment. “It’s a big transition going from one to many processors because we need at least 10 million zones to model an entire star,” says Dearborn. Fortunately, he says, Livermore has invested significant resources to figure out how to break up a complex physics problem, such as following fusion reactions in time, for efficient processing by hundreds and even thousands of processors.

Generating and monitoring large three-dimensional meshes containing millions of zones is a huge task. To aid computing, the Dhejuty team constructs a mesh sphere of seven blocks: one in the center and six surrounding it. The outlying six are distorted at their outer edges to make them spherical. Each block contains at least 1 million zones. Each zone represents thousands of kilometers on a side, and several thousand zones are assigned to a processor. All the processors must communicate efficiently with each other simultaneously. The key to Dhejuty’s simulation power is its ability to access many processors to efficiently compute the physics in each of the millions of zones. “We’re fortunate to have so many people who can develop a code like this,” says Dearborn.

The team has run simulations on increasing numbers of processors on the TC2K. Several simulations, using 128 processors and 56-million-zone meshes, were some of the largest astrophysics calculations ever performed; they generated close to a terabyte (trillion bytes) of data. The team has also begun to perform simulations on Livermore’s ASCI Frost, the unclassified portion of ASCI White, currently the world’s most powerful supercomputer. Simulations on ASCI Frost have used 128 of that machine’s processors to evolve stars with 60-million-zone meshes.

With the code running satisfactorily in a massively parallel environment, Dearborn and Eggleton focused on resolving a long-standing controversy in astrophysics. That controversy surrounds the discrepancy between the results from one-dimensional stellar models and data gained from astronomical observations concerning the size of the convection region inside a star. (See the box on pp. 6–7.) This region is where hot plumes of gas rise and fall. The team has simulated the cores of several stars, ranging from young stars before the onset of fusion reactions to old stars about half the age of the universe. Eggleton says that one-dimensional computer models are especially incomplete in simulating late stellar evolution, which is often characterized by deep mixing of gases and sudden pulses of energy.

Virtual Telescope at Work

Eggleton compares Dhejuty to a kind of virtual telescope that can take snapshots during a star’s lifetime of several billion years and examine in detail the star’s structure and the various physical processes at play. “There is no comparable three-dimensional code, although there have been heroic efforts to develop one,” he says. As a result of the early simulations, the Livermore team anticipates being able to accurately model in three dimensions, for the first time, a host of important stellar objects. For example, Dhejuty will be vital to understanding supernovas, the brightest objects in the universe, and about which much is unknown, as well as Cepheids.

Dearborn predicts that Dhejuty will provide an important link between theory and observation that will further our knowledge of stellar structure and evolution. Livermore’s Stefan Keller is conducting a number of observational studies to verify the Dhejuty simulations. One study uses a certain population of Cepheids to observationally determine the relationship between mass and luminosity that is dependent on the original amount of mixing in the star’s convective core. Preliminary results indicate that these Cepheids are considerably more luminous than predicted by standard one-dimensional models, a result suggesting a larger
degree of mixing than was previously thought. Djehuty simulations appear to confirm the observations.

In another study, astrophysicist Rob Cavallo is observing variations in the surface abundances of some elements in evolved red giant stars. The variations are caused by some form of nonconvective mixing process, which can only be determined with the use of a fully three-dimensional code such as Djehuty.

The team is also working to improve the code and better interpret its output. One goal is improving the accuracy of opacities. “There are a range of problems where a star’s behavior depends on the opacity of material whose composition is rapidly changing,” says Dearborn. The team plans to attack those problems by permitting the code to generate opacity levels using OPAL, a database of stellar opacity that was developed at Livermore several years ago. (See S&TR, April 1999, pp. 10–17.)

Another task is improving the techniques to better visualize and thereby understand the vast amounts of data generated by Djehuty. Analysis and visualization are the key for turning huge numerical simulations into scientific understanding, says Dearborn, and at present, “We must improve our ability to analyze three-dimensional structures. With longer, larger, and

Increasingly magnified sections of a star with four times the mass of the Sun can be seen in these Djehuty simulations. Here, (a) and (c) are the same as (b) and (d), respectively, but show the location of mesh zones. A closeup of the star’s convective core is shown in (e). Colors represent relative velocity (increasing from blue to yellow). The bulk of motion lies in the core, where convection currents driven by carbon–nitrogen–oxygen burning occur. The areas of convection appear to extend beyond what one-dimensional models depict, but Djehuty’s models are consistent with recent astronomical observations. (f) A two-dimensional slice of a Djehuty three-dimensional simulation depicting convection currents deep inside the core. The arrows signify the directions of the currents.
more realistic simulations, we must develop better tools to analyze our simulations to extract the greatest amount of information. We can’t eyeball 10 million zones in three dimensions. We must have ways for a computer to look for irregularities and flag them.”

Recently, the team began using MeshTV, a program that was designed at Livermore to visualize data for three-dimensional meshes. MeshTV can display an animation of data changing over time and permit a user to rotate, zoom, or pan an object while a movie assembled from the data is playing. (See S&T, October 2000, pp. 4–12.)

A Continual Code Development

Djehuty development will never be finished, although it will eventually become much less a development code and more a production code ready for use. The team continues to enhance Djehuty’s physics and refine its algorithms. Development is also under way to permit simulation of rapidly rotating stars and, in particular, binaries. Binary stars revolve around a common center of gravity and sometimes exchange some of their mass or even merge into one star. Often, one binary is distorted by the gravitational pull of the other, and the result is seen in varying brightness.

“Simulating binaries has become our main physics priority,” says Dearborn. “We want to see how mass comes off one star and is absorbed by the other.” One-dimensional codes don’t work for binaries because when two stars interact, the problem is three-dimensional.

Binary simulations require a more accurate means to simulate gravity, one that automatically changes to reflect a star’s size, shape, and internal physics. Once this enhanced gravity treatment is incorporated into Djehuty, the code will be able to represent binaries as well as stellar objects that are not perfectly spherical. “Once work on binaries begins,” says Dearborn, “we will enter completely new territory because calculations so far have been very crude.”

The Livermore effort to revolutionize stellar evolution and modeling calculations has been well received at two international conferences. The enthusiasm generated by this work has led to two proposals to the National Aeronautics and Space Administration from U.S. academic researchers interested in collaborating with the Djehuty team on binary star evolution. Other researchers have proposed using the code to study white dwarfs, the phase of stellar evolution that occurs late in stars’ lifetimes, depending upon their starting masses. Dearborn and Eggleton have also received inquiries about the possibility of modifying the code to run simulations of large planets and brown dwarfs.

Several postdoctoral scientists and university students have joined the Djehuty development team. With a user manual recently completed, the team is seeking university collaborators, both graduate students and visiting scientists, who would visit for several months at a time and join in astrophysical research that can be done nowhere else.

Dearborn and Eggleton hope to see a user facility established at the Livermore branch of the University of California’s Institute of Geophysics and Planetary Physics (IGPP). The Livermore IGPP currently collaborates with all UC campuses, more than thirty U.S. universities, and more than twenty international universities. “Djehuty is a unique institutional asset for attracting astronomers and physicists interested in stars and what can be learned from them,” says Eggleton.

—Arnie Heller

Key Words: Advanced Simulation and Computing (ASCI), ASCI Frost, ASCI White, binary stars, brown dwarfs, Cepheids, convective core, Djehuty, helium flash, Hertzsprung–Russell diagram, Institute of Geophysics and Planetary Physics (IGPP), Mesh TV, stellar evolution, supernovas, TeraCluster 2000 (TC2K), white dwarfs.

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Some postdoctoral scientists and the project leaders on the Djehuty development team. From left, Rob Cavallo, Stefan Keller, team leaders Peter Eggleton and David Dearborn, and Sylvain Turcotte.
Adaptive Optics Sharpen the View from Earth

Blur-free images reveal a wealth of astronomical detail.

FROM a remote outpost on the summit of Hawaii’s dormant Mauna Kea volcano, the world’s two most powerful telescopes, located at the W. M. Keck Observatory, are probing the deepest regions of the universe. Thanks to a Lawrence Livermore–Keck team of scientists and engineers, astronomers are obtaining images on the 10-meter Keck telescopes with resolution greater than that of other land-based telescopes or even the orbiting Hubble Space Telescope.

Many of the Keck images, together with those from the smaller Shane telescope at the University of California’s Lick Observatory near San Jose, are being taken by Lawrence Livermore astronomers working with colleagues from University of California (UC) campuses and the California Institute of Technology (Caltech). The images are shedding new light on the formation of stars and galaxies, revealing unexpected features on planets and moons in our solar system, and yielding new information on black holes in the centers of distant galaxies.

The key to the unsurpassed image clarity is adaptive optics that remove the blurring of starlight caused by turbulence in Earth’s atmosphere, resulting in a tenfold improvement in resolution. Adaptive optics measure the distortions of light from a natural star.
Adaptive Optics

scientist Deanna Pennington, “People are extremely pleased with the adaptive optics systems.”

Pennington, who served as laser guide star project leader at both Lick and Keck, says astronomers are clamoring to use the Keck laser guide star because “It makes possible entirely new kinds of observations that astronomers simply couldn’t access before.”

Livermore astronomers have been among the first to use the adaptive optics systems. Most of them are part of the Livermore branch of the University of California’s Institute of Geophysics and Planetary Physics. Since its establishment in 1983, the Livermore branch has been the focus of most astronomical activities at the Laboratory.

Livermore astrophysicists Claire Max, Bruce Macintosh, and Seran Gibbard have been observing objects within our solar system using both Lick and Keck adaptive optics. At Lick, they have been aided by Livermore’s Don Gavel, lead engineer for the adaptive optics system. The Livermore efforts focused on observations of Io, Jupiter’s largest moon; Titan, Saturn’s largest moon; the planets Uranus and Neptune; and various asteroids.

Surprising Storms on Neptune

Astronomers using the Keck telescopes have obtained the best pictures yet of the planet Neptune, the eighth planet from the Sun. Thanks to adaptive optics, the images reveal a

Exceptionally Clear Images

Astronomers are reporting exceptional results from the adaptive optics systems installed at the two observatories. At Lick, roughly 50 percent of images are taken using adaptive optics, and about half of those images are made with the laser guide star. At Keck, reports Livermore laser
wealth of small-scale features in Neptune’s atmosphere, including narrow, bright bands encircling the planet, similar to those observed on Jupiter. There appear to be waves within the bands and regions where the bands move apart and come together as if they are separated by a vortex.

The images suggest violent methane storms with wind speeds reaching more than 1,770 kilometers per hour. The imaging team, which has included astronomers from the UC campuses at Berkeley and Los Angeles (UCLA) and from Caltech, is working to understand what might be the source of the energy driving the extreme weather.

Working with UC Berkeley’s Imke de Pater, the team has also captured near-infrared pictures of the planet Uranus, which mark the first ground-based detection of the faint rings around that planet. Also clearly visible is a layer of methane haze on Uranus’s south polar cap, tiny cloud features at high northern latitudes, and, inside the planet’s bright epsilon ring, three fainter rings.

Keck images of Io have revealed many glowing volcanoes. Macintosh took the images in the infrared band to detect sources of heat on the moon. Other striking images, taken by Gavel, are of the asteroid Kalliope with its own moon. Gibbard has been using Keck to obtain images of Titan, the only solid body in the solar system besides Earth to have a substantial atmosphere (mostly nitrogen, with about 3 percent methane). Some astronomers believe that Titan’s atmosphere may be similar to that of Earth’s during our planet’s early development. Methane haze in the upper atmosphere obscures Titan’s surface features at visible wavelengths. However, in some narrow “transparency windows” in the near-infrared band, surface features can be seen through the haze.

Without adaptive optics, says Gibbard, “Titan looks like a fuzzy star.” She has been analyzing a large series of images to assemble the first map of Titan’s surface. “By taking many images over time, we can see which features do not change, and these belong to the surface,” she says. The use of adaptive optics has replaced a process called speckle imaging, which involved taking hundreds of very fast exposures and assembling them. “Adaptive optics is much simpler,” Gibbard says.

**Imaging Stellar Nurseries**
Macintosh and astronomers from UCLA are using adaptive optics on Lick and Keck to study the formation and evolution of planetary systems in the Trapezium (sword) region of the constellation of Orion. This region, the

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**Time-lapse photograph of the Lick Observatory and the laser guide star.**

(a) Astronomers using Keck’s adaptive optics have obtained the best pictures yet of the planet Neptune. The images show bands encircling the planet and what appear to be fast-moving storms of haze. (b) The same image without adaptive optics.
closest large-scale star formation to our Sun, serves as a stellar nursery.

“One of the most fundamental questions in modern astronomy is the possibility of the existence of other solar systems like our own, those with potentially habitable planets,” Macintosh says. He notes that although planetary systems have been detected through indirect methods, all are different from our solar system because they have massive, Jupiter-like planets occupying the inner part where Earth is located in our system. “It is unclear which type of system is more common in the universe,” says Macintosh.

The astronomers first use Lick to scout for promising young stellar systems and then travel to Keck to obtain high-resolution images. Bright stars found in the constellation serve as handy natural guide stars for the adaptive optics system.

Macintosh says that large planets (about the size of Jupiter) that are 10 million years old or younger radiate significant near-infrared light. Keck’s adaptive optics system can detect these planets even though they are a million times dimmer than the star they orbit. Macintosh has also imaged several of the Orion proplyds—protoplanetary disk envelopes surrounding young stars—that are being disrupted by intense radiation from nearby supermassive stars.

“Keck could be the first telescope to image a planet orbiting a star outside of our solar system,” Macintosh says. He adds, “Keck’s adaptive optics system represents the most significant advance in astronomical capabilities since the launch of the Hubble Space Telescope.”

Jennifer Patience is studying the binary star systems that are found among the young stars in Orion’s Trapezium. “We want to know how common it is for planets to form in binary systems,” she says. Astronomers believe that the presence of a nearby companion star may disrupt circumstellar disks surrounding young stars (circumstellar disks provide the raw materials for planet formation). Working with astronomers from UC Berkeley and UCLA, she uses Keck and Lick adaptive optics systems to look at star systems in the near-infrared spectrum and to see through clouds of galactic dust and gas that mask images in visible light.

The team has imaged 150 stars in Orion with resolution never before attained. Keck’s adaptive optics make it possible to resolve binaries with separations comparable to the distance
Adaptive optics systems have traditionally required the astronomer to find a bright star as a reference point of light. However, less than 1 percent of the sky contains stars sufficiently bright to be of use as a reference light. To extend the usefulness of adaptive optics, Livermore scientists developed a laser system that creates a virtual reference star high above Earth’s surface to guide the adaptive optics system. The laser guide star is created by projecting light from a dye laser on a layer of sodium atoms that are in the atmosphere 90 to 100 kilometers above Earth.

The main components of an adaptive optics system using a laser guide star are a wavefront sensor camera equipped with a charge-coupled device detector, a control computer, a deformable mirror, a pulsed dye laser that is tuned to the atomic sodium resonance line at a wavelength of 589 nanometers, and a set of solid-state lasers to pump, or energize, the dye laser. The dye laser, similar to that pioneered at Livermore for its Atomic Vapor Laser Isotope Separation program, creates a glowing star of sodium atoms measuring less than 1 meter in diameter at an altitude of about 100 kilometers above Earth’s surface. This artificial reference can be created as close to the astronomical target as desired so that the light from the laser star and the observed object pass through the same small part of the atmosphere.

At the telescope, wavefront sensors measure distortions due to atmospheric turbulence, using light from the guide star as a reference. The sensors relay this information to a computer, which in turn controls the movements of tiny actuators attached to the back of a deformable mirror. The mirror changes its shape hundreds of times per second to cancel out atmospheric distortion.

Near-infrared images obtained with the adaptive optics systems on the telescopes at the W. H. Keck Observatory in Hawaii are superior to images obtained with the Hubble Space Telescope because Hubble’s light-gathering mirror is much smaller. (Adaptive optics will not, however, replace space-based observatories, many of which are designed to sample certain bands of electromagnetic radiation such as ultraviolet light that are blocked by Earth’s atmosphere.)

Lick’s dye laser projects light into the sky through a 30-centimeter refractive telescope that is mounted on the side of the main telescope. The laser was designed and built by Livermore’s Herbert Friedman. The deformable mirror has 127 actuators to raise or lower a tiny part of the front surface by up to 4 micrometers.

The laser guide star at the Keck II telescope uses a 20-watt dye laser, the most powerful laser in use at a telescope. The laser light is projected onto the sky by a telescope with a 50-centimeter lens attached to the side of the 10-meter Keck II telescope. A 15-centimeter-diameter deformable mirror is adjusted continuously by 349 actuators.

Keck’s laser guide star was built at Livermore and then reassembled at the observatory’s headquarters in Waimea, Hawaii, which is slightly less than 1 kilometer above sea level. The observatory’s telescopes are located at the summit of the Mauna Kea volcano, over 4 kilometers above sea level. Scientists observe on these telescopes remotely from the Waimea headquarters to avoid the risk of sickness from extended exposure to Mauna Kea’s high altitude.

During the two-year temporary installation at headquarters, the Livermore team of Deanna Pennington, Curtis Brown, Pam Danforth, and Holger Jones made extensive improvements. “We installed a significant level of automation and diagnostics on the laser guide star system to make it more reliable and robust and permit it to be operated remotely from Waimea,” says Pennington, laser scientist and systems engineer at both Lick and Keck. She notes that installing the adaptive optics system and laser guide star at Lick gave the Livermore team valuable experience in designing the larger system at Keck. The laser system was installed and activated on the telescope at the 122-kilometer summit over a 6-month period, culminating in the “first light” demonstration on December 23, 2001.

Keck’s adaptive optics and laser guide star embody more than two decades of Livermore experience in adaptive optics technology. Adaptive optics systems with adjustable mirrors have been used on a succession of increasingly powerful lasers at Livermore, and they will be used on the National Nuclear Security Administration’s National Ignition Facility (NIF), under construction at Livermore.

Claire Max and Friedman started Livermore’s work on laser guide stars in the early 1990s. Feasibility tests conducted at Livermore in 1992 demonstrated the first laser guide star at usable power levels and determined the requirements for a telescope version.

Livermore scientists are working on the next generations of adaptive optics. About 20 Livermore employees belong to the Adaptive Optics program within the Physics and Advanced Technologies Directorate. One team is developing more reliable deformable mirrors based on microelectromechanical technology.

With funding from the Center for Adaptive Optics (see the box on p. 19) and the European Southern Observatory in Chile, Pennington will lead another group of Livermore scientists within the NIF Programs Directorate who are investigating fiber lasers to replace the current dye laser. Fiber lasers, widely used in the telecommunications industry, will be part of the NIF front end and will produce the laser beam before it is amplified. Pennington says that fiber lasers provide an “elegant solution” for generating 589-nanometer light because they are compact, efficient, and robust.
An overview of the layout within the dome of the Keck II telescope. (a) The laser equipment room on the dome floor houses the pulsed dye laser master oscillator, yttrium–aluminum–garnet pump lasers, and control systems. (b) The laser room on the elevation ring of the telescope houses an optics bench containing two stages of dye amplification, numerous diagnostics, and the bottom half of the projection telescope. (c) The 50-centimeter projection lens is located at the top end of the telescope.
between our Sun and Uranus, a distance that is less than the diameter of circumstellar disks. “We now have the capability of resolving most binary systems, including a range inaccessible to previous surveys,” Patience says. She notes that with the resolving power of Keck’s adaptive optics system, a person standing on Mauna Kea, located on the big island of Hawaii, could see objects as small as 1 centimeter tall on the island of Oahu, approximately 400 kilometers away.

**Peering into Black Holes**

Max, her colleague Gaby Canalizo, and astronomers from UC Santa Barbara, are using adaptive optics on Lick and Keck telescopes and Lick’s laser guide star to observe nearby active galactic nuclei, which are small, extremely bright central regions in some galaxies. Very distant and bright active galactic nuclei are known as quasars. Active galactic nuclei are thought to contain black holes at their centers, which suck up stars, planets, and gas from the surrounding galaxy in a process called accretion. In some cases, the material is then shot out from the region surrounding the black hole at high speeds in outflows known as jets.

Max notes that for 30 years, Department of Energy laboratories have been doing pioneering work on the high-energy processes involved in black-hole formation and emission. However, only in the past few years has direct evidence for black holes begun to emerge—in the form of high-resolution observations that probe the active galactic nuclei close to the central black hole.

Max and Canalizo’s team is observing energy outflow from the process of accretion of matter into the most massive black holes in nearby galaxies. The images enable astronomers to explore the region nearby and the evolution of the central black holes. In the process, the astronomers have found double active galactic nuclei suggestive of galaxy mergers, which are believed to be a cause of black hole formation.

**Looking to the Future**

When the Keck laser guide star becomes available for viewing, Livermore scientists will be among the first to use it and thereby help to make laser guide stars a more accepted tool of astronomical research. Pennington notes that a National Academy of Sciences panel has identified laser guide stars as a key technology for advancing astronomy. Most experts say that the next generation of giant telescopes will not be feasible without adaptive optics systems equipped with laser guide stars.

The first map of the surface of Titan, Saturn’s largest moon, is being assembled with the help of adaptive optics. Colors denote reflectance, with 1.00 corresponding to the reflectance of a perfect mirror. Data from current observations are filling in the blank areas.

Keck adaptive optics image of a protoplanetary disk envelope surrounding a young star in the Trapezium region of the constellation Orion.
New Center Spreads the Word

Lawrence Livermore is a major partner in the Center for Adaptive Optics, which is headquartered at the University of California (UC) at Santa Cruz. The center, funded by the National Science Foundation, began operations in November 2001. The 27 partner institutions in the center also include several other UC campuses, the University of Chicago, the California Institute of Technology, the University of Rochester, the University of Houston, Indiana University, and 17 other partners.

The center’s director is Jerry Nelson, professor of astronomy and astrophysics at UC Santa Cruz. Nelson designed the twin telescopes at the W. M. Keck Observatory in Hawaii. Livermore scientists Claire Max and Scot Olivier are associate directors, and Livermore scientists play important roles in center activities and sponsored research.

The center coordinates the efforts of researchers across the country involved in the growing field of adaptive optics for astronomical and vision science. The center also operates science education and outreach programs for scientists and college students.

“Our goal is to provide the sustained effort needed to bring adaptive optics from promise to widespread use by astronomers and vision researchers,” says Max. She predicts that most large ground-based telescopes will have adaptive optics systems within the next few years. Relatively few astronomers, however, have experience with adaptive optics, let alone laser guide stars. “We want to inform the broader astronomical community about adaptive optics through conferences and workshops,” she says.

Max points out that adaptive optics are also used in vision science to compensate for aberrations in the eye that affect vision and impede efforts to study the living retina. Adaptive optics has made it possible to obtain images of the living human retina with unprecedented resolution, enabling researchers to see individual light receptors. Adaptive optics may also provide normal eyes with supernormal vision. A team of Livermore researchers led by Olivier is developing a high-resolution liquid-crystal adaptive optics system for human vision correction that will be used at UC Davis to study the limits of human visual acuity.

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For online information on the W. M. Keck Observatory: www2.keck.hawaii.edu:3636

For online information on the Lick Observatory: www.ucolick.org/

For online information on the Center for Adaptive Optics: cfao.ucolick.org/

However, as a telescope gets larger, the requirements for an adaptive optics system become increasingly rigorous. The proposed California Extremely Large Telescope (CELT), a collaboration between UC and Caltech, is designed to have a 30-meter-diameter mirror, three times the size of Keck’s. CELT’s adaptive optics system will probably require multiple laser guide stars with several mirrors working together to correct for different layers of atmospheric turbulence. Each mirror may require about 5,000 actuators.

Thanks to increasingly powerful telescopes, more capable adaptive optics systems, and advanced guide-star lasers, the heavens are sure to be revealing more of their secrets in the new millennium.

—Arnie Heller

Key Words: active galactic nuclei, adaptive optics, atomic vapor laser isotope separation, binary star, black hole, California Extremely Large Telescope (CELT), deformable mirror, dye laser, Hubble Space Telescope, laser guide star, Lick Observatory, W. M. Keck Observatory.
Experiments Re-create X Rays from Comets

Earth is continually showered by x rays traversing the universe from our Sun and other hot stellar objects. A major branch of astronomy is devoted to detecting and studying x rays from distant stars and galaxies, and Lawrence Livermore scientists have long studied the x rays that are produced from nuclear detonations.

However, it came as quite a surprise to scientists in 1996 when the Rosat X-Ray Satellite detected low-energy (less than 1 kiloelectronvolt) x rays streaming from the comet Hyakutake. X-ray emission is usually associated with hot plasmas from stars, nuclear reactions, and black holes, not from ice-cold objects such as comets. Since the original discovery, other x-ray satellites have established that several other comets traveling through our solar system emit x rays with fluxes, or intensities, as high as $10^{25}$ photons per second.

To help resolve the apparent contradiction, a national team of scientists headed by Lawrence Livermore physicist Peter Beiersdorfer is working on the laboratory production of low-energy x rays identical to those produced by comets traveling near the Sun. The team is using Livermore’s electron beam ion trap (EBIT) to produce the x rays and an x-ray spectrometer (XRS) designed by the National Aeronautics and Space Administration (NASA) to detect them.

The research is providing much greater understanding about the x rays that are emitted by comets as they pass the Sun. The effort is also providing scientists with valuable information that will help them interpret data to be collected by a joint U.S.–Japan x-ray satellite mission scheduled for launch in 2005.

Primordial Chunks of Ice

Comets are odd-shaped chunks of ice (water and frozen gas) and dust a few kilometers to a few tens of kilometers in diameter. They are the oldest, most primordial objects in the solar system. X rays emanate from a comet’s nebulous atmosphere called a coma, which can stretch tens of thousands of kilometers in front of or behind the comet. The coma is formed when the comet gets close enough to the Sun so that some of the ice is vaporized.

More than a dozen theoretical models were first proposed to explain why comets give off x rays. Some models predicted that comet x rays are reradiated x rays from the Sun. Other models were based on some kind of interaction between the molecules.

The current explanation for comet x rays is called charge exchange. This process is believed to occur when heavy ions ($A^{i+}$) from the solar wind flowing from the Sun (right) collide with electrically neutral atoms and molecules (B) in the comet’s atmosphere (left). During a collision, a heavy ion captures one or more electrons from a comet’s atmospheric atom, ionizing it to $B^{(q-p)+}$. The solar wind ion, now $A^{i+}$, momentarily enters an excited state and kicks out an x ray as the electrons return to a low-energy state. The x ray can be detected by a spacecraft (lower left).
in the comet’s thin atmosphere and ions or electrons from the Sun’s solar wind, the stream of particles that blow off the Sun’s corona at 400 kilometers per second.

The current leading explanation is called charge exchange. This process is believed to occur when solar wind forces heavy ions of carbon, nitrogen, oxygen, and other elements to collide with the electrically neutral atoms and molecules found in a comet’s atmosphere. During a collision, a heavy ion from the solar wind captures an electron from a comet’s atmospheric atom or molecule and momentarily enters an excited state. The ion immediately kicks out an x ray as the electron returns to a low-energy state.

“Very little experimental data are available on charge-exchange-induced x rays and what the spectrum emission lines look like,” says Beiersdorfer. “The goal of our research is to re-create, in the laboratory, the same x-ray emissions that are produced when the solar wind and comets interact. In this way, we can better understand the nature of charge exchange and help other scientists interpret data taken by x-ray satellites.”

The research, supported by Laboratory Directed Research and Development funding and NASA, is a collaboration between scientists from Livermore, NASA’s Goddard Space Flight Center, and Columbia University. The investigators include Daniel Thorn, Mark May, and Hui Chen from the Laboratory; Richard Kelley, Scott Porter, Caroline Stahle, Keith Gendreau, Gregory Brown, Andy Szymkowiak, and Kevin Boyce from Goddard; and Steven Kahn from Columbia. In addition, space researchers Casey Lisse from the University of Maryland and Bradford Wargelin from the Harvard Smithsonian Observatory are aiding the research effort.

The team is using Livermore’s EBIT, which produces and traps highly charged ions by means of a high-current-density electron beam instead of traditional high-energy particle accelerators. The instrument was developed in 1985 by Laboratory physicists Mort Levine and Ross Marrs. Other electron beam ion traps, most of which are based on Livermore’s design, are used at research centers in the U.S., Europe, and Japan.

EBIT’s electron beam collides with selected ions to strip them of one or more electrons, depending on the beam’s energy. The current version, named SuperEBIT, can produce an electron beam energy of up to 250 kiloelectronvolts, enough to make uranium (U$^{92+}$) ions. “SuperEBIT can produce virtually any ion, x ray, or visible photon desired,” says Beiersdorfer.

**New Generation of Spectrometer**

The XRS was designed by NASA for Japan’s Astro-E X-Ray Satellite, but a failed rocket launch in February 2000 means a wait of five years before its replacement, the Astro-E2 Satellite, can be placed in orbit. Fortunately, the Astro-E’s engineering spare XRS was still available for laboratory x-ray astrophysics measurements. It was sent to Livermore after the failed launch.

At Livermore’s electron beam ion trap (EBIT) facility, scientists study the charge-exchange process and the effects of different ions and interaction gas molecules on the x-ray emission patterns recorded by the x-ray spectrometer (XRS) (front). The EBIT (in back) provides a source of ions to re-create solar wind particles. At the left is an old-style spectrometer. Also shown is the intersection of the XRS and EBIT.
Experiments Mimic Space Interactions

The EBIT experiments begin with the production of several million ions of either carbon, oxygen, neon, magnesium, silicon, or iron. These ions are found in the solar wind and are believed to be involved in charge-exchange reactions with comets. The beam is then turned off, and the trap is operated in the so-called magnetic mode, in which the ions are confined by a magnetic field to a volume of about 2 cubic centimeters. At this density, the physics is the same as that found in the vicinity of a comet passing close by the Sun. (A greater density of ions would introduce completely different physics regimes.) Next, neutral molecules of water, methane, nitrogen, or carbon dioxide, all of which have been identified in comets’ atmospheres, are injected into the trap.

For a few hours, the XRS records the x rays produced by charge-transfer collisions between the ions and the neutral molecules. The result is a catalog of emission lines that serve as tell-tale fingerprints of a particular ion’s x-ray-producing collision. Beiersdorfer says that the experiments are validating the hypothesis that charge exchange is a viable mechanism for producing comet x rays, although the exact mechanics of the process are probably more complex than is known.
The researchers discovered that the x-ray emission pattern changes with the kinetic energy of the ions. They found that the average x-ray energy emitted by the ions shifts to higher values as the kinetic energy of the ions is lowered. They also uncovered subtle changes in the x-ray emission lines when different neutral gases collide with the heavy ions. “The composition of the interaction gas is another important variable,” says Beiersdorfer.

Comets as Probes

Beiersdorfer predicts that careful detection and measurement of x rays produced by the interaction between the solar wind and comets will one day provide a powerful means to monitor space “weather” inside the solar system without the need for spacecraft circling the Sun. In this way, he says, comets could be used as probes to measure the intensity, speed, and composition of the solar wind, its intermittent “quiet time,” and the chemical composition of comet gases.

“Given that more than three bright comets with appreciable x-ray emissions enter the inner solar system each year, their x rays can provide a valuable diagnostic of the solar wind. This capability has opened up a whole new window to our solar system; it’s a very rich field.”

Some astronomers have conjectured that as the solar wind slows down throughout the heliosphere, it may generate weak x rays through charge-exchange reactions with natural gas streaming in from the interstellar medium (mostly hydrogen atoms). If this hypothesis is borne out by x-ray satellite data, astronomers will have to revise their assumption that the soft x-ray background that seems to permeate the universe may in fact be partly due to charge-exchange reactions from the solar wind.

Small Handbook on Comet X Rays

The result of the EBIT experiments will likely be a small handbook for scientists to guide their interpretation and understanding of the comet x-ray data sent back by Astro-E2, beginning in 2005. “The scientific community will be well prepared when Astro-E2 launches,” says Beiersdorfer. In the meantime, NASA has committed a second, advanced XRS for the EBIT team’s research.

As the EBIT experiments continue, other scientists are looking at the theoretical model of charge exchange. Atomic theorists Ronald Olson from the University of Missouri at Rolla; Jim Perez from Luther College in Decorah, Iowa; Charles Weatherford from Florida A&M University in Tallahassee; and Burke Ritchie from Livermore are aiding the research effort. Lawrence Livermore researchers have extensive experience in modeling short-wavelength radiation phenomena, and physicist Ritchie is using high-performance supercomputers to elucidate in greater detail charge-exchange reactions using the quantum theory of atomic collisions.

Clearly, primordial chunks of dirty ice still hold a few surprises for scientists.

—Arnie Heller

Key Words: charge exchange, comets, electron beam ion trap (EBIT), microcalorimeter, solar wind, x rays, x-ray spectrometer (XRS).

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Stepping Up to Extreme Lithography

A revolutionary microprocessor technology developed by Lawrence Livermore and Veeco Instruments Inc. could increase the speed of personal computers by 10- to 20-fold and their memory capacity by 100- to 1,000-fold. The Production-Scale Thin-Film Coating Tool is a highly precise deposition system that opens the door to advanced, high-volume manufacturing of the next generation of microprocessors. It is one of this year’s R&D 100 Award winners.

With the new technology, powerful desktop computers could be made that realize a wealth of exciting applications, including real-time multilingual voice recognition, translation, and human interfaces. “Applications such as these are impossible on today’s 1-gigahertz PCs,” says Regina Soufli, Livermore physicist and leader of the team that developed the coating tool. “Technology enabled by the tool will allow tomorrow’s PCs to approach the computing power of today’s multimillion-dollar mainframe systems that presently only exist in laboratories.”

Down the Optical Road

The semiconductor industry relies on optical lithography to manufacture computer chips. In the most advanced optical lithography in use today, light of 193-nanometer wavelength is projected through masks patterned with intricate circuit diagrams. The transmitted pattern is reduced by being relayed through a series of refractive lenses. In steppers (industry jargon for systems that repeat manufacturing steps over and over), the patterned image is reproduced onto thousands of silicon wafers, which are processed and developed into integrated circuits.

Presently, optical lithography can reduce circuit patterns to have features as small as 130 nanometers (the diameter of a human hair is 100,000 nanometers). This is approaching the limit of resolution, as dictated by the physics of light diffraction for the wavelengths used in current technology. But to increase the speed and power of computers, the semiconductor industry will need circuit patterns as small as 30 nanometers for computers operating at 10 gigahertz or faster. Thus, the industry has initiated a quest to find the next-generation lithographic technique that can further reduce feature size.

Extreme ultraviolet lithography (EUVL) has been recognized as the most feasible next step. It uses light of 13-nanometer wavelength, which is 15 times shorter than the wavelengths used by today’s technologies. Adopting EUVL, however, represents a giant challenge.

Going Extreme

Radiation at the extreme ultraviolet wavelengths is strongly absorbed by matter such as air or the lens material. For this reason, the entire EUVL system has to be maintained under a vacuum, and the light that produces the circuit image must be reflected from mirrors rather than refracted through lenses. Furthermore, the mirrors must consist of precisely figured glass substrates that have been coated with alternating layers of molybdenum and silicon to a thickness of 280 nanometers.

Shown against a backdrop of the projection optics for the coating deposition system they co-developed with private industry, members of the Livermore team are, from left, Jim Folta, Rick Levesque, Claude Montcalm, Swie-In Tan, Mark Schmidt, Regina Soufli, Fred Grabner, Chris Walton, and Eberhard Spiller. Missing from the photo is Steve Vernon.
This thickness can only vary by less than 0.05 averaged over the entire optical surface; such a variance is equivalent to one-quarter the diameter of a silicon atom.

If this stringent specification is not met, the printed circuits will be blurred and will fail. The challenge of making precision-coated optics and doing so in a reproducible manner is daunting and thus an obstacle to implementing EUVL lithographic steppers. “There were doubts that such thickness precision could be achieved repeatably,” says Soufli.

A daunting task to be sure, but Soufli and her team are receiving accolades for accomplishing it. Built on the basis of Livermore’s expertise in thin-film technology, the coating tool can deliver commercial-quality multilayer coatings on the optics used in the camera and illuminator of EUVL semiconductor steppers. The tool has achieved the 0.05-nanometer-thickness precision required on camera optics. As a demonstration of success, the same optics have also been used to print integrated circuit patterns as small as 39 nanometers. This is the best imaging resolution ever achieved with optical lithography and foreshadows the ability to print circuits at the 30-nanometer resolution required for next-generation microprocessors.

The Way It Works

The new coating tool is based on the magnetron sputtering method widely used for thin-film deposition. The coating takes place inside a chamber where molybdenum and silicon sputter sources have been placed 180 degrees apart. The sources, called magnetrons, have a magnetic field attached to the back of their surface. With the chamber maintained under vacuum, the magnetrons are ignited, and a small amount of argon gas is introduced into the system. Argon ions, excited by the electromagnetic field, impinge on the sources and sputter atoms off the two materials. The atoms land on the optical substrate that sits atop a rotating deposition platter. The rotating platter passes alternately under the magnetrons, resulting in alternating layers of the two materials being deposited onto the optical surface. The platter is rotated under the sources at speeds of about 1 rotation per minute, while the individual substrates are simultaneously spinning fast around their centers at several hundred rotations per minute, thereby equalizing the spatial variations of the sources.

The tool’s ability to control film thickness is based on a simple concept: The speed at which the optic passes under a sputtering source determines how much of that sputter material is deposited on the optical surface. Platter speed is modulated as the substrate passes under the silicon and molybdenum targets, depending on what thickness profile is desired.

The most critical step of the entire process is determining the right coating recipe for a given optic, and this is done with the help of computer simulation. First, using the substrate shape and desired coating thickness profile as input, a custom-designed computer model simulates the deposition process. The algorithm calculates the platter velocities and angles that should be applied and proposes a coating recipe that is tested on a surrogate optic. The resulting coating thickness on the surrogate optic is measured, compared with the desired profile, and fed back to the algorithm to adjust the recipe. The final recipe is arrived at after four or five iterations of simulation and adjustment. When put into use, the recipe must be calibrated only once for each set of optics and is stable enough to be repeatedly used for over a year.

The new coating deposition system can produce multiple sets of optics in a high-volume production mode with precisely identical thickness profile. This way of controlling coating thickness is accurate, quick, and inexpensive.

Riding the Wave of the Future

The coating tool represents a breakthrough in semiconductor equipment manufacturing. It enables the commercialization of EUVL. Beyond EUVL, the tool’s capabilities can be applied in other areas where thin films with precision thickness control are needed, such as astrophysics, magnetics, and biological x-ray imaging.

“We achieved commercial-level thickness control for the first time on large multilayer optics,” says Soufli. “By implementing a versatile design and a unique deposition algorithm, the tool has enabled commercialization of EUVL as the next-generation technology for highly advanced computers of the future.” The first EUVL-fabricated computer chips are scheduled to be developed in 2007. Expect to be able to buy your very own “supercomputer” shortly thereafter.

—Whitney Lacy

Key Words: extreme ultraviolet lithography (EUVL), magnetron sputtering deposition, production-scale thin-film coating tool, R&D 100 Award, semiconductor computer chips.

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To learn more about the early universe, scientists are attempting to create a state of matter that hasn’t existed since the first moments following the big bang.

Inside the accelerator, gold ions zoom toward each other at almost the speed of light. They crash together with enough force to melt the ions into a quark–gluon plasma. This hot, primordial quark soup is thought to have existed in the first millionth of a second after the big bang that created our universe. The entire universe, small though it was then, is thought to have been a quark–gluon plasma. As the universe began to expand and cool, the quarks and gluons bound together and have remained virtually inseparable ever since.

Whereas the alchemists of old tried to turn all sorts of materials into gold, modern-day physicists, including several from Livermore, are attempting reverse alchemy—turning gold into a different state of nuclear matter. By smashing gold ions together in the Relativistic Heavy-Ion Collider (RHIC) at Brookhaven National Laboratory in Upton, New York, they are working to free quarks and gluons and re-create a quark–gluon plasma on Earth.

The quark is the most elementary building block of matter. (See the box on p. 7.) By exchanging gluons—massless particles that make quarks stick together—groups of quarks constitute particles such as protons and neutrons. The binding force carried by both gluons and quarks is known as the strong force, and for good reason. Although theory says that at extremely high energy densities, protons and neutrons should dissolve into a quark–gluon plasma, no particle accelerator had been powerful enough to create the necessary conditions with high certainty.

The possibility of creating hot, dense nuclear matter by colliding large nuclei was first proposed in 1973 by several
BREATHTAKING images from the Hubble Space Telescope, with its 2.5-meter mirror lens, have delighted astronomers and the public for years. Now, the National Aeronautics and Space Administration (NASA) has announced plans for a progression of larger telescopes to be fielded in space over the next two decades. These include telescopes with primary optics whose apertures are 25 meters and more. The increased sensitivity and resolution of the giant space telescopes will allow astronomers to view extremely fine features on planets and their moons in our solar system, image the cores of distant galaxies, and probe the edges of the universe.

“The history of astronomy is dominated by the quest for larger and higher quality telescopes,” says Livermore physicist Rod Hyde. He notes, however, that using a giant optic in space raises this quandary: how to design large-aperture space optics that are both optically precise and can meet the size and weight requirements practical for launch and deployment. “Either of these challenges is, by itself, quite formidable; in concert, they have yet to be solved,” he says.

Hyde heads a Livermore team that has developed a radically new concept to overcome the difficulties inherent in building and fielding a high-quality space telescope far larger than ever deployed. The concept, called Eyeglass, uses diffractive optics (also called Fresnel lenses) instead of mirrors or conventional glass lenses.

A Fresnel lens is flat on one side and ridged on the other. It replaces the curved surface of a conventional lens with many concentric grooves that are etched into a thin sheet of glass, silica, or plastic to bend and focus light. Relatively crude Fresnel lenses are commonly found in traffic signal lights, vehicle headlights, and the rear windows of motor homes.

Neatly Packaged, Easily Fielded

Not only is the Eyeglass diffractive telescope lightweight, but it also is flexible and can be segmented and folded into a neat package that fits in a space launch vehicle, says Hyde. Eyeglass would be easy to field in space because as a thin, flat membrane, it would not need large, heavy backings, trusses, or motors to maintain its shape, as do telescopes using mirrors.

“Conventional glass lenses and mirrors are far too thick and heavy for large-aperture space optics.” Hyde says. “Diffractive optics would make an ideal lens in space; they would revolutionize deep-space astronomy.”

Hyde conceived the approach of using diffractive lenses for large-aperture space optics in 1996. Since then, the concept has been studied...
under Laboratory Directed Research and Development funding and, more recently, with support from federal agencies. About eight researchers were assigned to the project from Livermore’s National Ignition Facility (NIF), Chemistry and Materials Science, Engineering, and Physics and Advanced Technologies directorates.

The project takes advantage of long-standing Livermore experience in manufacturing diffractive glass optics for high-power laser systems such as the Petawatt (see S&T, March 2000, pp. 4–12) and NIF, currently under construction at Livermore. NIF will use nearly 1,000 diffractive optics components, mostly of 40-centimeter-diameter size. A significant number of the components are being manufactured at Livermore, which has the only facility in the world that can make precision diffractive optics of more than a few centimeters in diameter.

Diffractive optics can be made so that they either reflect light (like a mirror) or transmit it. Mirrors pose serious disadvantages because they are extraordinarily sensitive to the slightest bump or ripple on their polished surfaces. A diffractive optic that transmits light, however, is not severely distorted by surface ripples produced during its operation. Light passing through a surface ripple experiences the same optical path as light passing next to the ripple, thereby virtually eliminating distortion. And by making the diffractive optic slow—that is, by focusing the incident light farther away from the optic—its surface ripple tolerance can be made up to 100,000 times greater than for mirrors.

No Motors Required

Mirrors also commonly require a stiff external skeleton or small motors to maintain their precise shape to within a few tenths of a nanometer. Such ancillary systems, which increase weight and complexity, are unnecessary in transmissive diffractive optics.

Furthermore, transmissive diffractive lenses are themselves more lightweight. Compared to traditional lenses, the amount of optical material that is required to focus light with a diffractive lens is quite small. For example, Hubble’s 2.5-meter mirror weighs 800 kilograms. A 25-meter mirror made more lightweight by removing all unnecessary bulk would still weigh 7,000 kilograms, far too bulky and heavy to be launched. Likewise, a 25-meter traditional glass lens would probably measure 6 centimeters thick and weigh about 45,000 kilograms. In comparison, a 25-meter diffractive lens made of 10-micrometer-thick plastic would weigh only 10 kilograms.

One of the challenges of fielding a large space telescope is finding a method for stowing it in a space launch vehicle whose diameter is smaller than the lens’s. The Livermore team has found in origami, the ancient Japanese art of paper folding, a promising approach to temporarily contract a lens made of many repeating segments. The principles of origami are commonly used for map folding as well as product packaging. The team has worked with origami expert Robert Lang to identify and then simulate several folding patterns for lenses of various sizes, including a 5-meter lens. The sequences necessary to compactly fold lenses of many segments have proved workable in prototypes using plastic and glass panels.

“It’s difficult to fold something that is curved, like a mirror. It’s much easier to fold something that is flat, like a diffractive lens, especially one that is made of many flat segments,” says Hyde. He cites concerns about whether a lens made of many fragile glass segments can survive the severe
Foldable Optics

The Livermore team found in origami, the ancient Japanese art of paper folding, a practical way to fold and store a lens made of many segments. The team identified and then simulated several folding patterns for lenses of various sizes.

Early in 2002, the team, guided by computer simulations, assembled a two-thirds scale model of a 5-meter lens using unpolished and unetched plastic panels and successfully demonstrated the origami-like folding pattern. The folding process used strings attached from an overhead structure and secured to individual panels. Four of the steps of the folding process are depicted here. The final step (not shown) was folding the lens into a configuration measuring 1.2 meters in diameter and about 55 centimeters high.

The best approach appears to be to separate the panels with soft, disposable packing material so that the panels don’t touch one another and then to pack the assemblage tightly.

A Color-Corrected Telescope

The team has been building and testing increasingly advanced diffractive lenses with materials that are considered suitable for space missions. They started by defining the requirements for a space mission, selecting and characterizing the best materials to make a diffractive lens, and developing fabrication technologies. Then they built a series of progressively larger diffractive telescopes and demonstrated a way to correct for chromatic (color) aberrations.

One of the great challenges of making diffractive lenses suitable for astronomical imaging, says Hyde, is that a diffractive Fresnel lens focuses different wavelengths of light at different points in space, thereby distorting the color characteristics of the image. Because of this effect, diffractive lenses are mostly used for applications needing only one wavelength—a monochromatic application—such as for lasers. In principle, chromatic aberrations can be eliminated by using a relay lens to reimage an object from the first diffractive lens onto a second diffractive lens, or inverse Fresnel lens, which then corrects the aberrations.

In 1999, the team developed a color-corrective optic and incorporated it into the first large-aperture diffractive telescope. The primary Fresnel lens was 20 centimeters in diameter and had a focal length of 20 meters. The lens was fabricated by a photolithographic process that etched a series of diffractive grooves into 10-millimeter-thick glass. The chromatic correction...
system included a 4-centimeter relay lens and a 2.2-centimeter inverse diffractive lens. The team demonstrated the color correction function of the system by bringing broadband light (from 470 to 700 nanometers) to a common focus. Without the correction system, numerous focal spots generated by the primary lens would span a 7-meter distance.

The team then used the telescope to obtain full-color images of the lunar surface, solar flares, Jupiter, and Saturn. “This telescope successfully demonstrated that diffractive lenses can be used for imaging over more than an extremely narrow bandwidth,” says Hyde.

Four years ago, Eyeglass received its first external funding, which was used to construct a 50-centimeter-diameter, color-corrected, f/100 (lens aperture setting) diffractive telescope. The relatively large diameter and slow f-number of this lens produced a 50-meter-long telescope. The team used the laser bay of the Laboratory’s now-disassembled Nova laser to provide a large, vibrationally and environmentally controlled beam path, which is needed for optically testing the telescope.

First Segmented Lens

Satisfied that they could manufacture diffractive telescopes capable of operating over all the wavelengths of visible light, the team began work on overcoming the packaging challenge for deploying a diffractive lens in space. Livermore physicist Sham Dixit, who oversaw fabrication and assembly of the Eyeglass lenses, notes that fabricating a single precision diffractive optic of 5 meters, let alone one measuring 25 meters, is far beyond current capabilities. However, even if the team could manufacture a 25-meter piece of glass, it could never be stowed in a spacecraft and launched into space. As a result, the Livermore team focused its efforts on designs that stitch many individual pieces into one large lens.

Dixit says the multipanel approach is attractive because it splits the fabrication task into two efforts: optical engineering for creating many meter-scale lens panels and mechanical engineering for precisely aligning and joining the panels. The use of multiple panels also provides a practical way to fold the lens because all folding occurs at metal joints connecting the flat panels. “The joint has to fold, but the panels do not,” says Dixit.

In 2001, in an attempt to demonstrate the feasibility of the multipanel approach, the team built its first segmented lens. The lens measured 75 centimeters in diameter and was assembled from six panels precisely aligned and joined to each other. In optical tests, the lens produced a tightly focused spot. Following this demonstration, the team folded the lens into the shape of a piece of pie, unfolded it into a flat lens again, and observed that the focal spot did not degrade from the folding–unfolding operation. “We achieved our goal of demonstrating that high-quality, thin, segmented diffractive lenses could be built with sufficient alignment and seaming accuracy,” says Dixit.

Hyde acknowledges some disadvantages to making a large lens from smaller pieces. The 2- to 4-centimeter gaps between the segments scatter a small amount of light that could obscure tiny details, for example, during an attempt to detect a planet rotating around a much brighter star. Also, the metal seams holding the panels together expand at a different rate than glass, thereby...
causing a small amount of distortion at
the panels’ edges. Nevertheless, Hyde
says, the advantages of a design of
multiple segments far outweigh the
disadvantages.

Last year, the team began work to
produce 72 glass panels and precisely
assemble them into a 4.7-meter
diffractive lens that could be compactly
packaged and deployed in space to meet
the space and weight requirements of
NASA and other federal agencies. “Our
objective was to fabricate a diffractive
lens that is lightweight, foldable, of high
resolution, and that can be scaled up for
larger space-based lenses,” says Dixit.

Panels Polished and Etched
To make the individual lens panels,
the team started with sheets of
commercial zinc borosilicate glass
measuring 1,150 by 850 by
0.7 millimeters. This type of glass was
selected because it is not expensive and is
widely used in laptop computer displays
and microscope slides. Forty 700- by
800-millimeter panels were required for
fabricating the 72 panels.

The glass sheets contained several
micrometer-deep ripples; they needed to
be smoothed to a flatness within about
0.1 micrometer to obtain the required
optical quality. Because traditional grind-
and-polish techniques are expensive and
become increasingly risky for thinner and
thinner sheets of glass, the team explored
other methods. The most promising
approach was a wet-etching method
developed by Livermore scientists Jerry
Britten and Mike Rushford. They
polished thin glass sheets using a
controlled application of acid etchant.
This technique polishes the glass without
stressing it. In 2001, the team
demonstrated the effectiveness of this
process and built a machine for
smoothing glass sheets.

The thin glass sheets were inscribed
with a precise pattern of 0.5-micrometer-
deep grooves. To inscribe the grooves,
the team used photolithographic surface-
patterning methods similar to those used
in the semiconductor industry. A coating
technique, developed at Livermore, laid
down a precise thickness of liquid
photoresist on the lens surface, and an
optical pattern was illuminated through a
mask onto the photoresist.

All told, the 72 panels contain
19,105 circular grooves. The grooves,
about 0.5 micrometer deep, range from
60 micrometers to several millimeters
wide. The grooves are arrayed
centrically, starting from the
centermost panels and continuing to the
perimeter of the outermost panels. The
concentration of grooves ranges from
about 1 line per centimeter at the very
center of the assembled lens to about
16 lines per millimeter at the outer edge.

Assembling the Panels
The 72 lens panels were cut into
precise rectangular and triangular shapes
for assembly into the complete lens.
The assembly, done by a group led by
engineer Andrew Weisberg, used the
same process demonstrated on the
75-centimeter lens but upgraded to
account for the larger size, panel count,
and tolerance requirements of the
5-meter lens. Dixit notes that when
working on individual panels, one must
never lift them by the edges but rather slide them on a smooth backing, much like using a pizza paddle.

Once a panel was in the proper location, it was joined to its neighbors by gluing each piece to foldable metal. Having panels out of register, says Dixit, would be disastrous to image quality. Precision alignment can be ensured by matching fiducials (tiny marks) etched along the common borders of neighboring panels to a precision of 1 to 2 micrometers. About 250 micrometers thick, the seams can withstand forces much greater than those it would likely experience during deployment in space.

The assembled 5-meter lens has a focal length of 250 meters and an optical speed of f/50. Its 72 panels include 16 rectangles measuring 654 by 790 millimeters, 32 right triangles measuring 327 by 790 millimeters, and 24 isosceles triangles measuring 654 by 790 millimeters. The panels form eight “petals,” each consisting of three isosceles triangles, four right triangles, and two rectangles. Each petal covers 45 degrees, or one-eighth of 360 degrees.

With this configuration of repeating triangles and rectangles, the entire lens can be folded in an intricate but foolproof manner and fit into a hatbox measuring 1.75 meters in diameter and about 80 centimeters high. The team gained confidence in the folding patterns by building subscale models from plastic and glass panels.

Following assembly, the lens was mounted in a steel frame and a mesh of aluminum bars on each side to keep the lens rigid for transportation to an outside testing location and to protect it against winds. Although the team verified the characteristics of the individual panels during the fabrication and assembly process, optically testing the complete lens was still required.

Upon delivery at its testing location, the horizontal lens was lifted by a crane to a vertical position and then secured.
On the Map

The lens is, by a wide margin, the largest optical-quality lens in the world. For example, it has twice the diameter of the primary mirror for the Hubble Space Telescope, yet is 10 times lighter.

“A 5-meter lens is a big-league optic. Demonstrating such a large Fresnel lens places diffractive optics firmly on everyone’s map,” says Hyde. “By making the lens from technology that is scalable to much larger sizes and from space-deployable materials, we have demonstrated the technology and the here-and-now reality of diffractive telescopes.”

A 5-meter diffractive space telescope could be deployed in space within two to three years, says Hyde. A 25-meter or larger version could be deployed within a decade.

The team is exploring preliminary partnerships with U.S. agencies that could benefit from diffractive telescopes. Discussions have focused on design, technology development, and demonstrations of lenses of 5 meters and larger. Hyde also plans to establish partnerships with traditional space contractors. The Livermore role in these partnerships would be to support the optical and deployment designs and serve as the fabrication house for the lenses.

One option under exploration is obtaining even thinner glass sheets to save additional weight. Another option is fashioning a lens from segments made of polymer films. A plastic lens would be less prone to damage from launch vibration, would weigh less, and could be fashioned from multiple panels that are larger than their glass counterparts. The Livermore team has carried out research on polymer films and done etching on several meter-size panels.

Hyde adds that the technology developed at Livermore could be used for more than astronomy. Lightweight diffractive optics of greater than 10 meters would likely be used in applications such as Earth observation and optical communications. Closer to home, “Everything we’re learning about making diffractive optics benefits the National Ignition Facility and high-powered lasers everywhere,” he says.

The Livermore team has put diffractive telescopes on the map. The next job is putting them into space.

—Arnie Heller

Key Words: diffractive telescope, Eyeglass, Eyepiece, Fresnel lens, Hubble Space Telescope, Magnifying Glass, National Ignition Facility, photolithography.

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For more information about diffractive optics:
www.llnl.gov/nif/lst/diffractive-optics/newtecheye.htm
Livermore physicists, including George Chapline and Edward Teller (Physical Review D 8, 4302–4308). They predicted that experiments using Lawrence Berkeley National Laboratory’s Bevelac, then the most powerful particle accelerator for heavy nuclei, would probably result in the “production of matter in a new regime of temperature and density.”

They recognized that “since the experiments explore regions very far from our experience, it is reasonable to expect surprises.” In fact, they surmised that the main result of the experiment would be the “unexpected phenomena.” That is what great science is often all about.

The Experiment Today

More than 25 years later, in 1999, physicists from institutions all over the world believed they might have finally established the laboratory conditions required to create not only the hot and dense region described in 1973 but also a new phase of matter. (See the box on pp. 8–9.)

Beams of gold ions or nuclei—atoms that have been stripped of their electrons—are propelled around RHIC’s loops in opposite directions at 99.9 percent of light speed. When any two nuclei collide, the collision acts as a pressure cooker, liberating more than a trillion electronvolts of energy in a volume the size of an atomic nucleus. Some of the energy each nucleus had before the collision is transformed into intense heat and new particles such that new matter is created at a temperature ten thousand times that of the Sun. The collisions are highly explosive, and if a quark–gluon plasma is created, it decays into particles (bound quarks) almost as quickly as the plasma is formed.

To determine whether a quark–gluon plasma existed during an experiment, scientists look for signatures in the distribution and composition of the particles that reach the Pioneering

![Aerial photograph of the 3.8-kilometer-circumference Relativistic Heavy-Ion Collider and associated particle accelerators at Brookhaven National Laboratory.](image)

(a) A schematic of the Pioneering High-Energy Nuclear Interaction Experiment (PHENIX) detector. (b) Inside the PHENIX detector.
High-Energy Nuclear Interaction Experiment (PHENIX) detector, which Livermore helped to design and build during the 1990s.

“If the experiment continues according to plan, we will have made a quark–gluon plasma,” says Livermore physicist Ron Soltz, a principal investigator for Livermore’s work at RHIC. “What we’re essentially trying to do is find the boiling point of nuclear matter.”

(a) Inside Brookhaven’s Relativistic Heavy-Ion Collider, two gold nuclei approach one another at almost the speed of light. Traveling at relativistic speeds causes them to look flat rather than spherical. (b) As the two nuclei collide and pass through each other, some of the energy they had before the collision is transformed into intense heat and new particles. (c) If conditions are right, the collision liberates the quarks and gluons in the nuclei to form a quark–gluon plasma. (d) As the area cools off, thousands more particles form. Many of these new particles will travel to a detector where their distinctive signatures give physicists clues about what occurred inside the collision zone.

### Measuring Success

Soltz’s team, including physicists Stephen Johnson and Ed Hartouni and postdoctoral fellows Mike Heffner and Jane Burward-Hoy, are measuring the volume, lifetime, and violence of the collision zone (or source). A large volume and long lifetime are one of the purported signatures of a quark–gluon plasma. To take the measurements, the team examines the production of pions, a two-quark particle that is the most prevalent product of these collisions. The team is exploiting a simple property of quantum mechanics, which is that the more highly correlated the pions are in a given direction, the larger the emission volume is along that axis. A long-lived source should appear as an apparent elongation of the fireball in the direction of the detector relative to the geometric radius of the fireball. The Livermore team found almost no elongation, in contradiction to most recent theoretical expectations.

However, the story does not end there. Even before the Livermore team had finished its analysis, other collaborators were finding signs of the plasma in another signature.

“If no plasma is formed, particles with high momentum escape the collision unscathed,” notes Johnson. “But if a quark–gluon plasma has been created, the interaction between high-momentum particles and the medium increases dramatically, significantly lowering the velocity of the particles.”

Quantum chromodynamics theory (see the box on p. 7) predicts that in the presence of a quark–gluon plasma, a paucity of high-momentum particles during the collision of gold nuclei, which is the result of an opaque source, is consistent with theory and indicates the existence of a quark–gluon plasma.

Results from the STAR and PHENIX detectors show that the elongation of the collision zone (indicated by the ratio of two radii) was considerably less than theory predicted. In fact, there was no elongation at all, with ratios of about 1.
substantially fewer high-momentum particles will make their way to the detector. That relatively low number is, in fact, what PHENIX found by counting high-energy pions.

So right now, the data are inconclusive. “Obviously, we need more information,” says Soltz. “We’re considering two options at this point. One is to study rarer particle signatures, which would require a lot of data that we don’t have. The other option is to go to a simpler experiment whose results will be easier to interpret.”

A Simpler Experiment

When two gold nuclei collide, many interactions occur between all of the nucleons (protons and neutrons). Although these numerous interactions are responsible for creating the conditions necessary to form a quark–gluon plasma, researchers have difficulty differentiating between signals resulting from the plasma and those that may be caused by other interactions of the nucleons.

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**Atomic Parts and Particles**

All things, living and inanimate, are made of atoms. Almost all of an atom’s mass is in its nucleus, where protons and neutrons reside. Protons and neutrons consist of various combinations of quarks. At the moment, scientists believe that quarks are the smallest particles in our universe and that they form the basis for all matter. However, just as scientists until the late 19th century believed that the atom was the smallest particle, they may someday discover particles smaller than quarks.

In the meantime, theory holds that quarks, with the help of gluons to hold the quarks together, make up everything in the nuclei of atoms. Up, down, charm, strange, top, and bottom—these are the six “flavors” of quarks. Up and down quarks are the least massive and are more prevalent than other types. Protons always have two up quarks and one down quark, whereas neutrons have two down quarks and an up quark. Other more exotic and more massive particles are composed of other quark combinations. A lambda particle, for example, has an up, a down, and a strange quark, while a kaon has a strange and an up quark. Gluons carry the strong force that glues quarks together to form protons, neutrons, and other particles and keeps them together in an atom’s nucleus.

In contrast, the electron is not made of quarks and is not subject to the strong force. Instead, the electromagnetic force keeps an electron in its orbit spinning around an atom’s nucleus.

After discovering that the atom was not the most elementary particle, scientists realized that subatomic particles behave differently from larger, bulk quantities of matter. The field of quantum mechanics was developed to explain this apparently eccentric behavior.

Then they discovered quarks and gluons, whose existence was first inferred from the spectra of elementary particles and from electron-scattering experiments in particle accelerators. Quarks and gluons possess a type of charge that has been whimsically termed color. Color is the source of the powerful forces that first cluster the quarks and gluons to make protons and neutrons and, in turn, grip these nucleons to one another to form atomic nuclei. A new theory, quantum chromodynamics, was developed late in the 1960s and early 1970s to describe these phenomena.

Quantum chromodynamics, which explains the strong force, bears many similarities to quantum electrodynamics, which explains electrical charges and light. Atoms can be ionized and the fundamental electrical charges of quantum electrodynamics can appear in isolation, but in quantum chromodynamics, the fundamental quark and gluon constituents of protons and neutrons can only be liberated in conditions identical to those of the big bang. This property of quark–gluon confinement gives stability to all matter as we know it.

Quantum chromodynamics theory predicts that deconfinement will occur at sufficiently high temperatures, nuclear densities, or both. Quarks and gluons will break free of their bondage in atomic nucleons, re-creating the earliest moments of our universe.
Simpler to study than the collision between two nuclei is a collision between a single proton and a nucleus. While one proton may have several interactions within a nucleus, scientists do not expect that these interactions will create a plasma. But exactly how many such interactions are there? Finding the answer to this question for each proton–nucleus collision will allow scientists to make proper comparisons with the results from nucleus–nucleus collisions. If scientists can measure the number of interactions, they should be able to verify the underlying signatures of a quark–gluon plasma.

Under Johnson’s leadership, the Livermore team has begun adding a detector to PHENIX that will make these measurements in proton–nucleus collisions. The new detector is a calorimeter that measures the pieces of the fragmenting nucleus after a proton has blasted through it. To provide this entirely new capability in short order at a minimal cost, the Livermore group adopted detectors and equipment from previous Brookhaven experiments. The result is what they jokingly refer to as the “Scrounge-a-Cal.” The calorimeter is being instrumented in PHENIX now, and the first results will be analyzed this spring.

Answering Quark Questions

Research at Brookhaven and elsewhere is beginning to answer some new and old questions about quarks. Researchers at the National Aeronautics and Space Administration’s Chandra X-Ray Observatory recently discovered what appears to be a collapsed star with

PHENIX and RHIC Rise

Only massive experimental equipment such as the Relativistic Heavy-Ion Collider (RHIC) and the Pioneering High-Energy Nuclear Interaction Experiment (PHENIX) detector at Brookhaven National Laboratory make it possible to study the almost infinitesimally small dot known as the quark.

An inverse relationship exists between the size of the object being studied and the size and expense of the equipment needed to examine it: the smaller the object, the greater the energy needed to probe it, and thus, the larger the equipment required. Particle and nuclear physicists, who want to examine the fundamental building blocks of matter up close, need hugely expensive machines often measuring a kilometer or more in diameter. Given their expense and size, few such machines can be built. Many nuclear and particle physicists must concentrate their efforts on the few particle accelerators and colliders available around the world.

Lawrence Livermore is just 1 of 55 institutions from 11 countries involved in the quark–gluon plasma experiments being performed on the PHENIX detector at Brookhaven. There are 450 scientists participating, each

![PHENIX and RHIC Rise](image_url)

A schematic of the Relativistic Heavy-Ion Collider (RHIC) complex.
a quark core. If accurate, this discovery complements the current search for the quark–gluon plasma at RHIC. It also confirms a prediction made 25 years ago by Livermore physicist Chapline about extremely dense stars with a quark–gluon plasma at their core rather than the bound quarks usually found in neutron stars.

Equally important—for basic science and a better understanding of how our universe got started—the experiments at Brookhaven’s RHIC hold the key to answering one of the questions posed recently by the National Research Council Committee on Physics of the Universe. In its report, *Connecting Quarks with the Cosmos: 11 Science Questions for the New Century*, number 7 on the council’s list was “Are there new states of matter at ultrahigh temperatures and densities?” Livermore researchers and their collaborators hope to answer that question soon.

—Katie Walter

**Key Words**: Brookhaven National Laboratory, particle physics, Pioneering High-Energy Nuclear Interaction Experiment (PHENIX) detector, quark–gluon plasma, Relativistic Heavy-Ion Collider (RHIC).

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www.bnl.gov/RHIC

The team celebrates completion of testing of the PHENIX detector.
An Elusive Transformation

The Mystery of Oscillating Neutrinos

An experiment to determine whether one type of neutrino spontaneously transforms into another type will improve understanding of particle physics and the forces that guide the universe.

Neutrinos are enigmas in the world of particle physics. Cosmically created in stars and supernovas, produced by cosmic rays colliding with the Earth’s upper atmosphere, and unleashed in nuclear reactors and in the detonation of nuclear weapons, neutrinos are one of the most pervasive forms of matter in the universe. They are also elusive and difficult to detect. Unlike other particles in the pantheon of particle physics, neutrinos almost never interact with other forms of matter. These chargeless, seemingly massless particles stream through space, planets, and solid walls, leaving nary a trace.

Even as scientists invent ways to measure the occasional rare interaction as a means of studying neutrinos, the mystery surrounding these elusive particles intensifies. For instance, scientists now know that three types of neutrinos exist—the electron neutrino, the muon neutrino, and the tau neutrino, which are related, respectively, to the common electron and the less common muon and tau particles. The fusion process—the process that powers our Sun—produces electron neutrinos, and scientists have calculated how many electron neutrinos should arrive on Earth. But more than two decades of experiments have found less than half the predicted number. The same conundrum appears with the neutrinos produced by cosmic rays. Theory says that twice as many muon neutrinos should exist at ground level as electron neutrinos because of the interaction of cosmic rays with the upper atmosphere. But experiments find muon and electron neutrinos in about equal measure.

So where are the missing neutrinos?

Neutrinos, they are very small.
They have no charge and have no mass
And do not interact at all.
The earth is just a silly ball
To them, through which they simply pass,
Like dustmaids down a drafty hall
Or photons through a sheet of glass.
They snub the most exquisite gas,
Ignore the most substantial wall, . . .

—From John Updike’s “Cosmic Gall,” which originally appeared in The New Yorker and was published in Telephone Poles and Other Poems (Knopf: 1960, 1988).

In the late 1950s, physicists first suggested that neutrinos might be able to transform from one type to another. If true, this transformation would explain the “missing” particles. Even more importantly, these oscillations would prove that neutrinos are not massless—as originally theorized in the 1930s by physicist Wolfgang Pauli and declaimed in 1960 by writer John Updike—but “weigh” something after all, albeit very
little. (See the box below.) If the electron neutrino has a mass, it would be less than one-hundred-thousandth that of the electron.

If these subatomic particles do indeed have mass—and more and more evidence seems to point in that direction—that fact will have vast implications for understanding cosmology and for the prevailing physics theory that describes the elementary particles and forces of the universe.

Since measuring neutrino mass directly is beyond present-day technology, scientists must use indirect methods, such as determining whether neutrino oscillations occur. A team from Lawrence Livermore—including physicists Peter Barnes, Douglas Wright, and Edward Hartouni—are part of an international collaboration of 200 scientists from 26 institutions taking part in an experiment centered at the Fermi National Accelerator Laboratory (Fermilab) to look for neutrino oscillations and begin to understand their particulars. Results from the Main Injector Neutrino Oscillation Search (MINOS) will help illumine the nature of neutrinos and, ultimately, the universe.

MINOS to Shed Light on Mystery

The job of detecting neutrino oscillations is a daunting one. The neutrinos must travel far enough (that is, travel a long enough time at nearly light speed) for a significant portion of them to change into a different neutrino type. The beam of neutrinos must also be intense enough to produce measurable interactions at the detector, because the neutrino beam, like a flashlight beam, will fan out over distance, going from about 30 centimeters wide about 1 kilometer from the source to nearly 1 kilometer wide at a detector over 700 kilometers away. Finally, out of 5 trillion neutrinos a year passing through the detector, only about 9,000 will interact and produce a measurable signal.

The MINOS experiment will use a beam of neutrinos generated at Fermilab,
40 miles west of Chicago, one of the few facilities able to generate a beam intense enough for the experiment. Fermilab is constructing a new particle beamline to direct a nearly pure beam of muon neutrinos at a detector deep in a former iron mine in Soudan, Minnesota, 735 kilometers away. “Fermilab will tune the beam to an energy spectrum of 0.5 to 8 gigaelectronvolts,” says Barnes, “which, according to calculations, is the energy range that allows the most neutrino oscillations for the distance the beam needs to travel to the ‘far’ detector.”

Before reaching Soudan, though, the neutrino beam will zoom through a smaller “near” detector a mere 1 kilometer from the beam source. This detector will measure how many muon neutrinos are at each energy. During the next 2 milliseconds, the beam will flash beneath northern Illinois and Wisconsin—2 milliseconds during which some of the muon neutrinos are expected to oscillate into tau neutrinos. The beam will then encounter the far detector, 800 meters deep in the Soudan mine. Some of the remaining muon neutrinos—about one in a million—will interact with the detector. “We won’t be able to identify the tau neutrinos,” explains Barnes, “but we will see a decrease in the number of muon neutrinos, and we’ll be able to measure how many remain at each energy. The decrease will tell us that some of the muon neutrinos in the beam have changed into another type. The oscillations will help confirm that neutrinos have mass.”

Physicists hope to uncover other details about the nature of neutrino oscillations as well. For instance, they hope to discover the oscillation probability of the beam—that is, the fraction of a beam that can change from one type to another at a given energy—by measuring the fraction of oscillations at each energy. In addition, they hope to determine the oscillation length, which is the distance a beam of neutrinos of a particular energy must travel to transform from one neutrino type to another and back again.

**Down in the Mine**

The experiment itself is impressive enough—but putting it all together presents another set of challenges no less daunting. A key issue is how to design the steel planes of the detectors. Each plane is 8 meters in diameter and weighs 10,000 kilograms, and 450 of them must be transported 800 meters underground. Plus the only access and egress underground is a mine shaft 2 meters across.

Several designs were put forth by different collaborators, including making the plate in one long, coiled strip—like an old-fashioned watch spring—that could be uncoiled and snaked downhole. Because much of the Laboratory’s research has coupled physics and engineering, Livermore’s Douglas Wright, a physicist with engineering training and experience, was selected to lead the steel design work for the MINOS collaboration. By 1995, Livermore engineers Marcus Libkind and Johanna Swan came up with the selected solution: make the planes from plates of steel—2 meters across, 8 meters long and 1.25 centimeters thick—that could be uncoiled and snaked downhole. This concept was fully developed at Livermore by engineer Tony Ladran (now with Lawrence Berkeley National Laboratory). The crucial feature of the design is that each plane is composed of...
two layers of steel formed by strips laid at right angles. The two layers are joined by welds through precut holes in the steel. The technique results in a monolithic plane that is exceedingly flat and magnetically similar to a solid plane.

Even this solution presented challenges. The long, wide, thin plates were the steel equivalent of strips of paper. Unfortunately, unlike paper, which can bend but keep its structural integrity, steel doesn’t have as much yield strength, and excessive bending causes it to tear. Also, once assembled, the steel planes could not be simply mounted on the floor with all the weight on the bottom edge. In addition, the edges all around the detectors had to be kept free for optical and electrical cables to snake in and out.

But how can 450 such planes be supported so they don’t buckle under their own weight? The answer lies in a filing cabinet, says Barnes. “We decided to suspend them like hanging file folders, using two metal ears on each plane that rest on metal rails.” For each plane, 9,000 kilograms of steel plate and 900 kilograms of plastic scintillator strips are supported on two 5- by 10-centimeter areas, one under each ear, resting on 10-centimeter-wide rails.

By July 2003, the entire detector system will be assembled in the mine. Fermilab is using the same design on a smaller scale for the near detector, and the MINOS experiment is expected to be up and running in early 2005.

**Bring on the Beam**

Livermore is also a key participant in another MINOS-related effort to look at exactly what happens in creating the neutrino beam—or indeed, any beam of particles. The answers will have important ramifications for Livermore’s basic science and stockpile stewardship missions.

To produce neutrinos for MINOS, a 120-gigaelectronvolt proton beam will slam into a graphite target, producing pions and other particles as well. Because

**Livermore engineers and physicists worked together to come up with a design that would allow sections of the 450 detector planes to be lowered into the mine and assembled underground. All equipment must be broken down to fit into the 2 meter by 2 meter shaft and then reassembled underground.**
pions—precursors to muon neutrinos—are charged particles, they can be focused with magnetic fields and directed into a vacuum pipe of sufficient length to give them time to decay into neutrinos. (See the box at the right.)

“The focusing properties of pions are well understood,” says Barnes. “Propagation in the decay pipe is also well understood. What isn’t well characterized is the nature of the stuff produced at the target by the proton beam. How many of what particles? And at what angles do they leave the target and at what energies? We need to characterize these details better. In addition, we know that the muon neutrino

### Recipe for a Neutrino Beam

1. Take a beam of 120-gigaelectronvolt protons.
2. Aim the beam on a graphite target, where the protons can interact with the carbon atoms.
3. Take the beam produced from this interaction (which will contain mostly pions and kaons), and use magnets to focus the positively charged particles.
4. Direct these positively charged particles down a decay pipe. The pions will decay into muons and muon neutrinos. The kaons will also decay into muons and muon neutrinos and sometimes into electrons and electron neutrinos as well.
5. Send the subsequent beam through 229 meters of rock and steel to remove unwanted particles and muons.

Result: A beam of muon neutrinos, with a few scattered electron neutrinos.

A CAUTION TO THE COOK: Neutrinos, being neutral, cannot be steered, so be sure your focusing system and decay pipe are pointing in the direction of the desired beam. For the Main Injector Neutrino Oscillation Search (MINOS) experiment, point the pipe 3 degrees down and north-northwest toward Minnesota.
beam produced in the decay pipe is not pure—it contains some electron neutrinos. We need to know more about these particles as well.”

Because the beam will be only 30 centimeters in diameter at the MINOS near detector, the entire beam will pass through it. But only a small fraction of the beam ends up aimed at the far detector, explains Barnes. “Since the beam spreads out to a diameter of 1 kilometer at the far detector, we won’t be measuring the whole beam. We need to know the angular distribution of the particles produced at the target and their energy spectrum. This information will help us understand the differences between the whole beam seen by the near detector and the subset seen by the far detector.”

The lack of information about the particle production of the proton beam is the largest systematic uncertainty in the MINOS system. Details of particle production also turn out to be important for other efforts where particle beams interact with targets, such as future accelerator concepts like muon colliders and Livermore’s stockpile stewardship work with proton radiography. (See the box below.)

To better understand the details of particle production, Livermore is leading the Main Injector Particle Production (MIPP) experiment in collaboration with Fermilab and a group of 10 universities, colleges, and institutes of technology. In preparing for MINOS, MIPP will examine what happens when 120-gigaelectronvolt protons hit graphite targets. Beams of protons, kaons, and pions at energies from 5 to 100 gigaelectronvolts will also be generated to examine particle production on target materials as diverse as hydrogen and lead. The experiment, which takes place at Fermilab, is just getting under way. MIPP begins this summer and will continue until MINOS comes on line.

**Bringing in the Next Generation**

In addition to providing results of interest to basic science and stockpile stewardship efforts, the MIPP and MINOS experiments are introducing postdoctoral fellows and others just entering the field of high-energy nuclear and particle physics to some of the work being done at Livermore. Barnes explains, “Most of the particle and high-energy nuclear physics experiments take a long time to plan and execute. One set of postdoctoral fellows works on the early part of the experiments—setting up the systems, doing early calculations, and so on—and then, years down the road when they’ve moved on, another set comes in to better understand the details of particle production, Livermore is leading the Main Injector Particle Production (MIPP) experiment in collaboration with Fermilab and a group of 10 universities, colleges, and institutes of technology. In preparing for MINOS, MIPP will examine what happens when 120-gigaelectronvolt protons hit graphite targets. Beams of protons, kaons, and pions at energies from 5 to 100 gigaelectronvolts will also be generated to examine particle production on target materials as diverse as hydrogen and lead. The experiment, which takes place at Fermilab, is just getting under way. MIPP begins this summer and will continue until MINOS comes on line.

**Proton Radiography**

In addition to supplying information critical to the Main Injector Neutrino Oscillation Search (MINOS) experiment and other basic physics experiments, results from the Main Injector Particle Production (MIPP) experiment will contribute to Livermore’s stockpile stewardship efforts. For seven years, Livermore has been exploring whether beams of high-energy protons could be used to create three-dimensional images or movies, much the way that x rays are used to create medical computed tomography scans. (See S&TR, November 2000, pp. 12–18.)

Such proton radiographic systems could be used in stockpile stewardship to image deep inside dynamic systems and obtain information about materials too dense for x rays to penetrate. One of the roadblocks to using proton beams is the tendency for protons to scatter at small angles off other particles, leading to blurry images. In 1995, researchers at Los Alamos National Laboratory came up with the idea of using a magnetic lens to refocus the charged protons, much as an optical lens refocuses a blurry image.

Such focusing techniques can be effective but present another problem. Just as MINOS physicists need to understand the scattering processes in detail, so physicists need to understand the scattering processes of proton radiography in detail. The beam that reaches the film also contains other particles produced as the beam passes through the target material. “We need to better understand these other particles,” says physicist Peter Barnes. “Some of them reach the radiographic film and add their own signal. Not only do they blur the image, but their added signal also lightens the image, making the imaged materials appear to be less dense than they really are.”

Because sharpness and density of image are critical to interpreting what is happening inside these complex systems, stockpile stewards need to know what the secondary particles are and how they affect the final image. MIPP will provide a more complete picture of the particles produced, including their energy spectrum and angular distribution.
and gathers and interprets the data. But for MIPP, we started work a year ago and now we’re almost ready to take data. It’s a three-year project, from building the system, to taking data, to producing a paper. It has a much shorter cycle than most experiments, allowing someone in a postdoctoral position to be involved in the project from start to finish.” Through MIPP, a new generation of researchers is introduced to the Laboratory.

“The work on neutrino oscillations and proton radiography is a good example of how the Laboratory integrates basic science research with its missions,” says Barnes. “Ultimately, the answers gained about neutrino oscillations through MINOS will connect to the early history of the universe. With MIPP, we’re supporting that search for answers as well as supporting the Laboratory’s stockpile stewardship work. It’s a perfect example of what high-energy physics at the Laboratory can achieve.”

—Ann Parker

Key Words: Fermi National Accelerator Laboratory (Fermilab), high-energy physics, Main Injector Neutrino Oscillation Search (MINOS), Main Injector Particle Production (MIPP), neutrino oscillation, particle physics, proton radiography.

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For more information on the MINOS experiment, see:
www-numi.fnal.gov/index.html
A New Way to Measure the Mass of Stars

When an international collaboration began a search for dark matter in the Milky Way Galaxy, measuring a star’s mass was not the goal they had in mind. But as the team examined more closely the massive compact halo objects (MACHOs) they had found, they realized that all the information they needed for measuring a single, isolated stellar mass was right in front of them.

Measuring the mass of a star or a satellite such as planets or moons used to be a relative affair: How does the presence of one body affect the position of the other? The movement of the Sun as the Earth and other planets revolve around it is largely a function of their relative masses. The same is true for our Moon as it revolves around our home planet. New discoveries about the existence of planets around other stars are inferred by observing wobble in a star’s position. More wobble means more mass is revolving around it. Careful observations of the wobble can reveal how many planets are acting on the star.

Astrophysicist Kem Cook, who leads the Livermore contribution to the team, notes, “Measuring the mass of a star has never been possible when it was in physical isolation. Always before, we were looking at two bodies—the Sun and Earth or binary stars. Now we can do just one, but it takes lots of time and data.”

The Critical Image

From 1992 to 2000, the MACHO collaboration, including researchers from the U.S., Australia, Chile, Germany, Britain, and Canada, searched the outer regions of the Milky Way for MACHOs using the Large Magellanic Cloud (LMC) as a backdrop (see the box on p. 22). They were looking for events in which the gravitational field of a MACHO came between their detector and a distant star, causing the distant star to brighten significantly. Gravity acts as a lens in a process called microlensing. Six years of observational data have been analyzed thus far, revealing 17 microlensing events in the Milky Way’s halo, including the first event ever positively identified.

Of particular interest was the brightest event, known as LMC-5. The distant, or source, star became at least 15 times brighter when it was behind the microlensing object. The unmagnified color of the patch of sky occupied by both the lens and the source star was redder before and after the peak of the microlensing event. Researchers suspected that the source star was a blue star in the LMC that, because of atmospheric blurring, was confused with a red star, whose color and brightness suggested a red dwarf star in the Milky Way.

To better characterize the source stars of all microlensing events, the team obtained images taken by the Hubble Space Telescope, which operates well above Earth’s atmosphere. The 1999 Hubble image for the LMC-5 region, taken 6.3 years...
after the peak of the LMC-5 microlensing event in February 1993, revealed a faint red object in addition to the source star. The two stars were still so close to one another that even on the Hubble image, they appeared slightly blended.

The team went back to reexamine the details of the LMC-5 microlensing curve. By analyzing perturbations in the curve caused by Earth’s movement around the Sun, they were able to predict the direction that the lens would move across the sky. They found that the red star shown in the Hubble image was in the place that their calculations predicted and must be the lens. But the team didn’t stop there.

**Adding It All Up**

Over 30 years ago, researchers suggested that gravitational microlensing could be used to measure the masses of nearby stars, although no one had yet seen a microlensing event in action.

Data collected in microlensing events are insufficient to measure the mass of the lens: The duration is proportional to the mass of the lens, the relative distances of the lens and the

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**The Search for MACHOs**

Massive compact halo objects (MACHOs) are thought to be one kind of the invisible dark matter that surrounds and permeates our galaxy and other galaxies like it. Astronomers have determined that the Milky Way Galaxy must be much more massive than the amount of mass that is visible. Without the additional mass, the galaxy would fly apart. In fact, as much as 90 percent of the Milky Way’s mass cannot be detected with available techniques. There is no question that dark matter exists. Finding it is the challenge.

Earlier studies suggested that MACHOs would produce gravitational microlensing, a process by which the gravity of one object comes between an observer and a distant star and causes the light of the distant star to be briefly magnified. Because a microlensing event requires that the two bodies be lined up almost perfectly, microlensing events are quite rare. Although a star could act as a microlens, the relative lack of stars in the outer regions of the Milky Way made it likely that any microlenses seen would prove to be MACHOs.

Using the Large Magellanic Cloud (LMC) Galaxy as a backdrop of distant, or source, stars, researchers from around the world searched for MACHO microlensing events with a special camera developed at Livermore. Scientists monitored millions of stars in the LMC at Mount Stromlo Observatory in Canberra, Australia, from 1992 to 2000. This observatory was chosen because the LMC is only visible from the southern hemisphere.

By observing whether the brightness of any source stars varied over time as a gravitational lens passed between the star and the observatory’s detector, the team identified numerous microlensing events toward the Large Magellanic Cloud. Their data to date indicate that between 8 and 50 percent of the Milky Way’s mass is in the form of MACHOs.

Using Hubble Space Telescope images to more closely examine the source stars of LMC microlensing events, the team has thus far found that only LMC-5 involved a visible star acting as a lens. All the rest were apparently caused by the gravitational field of a MACHO.

Astronomical research came to a screeching halt at the Mount Stromlo Observatory in January 2003 when a raging bush fire destroyed many buildings, including four telescopes, computers, and a spectrograph being constructed for the 8.2-meter Gemini North telescope in Mauna Kea, Hawaii. The fire destroyed about one-third of Australia’s astronomical research program.
source star from Earth, and the motion of the lens across the line of sight of the source star.

With LMC-5, much more information was available, thanks to the image from the Hubble Space Telescope. “If we assume that the red star is the microlens and the other star is the source star, then we have a physical measurement on the sky of the motion of the lens,” says Cook.

The team had already determined the apparent direction and motion across the line of sight of the lens from the distortion in the light curve due to the motion of the Earth. Combining that information with the known distance to the Large Magellanic Cloud, which is very shallow, and the time between the original image and the Hubble image, allowed them to determine the distance the lens had traveled and, hence, its velocity. With the Hubble image—the first ever of a microlens scooting across the heavens—the team had all of the elements needed to determine the distance of the lens and its mass. They found that the mass of the LMC-5 lens was about one-tenth the mass of the Sun.

**A Better Way Soon**

An even better way to measure the mass of stars will be available in 2009 or so when National Aeronautics and Space Administration launches the Space Interferometry Mission (SIM). SIM will use optical interferometry to measure the tiny, apparent motion of stars, which is caused by microlensing, to determine the masses and distances of stars with much greater accuracy than previously possible. Measuring the mass of individual stars with data from SIM will be a veritable walk in the park.

—Katie Walter

**Key Words:** gravitational microlensing, massively compact halo objects (MACHOs).

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When Every Second Counts
Pathogen Identification in Less than a Minute

WHEN there’s anthrax in the air—or indeed, any pathogen—the sooner one knows, the better. Ideally, a detector would identify the pathogen in time to take action, an interval referred to as detect-to-warn, which is generally considered to be a minute or less.

Commercial systems exist that can identify airborne pathogenic spores, but they take days or, at best, hours to produce results. Far too long to hold one’s breath.

A system being developed by Lawrence Livermore to identify such spores—the bioaerosol mass spectrometry (BAMS) system—recently broke that critical 1-minute time barrier. Livermore chemist Eric Gard heads up a team developing this mass-spectrometry technique, which can successfully distinguish between two related but very different spore species. It can also sort out a single spore from thousands of other particles—both biological and nonbiological—with no false positives.

The biomedical aspects of this work are funded by the Laboratory Directed Research and Development (LDRD) at Livermore, and the biodefense aspects are funded by the Technical Support Working Group and Defense Advanced Research Project Agency of the Department of Defense.

When Time Is of the Essence

The premise of a detect-to-warn system is to allow time to react. “A minute gives people enough time to put on masks, leave the room, hold their breath. The challenge was to actually make a device that could provide answers in less than a minute,” explains Gard.

Coming up with techniques for identifying pathogens in such a short time has proved difficult for a number of reasons. The small size of the particles involved can, of itself, make rapid detection difficult because they can be widely dispersed in the atmosphere. For example, an aerosol particle containing a single Bacillus anthracis spore has a mass of approximately one-trillionth of a gram. Of the methods available to detect anthrax and other airborne uglies, most take hours, even days, to yield results, making timely actions impossible.

The issue of false alarms is also critical—some techniques have difficulty separating organisms that are benign from those that are pathogenic but very similar. The situation becomes even more complicated because some pathogens, such as smallpox, are highly contagious, requiring just a few organisms to infect a person. The system should ideally be sensitive enough to find and identify a single particle among other naturally occurring background particles, which could be present at concentrations thousands of times higher.

The BAMS technique, which Gard and others have been working on for nearly five years, can successfully identify a single airborne particle in about 100 milliseconds. This technique has other applications as well, Gard notes. “In the future, BAMS could also be used as a medical diagnostic to, for instance, track small subpopulations of cancerous cells that deviate from their normal development cycle. As such, BAMS may make far-reaching contributions in the fields of oncology, microbiology, and public health.”

Zap ‘Em with Lasers

BAMS operates by sucking air and any particles (dust, spores, smoke, and the like) through a nozzle into the system,
which is under a vacuum. While entering the vacuum, each particle accelerates to its own specific terminal velocity—a velocity that depends on a particle’s size and shape but averages about 300 meters per second. The particles then pass, one at a time, through two continuous scattering laser beams, which are set serially in the path of the particles. Each particle scatters laser light as it passes through each beam. The time between the two scattering events provides information on a particle’s velocity and size. Each particle continues on, zipping into the path of a third, pulsed ionization laser. The pulsed laser fires, desorbing and ionizing the particle and producing both negative and positive ions. The particle’s journey—from entering the nozzle to annihilation by the ionizing beam—takes about 100 milliseconds. (See the figure at left.)

Spectra from these resulting ions are collected simultaneously by separate mass spectrometers. The spectra for each type of material are as unique as snowflakes. The spectra from one spore species differ in varying degrees from those of other Bacillus spores and are even more different from the spectra from a smoke particle, for instance. The spectra are first analyzed and categorized using real-time

Spectra of (a) Bacillus subtilis var. niger and (b) Bacillus thuringiensis, showing the peaks of greatest difference.
pattern recognition software developed at Livermore. Then, in a two-stage process, they are compared with spectra in a database of various substances gathered previously.

In the first stage, nonmicrobial (nonliving) particles such as smoke and flour are identified and removed from further analysis, while spectra of bacterial spores proceed to the next stage. In this second stage, the spectra of the bacterial spores are analyzed and classified by species. “A lot of data come in very quickly,” says Gard. “We need to be accurate, first time out. For instance, a natural insecticide containing spores of *Bacillus* is similar in chemical structure to the anthrax pathogen. We need to be able to differentiate between them the first time, every time.”

**Tests Show the Difference**

To test their system, the team used surrogates of anthrax (*Bacillus subtilis var. niger*) and a commonly used organic pesticide (*Bacillus thuringiensis*) that differs from *B. anthracis* in two short sections of its DNA. One technical reality the team had to work around is that the fast-traveling microorganism may encounter the ionizing laser beam at any point in the beam field. Because irregularities in the beam field exist—even in a beam of specific wavelength, pulse length, and fluence—this inhomogeneity results in the particle fragmenting into slightly different ions, depending on what part of the beam field it hits. The variation in the resulting ions makes it more difficult to identify the original material. Even so, subtle differences between the spectra of *B. subtilis var. niger* and *B. thuringiensis* can be detected. (See the lower figure at left.) In recent tests, the BAMS systems success rate was 93.2 percent.

A prototype of the system was taken to Florida in 2001 to help screen the overwhelming number of suspicious powders sent to the Florida Department of Health shortly after the anthrax exposures in the U.S. Postal Service. “The Department of Health was using methods that took three days to turn around a single sample. At the time, we wanted to see if we could do the analysis with our system in a few seconds,” says Gard.

In earlier tests at a biosafety level 3 facility in Florida, the system detected *B. anthracis* spores from nonmicrobial background particles. These proof-of-principle experiments showed how *Bacillus* spores could be detected when mixed with biological and nonbiological materials. Some of the other materials included white powders, such as aspartame, medicated foot powder, gelatin, growth medium, baking soda, and powdered sugar as well as cigarette and wood smoke. In all these cases, the BAMS system was easily able to detect spores from all other materials.

The team is working on the next-generation system, with which they hope to improve the rate of detection by focusing on specific optical properties of particles of interest.

**Identifying Cancer, Tracking Tuberculosis**

The ideal method for identifying bioagents would be instantaneous and absolute. BAMS is heading in that direction.

The technique also holds great promise in the arena of public health. The team is in the final year of an LDRD project, headed by Matthias Frank and Eric Guard. The goal is to develop the BAMS technique primarily for biomedical applications, such as detecting cancer by analyzing individual cells in clinical biopsies or identifying the bacteria that cause tuberculosis.

“Some day, when the system is perfected for field use, BAMS could be smaller than a breadbox and detect particles in about a millisecond,” says Gard. “A person would breathe into a mask. BAMS could sample the particles from the lungs and then identify and characterize the particles—instantaneously.”

—*Ann Parker*

**Key Words**: anthrax, bioaerosol mass spectrometry (BAMS), bioterrorism, airborne pathogens.

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The bioaerosol mass spectrometry (BAMS) team includes (left to right) in the front row: Maurice Pitesky, Herb Tobias (aerosol science), Joanne Horn, David Ferguson (data analysis), and Eric Guard (team leader); middle row: Jim Birch, Vincent Riot, Matthias Frank (laser–particle interactions) and Bruce Woods; and back row: Paul Steele, Norm Madden, and Keith Coffee (next-generation system).
Research Highlights

Portable Radiation Detector Provides Laboratory-Scale Precision in the Field

UNTIL recently, the U.S. relied on large oceans and friendly bordering countries to provide security against a terrorist attack. It was believed that an attack would most likely arrive in the form of missiles launched from land, air, or sea.

The terrorist threat now lies much closer to home. Experts believe that a possible method of weapon delivery will be a suitcase concealing contraband radioisotopes hidden in a car or plane’s luggage compartment. Or a seemingly harmless shipment of medical or industrial radioisotopes could mask potent radioisotopes destined for a dirty bomb—an ordinary explosive laced with radioactive material. To counter such threats, security agencies are looking for a new generation of portable radiation detection devices that will allow military, law-enforcement, public-health, and medical personnel to easily and quickly identify radioactive materials and distinguish among them.

Devices that detect x and gamma rays have been available for a few decades. However, precision energy-resolution detection devices, which unambiguously identify radioisotopes, are large and power-intensive and require a consumable liquid cryogen, all of which make them difficult to use in the field. A Lawrence Livermore team has developed a portable, handheld germanium radiation detector called CryoFree/25 that can duplicate the energy resolution and efficiency of a laboratory gamma-ray spectrometer. Physicist John Becker and engineers Norman Madden, Lorenzo Fabris, and Chris Cork are collaborating on the project. Begun in 1998, the project is sponsored by the Department of Energy’s Office of Nonproliferation Research and Engineering, which is part of the Office of Defense Nuclear Nonproliferation.

In CryoFree/25, a hermetically sealed germanium gamma-ray detector is coupled to a small, low-power cooler that is available commercially. The unit weighs 4.5 kilograms and can operate for 7 to 8 hours on two rechargeable lithium-ion batteries.

“The team’s goal,” says Madden, “was to create the smallest possible handheld, mechanically cooled gamma-ray spectrometer with the largest amount of germanium. The more germanium, the higher the detection efficiency.” As part of Livermore’s Measurements Science Team, originally formed at Lawrence Berkeley National Laboratory and now part of the Physics and Applied Technologies Directorate, the team had previously developed technology for a radiation detector that is onboard a NASA spacecraft. Becker thought it would be worthwhile to explore terrestrial applications for the radiation detector.

Powerful and Lightweight

Developed under the name Cryo3 but now dubbed CryoFree/25, this technology makes a quantum leap forward in portable radiation detection. The detector system features a handheld, gamma-ray spectrometer and book-size auxiliary equipment, such as a portable computer, power supply, and conditioning units. The gamma-ray spectrometer nearly replicates the precision energy resolution found in the larger, less-portable laboratory units used for unambiguous radioisotope identification.
The unit weighs less than 4.5 kilograms and can run for 7 to 8 hours on two rechargeable lithium-ion batteries. CryoFree/25 operates on only 16 watts of dc power and can operate continuously for more than 6 months before the unit’s cooling mechanism needs a short recycling period. “The beauty of CryoFree/25 is that the device can deliver the level of gamma-ray energy resolution associated with laboratory germanium spectrometers in a portable, lightweight, germanium detector without liquid nitrogen and with long field life,” says Becker.

Germanium has long been the detector material of choice for precision gamma-ray spectroscopy. Compared with other semiconductor materials used in detectors, such as silicon or cadmium telluride, germanium provides better detection efficiency, line-shape characteristics, and precision energy resolution, which are needed to produce the detailed x- or gamma-ray spectra for identifying radioactive materials. The germanium crystals must be cooled to approximately 90 kelvins (about –300°F) to operate. Liquid nitrogen has been the cryogen of choice, but more than 10 liters per week of liquid nitrogen are required to cool an average laboratory-size detector. This cooling requirement makes standard detectors awkward to transport, store, and handle in the field. Access to liquid nitrogen is a requirement for routine use.

Becker’s team overcame the size and access problems by joining the germanium crystal to a commercially available mechanical device commonly used to cool low-noise cell-phone antennas. The device, originally designed for the aerospace industry, requires only 12 watts to cool the germanium. “Our innovation is coupling a germanium radiation detector with a small, low-power cryogenic cooling mechanism,” explains Madden. “This combination offers extremely high-resolution gamma-radiation analysis in a portable package.”

As gamma-ray photons interact with the germanium in CryoFree/25, their energy is converted into charges that can be measured and recorded. Every radioisotope has a unique gamma-ray signature, which can be inferred by measuring the magnitude of the charge created in the detector and processed by the detector’s electronics. Unlike many other detectors, CryoFree/25 can identify all of the gamma rays originating from the known radioisotopes.

Adaptable for Multiple Applications

“CryoFree/25 is a forensics science tool for gamma-ray detection,” says Madden. “The resolution of the CryoFree/25 is so precise that it provides a unique fingerprint of the sample. For example, the detector can reveal not only...
what radioisotope is present but also the history of the radioisotope—whether, for instance, it came from a spent fuel rod or another source and how long ago the chemical alteration to the radioisotope occurred. The device might even reveal approximately where the alteration occurred.”

In addition to finding a cooling mechanism for the portable unit, the Livermore team added signal-processing electronics to minimize electronic noise that would otherwise obscure the detector’s energy resolution. A readout that shows detector pulse height with sharp, defined peaks accurately depicts the types and amounts of radiation present.

The Livermore team is working with the Coast Guard to adapt the unit for use on shipping vessels. “The Coast Guard needs the least obtrusive, most rugged and lightweight unit with proven reliability,” says Madden. CryoFree/25’s small size makes it particularly attractive for applications where small spaces may obscure field use of other detectors, such as at border crossings, airport terminals, and cargo ports.

The group is applying the same detector technology used in CryoFree/25 for space applications. Last year, an expanded team from Lawrence Livermore and the Space Science Laboratory at the University of California at Berkeley, delivered a flight detector to Johns Hopkins Applied Physics Laboratory for research on a NASA spacecraft designed to retrieve radioisotope data on the geochemistry of Mercury. CryoFree/25 technology may also prove valuable for the Department of Energy’s work in monitoring the nation’s nuclear weapons stockpile and protecting the weapons and nuclear energy facilities from terrorists.

The team is hopeful that government agencies will take advantage of the portable unit’s technology, which can be adapted to many applications. In emergencies, where time and power outages may limit the ability of laboratories to process radiation samples, CryoFree/25 provides the unambiguous radioisotope identification that is required to protect vital resources.

—Gabriele Rennie

Key Words: counterterrorism, CryoFree/25, portable germanium radiation detector.

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MICROELECTRONICS permeate our lives. They are in our cars, our kitchen appliances, our computers, and thousands of other products that drive our modern-day existence. Now, researchers at Lawrence Livermore, Sandia, and Lawrence Berkeley national laboratories have developed a system that will keep microchips rolling off the line with ever-smaller features.

The extreme ultraviolet lithography (EUVL) full-field step-and-scan system is the first tool that demonstrates all of the key technologies needed for production of next-generation microprocessors. This fully integrated system prints 50-nanometer features—less than half the size of those made by current production tools—and it writes the full field size of the chip—24 by 32 millimeters. The projection optical system, which was developed at Livermore, is the first large-field diffraction-limited camera for extreme ultraviolet (EUV) wavelengths and may rank as the most accurate imaging system ever constructed.

Because it prints smaller features, the system produces chips that are higher in density. That is, they can “do more” in less space, which will dramatically improve the speed and memory capacity of computer systems. Microchips with features smaller than 50 nanometers may well lead to systems for facile speech recognition, improved weather prediction, enhanced medical diagnostics, three-dimensional image processing, microcontrollers for “intelligent” machinery, and more powerful supercomputers for scientific and defense research.

Physicist Regina Soufli, one of Livermore’s principal investigators on the multilaboratory team, says such applications will be possible because the system embodies a set of groundbreaking technologies. In fact, until a few years ago, the science and technology community considered many of them impossible to develop.

Making the Jump for Moore’s Law

For several decades, integrated circuits have steadily gotten faster, smaller, and cheaper. Circuit performance has basically doubled every two years—a pace of development referred to as Moore’s Law. This rapid development rate is primarily responsible for the remarkable advances in computer technology that have occurred over the past few decades.

Unfortunately, fundamental physics laws on the diffraction of light are threatening to put the brakes on this progress. Photolithography uses light to print features onto a circuit substrate, which is usually silicon. The wavelike nature of light makes it extremely difficult to print images whose features have
a resolution less than the wavelength of the light being used. To print 100-nanometer features—the current size for computer chips—manufacturers have had to add expensive enhancements to lithographic systems. The enhanced systems use light in the deep ultraviolet part of the spectrum with wavelengths of 193 to 248 nanometers.

The EUVL full-field step-and-scan system goes beyond deep ultraviolet into the EUV part of the spectrum, using light with wavelengths of about 13 nanometers—more than a factor of 10 shorter than the wavelength of even the most aggressive deep ultraviolet system. The current resolution for the EUVL system is 50 nanometers, but Soufli says that a resolution of 20 nanometers will ultimately be possible. She adds that such a fine resolution is not likely to be attained with other semiconductor technologies for high-volume manufacturing.

Because it uses EUV light, the new system will also have a greater depth of focus than systems using longer wavelengths, which will guarantee more robust processing capabilities. In addition, the mask patterns for imaging onto the silicon wafers can be relatively simple, which eliminates the complex and expensive pattern modifications that non-EUV systems use to enhance the resolution of the printing process.

Bringing the EUVL full-field step-and-scan system into reality for the next Moore’s Law jump required the multidisciplinary team to rapidly develop several technologies. Many of these technologies were thought to be too difficult or even impossible to develop in time for EUVL to play a role in manufacturing.

For example, the team developed highly accurate metrologies to fabricate and align the system’s mirrors (see S&TR, October 1997, pp. 6–7) because no existing method came even close to measuring figure and smoothness with the accuracy required. With the new metrologies, these measurements are accurate down to atomic dimensions. The team also developed the world’s most precise multilayer reflective coatings, which are necessary for EUVL optics (see S&TR, October 2002, pp. 10–11; October 1999, pp. 12–13), as well as a clean, 13-nanometer light source with a high-power laser-produced plasma. The source provides enough light for rapid scanning without creating contaminants that would damage the system.

Since EUV radiation is absorbed by gases, new controls were needed to ensure a suitable, ultrahigh-vacuum environment in which to operate the system. The team developed magnetically levitated precision stages compatible with the vacuum environment. Custom sensors were also created that could operate in the EUV environment, and control hardware and software were designed to provide full step-and-scan capabilities.

The EUVL full-field step-and-scan system is the central element of the largest Cooperative Research and Development Agreement (CRADA) between the U.S. national laboratories and private industry. This unprecedented CRADA is a 6-year, $250-million program, funded by the EUV LLC, a consortium of six semiconductor manufacturers. The system’s development was key in convincing the microelectronics industry that EUV systems could follow deep ultraviolet systems as the next-generation lithography technology for producing microelectronics. In fact, Charles W. Gwyn, general manager of EUV LLC and a program director at Intel, noted that the success of this system led EUVL to be selected by international semiconductor organizations as the best candidate technology for use with circuit features below 50 nanometers.

The EUVL system also has potential applications outside the semiconductor manufacturing industry. Various nanotechnologies could benefit from the large surface area that can be imaged with features smaller than 50 nanometers. Possibilities include photonic crystals, surface-acoustic-wave detectors, and molecular electronic devices.

Set for the Future

With the success and acceptance of the system, EUVL now appears on the road maps of all the major semiconductor manufacturers. Soufli notes that subsequent versions of this system most likely will be used to fabricate microelectronics that are 100 times faster than those currently available. With Moore’s Law now in good shape for well into the next decade, microelectronics will continue to advance at the pace we have all come to take for granted for nearly half a century.

—Ann Parker

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A frantic race is under way in the microelectronics industry to integrate more and more capability onto computer chips. Yet conventional optical lithography—the current practice of directing light through a mask, or reticle, to print integrated circuits on chips—is being pushed to its limits. When beams of light cannot be made thinner, the number of circuits that can be written on a given chip can go no higher. Extreme ultraviolet lithography (EUVL), which has emerged as the lithographic method of the future, is expected to be capable of reducing the feature size from 130 nanometers to less than 50 nanometers.

“One of the highest risk areas for EUVL technology was the development of the reflective reticle,” says materials scientist Paul Mirkarimi. Mirkarimi’s team has not only overcome that concern but also won an R&D 100 Award for the ion-beam thin-film planarization process, which generates nearly perfect surfaces for reticles and other critical components for EUVL. With this novel deposition and etching process, surfaces that have been contaminated with particles piled up to 70 nanometers high can be made almost perfectly smooth. The resulting profile of the thin-film coating is less than 1 nanometer high. Imagine “smoothing” a 70-story skyscraper to the height of a single-story house.

Almost Perfect Surfaces

An EUVL reticle blank consists of a substrate coated with a molybdenum–silicon (Mo/Si) multilayer film designed to have optimal reflectivity at extreme ultraviolet (EUV) wavelengths of 13 to 14 nanometers. Reflectivity is critical because EUVL uses strongly attenuated EUV light directed at reflective optical components to create minute features. The film is coated with a buffer layer and an absorber layer and is processed with an electron-beam lithographic tool to form a patterned EUVL reticle. The finished reticle absorbs EUV light at specific locations and reflects it everywhere else.
The key challenge in developing this reticle technology is to manufacture reticle blanks that are virtually defect-free. The allowable defect density is about 0.0025 defects per square centimeter for defects of approximately 50 nanometers and larger. This density corresponds to just one defect for every two 15-centimeter-square reticle blanks—or a single defect the size of a basketball on a flat surface slightly larger than the states of Oklahoma and Texas combined. Says Mirkarimi, “To our knowledge, these are the most stringent defect specifications ever required for a coating process.”

The Livermore team’s technology smooths, or “planarizes,” substrate particles during the multilayer coating process. A primary ion source sputters material off a target onto the substrate, and a second ion beam etches, assisting in the formation of a smooth, uniform film with remaining defects less than 1 nanometer high. Defects that small—just a few atomic layers thick—are considered to be benign according to EUVL printability modeling.

Two other deposition processes—magnetron sputtering and ion-assisted electron-beam evaporation—can also be used to print computer chips. But magnetron sputter deposition results in larger substrate particles. And at least for Mo/Si coatings, there are no data to suggest that ion-assisted electron-beam evaporation smooths out defects.

Mirkarimi’s team also demonstrated that their planarization process smooths rough substrates, making it applicable to projection optics, another critical EUVL component. The figure and finish specifications of these optics are about 0.1 nanometer, which are extremely challenging and expensive to achieve simultaneously. “There is the risk that sufficient quantities of these optics won’t be produced because of the difficulty in fabricating them,” says Mirkarimi.

With the planarization process, coatings with EUV reflectivities of about 67 percent can be obtained on substrates with roughness of approximately 0.4 nanometer, which is sufficient for projection optics. Thus, finish specification for the optics could be relaxed, significantly reducing the production costs and increasing the availability of these optics. Livermore’s process is equally effective for smoothing homogeneous films. By successively depositing and etching thin silicon layers, the team achieved a level of particle smoothing with homogeneous silicon films similar to the level accomplished with Mo/Si multilayer films.

**Putting EUVL to Use**

With the smaller feature size that’s possible with EUVL, many more transistors can be placed on an integrated circuit. Desktop computer microprocessor chips will operate at more than 10 gigahertz, and random access memory chips can have gigabyte capacities. Such powerful, affordable computers are expected to make a variety of computationally intensive applications practical. Real-time, multilanguage voice recognition and translation are just two examples.

In 2001, the Semiconductor Industry Association reported that the industry was annually manufacturing about 60 million transistors for every man, woman, and child on earth. By 2010, this number is expected to be 1 billion transistors, as integrated circuits make their way into even more devices used in our daily lives. If we think our lives are computerized now, we obviously haven’t seen anything yet.

—Katie Walter

**Key Words:** extreme ultraviolet lithography (EUVL), ion-beam thin-film planarization, R&D 100 Award, reticle.

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Millions of people use eyeglasses or contact lenses to correct their vision, and many are opting for laser eye surgery. But determining the needed correction is not an exact process. When we have our eyes checked, we sit in a darkened room, peer through a device called a phoropter, and look at a focusing target, often an eye chart, projected in front of us. As we read the chart, an optometrist or ophthalmologist changes the lenses we’re looking through while we repeatedly answer the doctor’s only question: “Which one looks better—number one … or number two?”

A new optical device, called the microelectromechanical systems– (MEMS-) based adaptive optics phoropter (MAOP), will greatly improve this process. It allows clinicians to integrate a computer-calculated measurement of eyesight with a patient’s response to the target image. Patients can immediately see how objects will look—and the clinician can adjust the prescription—before they are fitted for contacts or undergo surgery. As a result, patients will experience better vision correction outcomes, especially with custom contact lenses or laser refractive surgery.

MAOP was developed in a collaboration among universities, national laboratories, and industry, including a team of researchers from Lawrence Livermore. Funded by the Department of Energy and the Center for Adaptive Optics—a National Science Foundation Science and Technology Center—the project brings together optical component manufacturers and one of the world’s leading providers of custom contact lenses and refractive eye surgery equipment. The MAOP team received an R&D 100 Award for developing an eye-correction system that combines technologies to improve the diagnosis and treatment of eyesight aberrations and ophthalmic and retinal disease.

An Objective Measure of Eyesight

The current phoropter used to measure vision addresses only the lower-order aberrations, such as defocusing and astigmatism. MAOP is designed to help patients with higher-order problems, such as coma, spherical aberration, trefoil, and quadrifoil. Scot Olivier, who led Livermore’s MAOP effort, says future versions of the system will incorporate retinal imaging, so clinicians can more successfully diagnose and treat retinal diseases—such as retinitis pigmentosa, glaucoma, diabetic retinopathy, and macular degeneration—that cause blindness.

MAOP combines adaptive optics technology—a technology used on the world’s largest telescopes for high-resolution imaging of astronomical objects—with MEMS deformable mirror technology. By using the MEMS deformable mirror, says Olivier, the team significantly reduced the size of the phoropter and could build it with commercial components, thus making MAOP compact and affordable.

Adaptive optics compensates for optical aberrations by controlling the phase of the light waves, or wavefronts, as they hit the retina—much like waves breaking on a shoreline. The optical structures in the eye, particularly the cornea and lens, can distort...
these wavefronts and thus produce the aberrations we encounter in our natural vision. An adaptive optics system measures aberrations with a wavefront sensor and uses a wavefront corrector to compensate for the distortion.

With MAOP, a patient looks through the phoropter viewport at a focusing target. A light source, a superluminescent diode, is projected into the patient’s eye and creates an image on the retina. A flip-in mirror allows a computer to calculate the needed correction. By pushing a button, the clinician can apply the computer-calculated prescription and ask the patient if the image is clear.

A beam splitter can be incorporated with the system to combine these two steps. Then the patient can simultaneously view the focusing target while the computer corrects the aberrations. The MEMS deformable mirror uses a standard Shack–Hartmann wavefront corrector. Light from a laser or superluminescent diode passes through the beam splitter, flip-in mirror, adjustable lens, and telescopic lenses and is then reflected off the corrector. Another set of telescopic lenses directs the light through the eye and creates an image on the retina. The wavefront sensor sends information to the computer interface, telling the computer how to adjust the corrector.

MAOP is the first system to use the much smaller and less expensive MEMS deformable mirror for adaptive optics and ophthalmic applications. The wavefront sensor determines how much the wavefront is distorted as it passes through the eye’s cornea and lens. A computer uses this information to create an internal, three-dimensional (3D) representation of the distorted wave. That 3D shape is then used to instruct the 144 MEMS actuators to move to positions that will minimize the distortion and “flatten” the wavefront.

Hope for Fighting Retinal Disease

Because MAOP features a modular design, it can be adapted for other applications. Modules under construction will enable the system to also perform retinal imaging. Traditional retinal imaging systems cannot apply wavefront corrections and thus produce images with a limited resolution, which hinders a doctor’s ability to diagnose early-stage retinal disease. Adaptive optics systems, which can correct wavefronts, produce far superior retinal images.

Higher-order aberrations, such as distorted vision from halos or glare, increase with an individual’s age. Previous computer-calculated methods do not correct for these problems and have not produced acceptable results. MAOP not only measures and corrects these aberrations, but it also can be used to evaluate eyesight under conditions that limit vision, such as while driving at night.

Clinical studies at the University of Rochester, which were conducted with earlier versions of MAOP, showed the benefits of correcting higher-order aberrations. Patients with extremely poor vision—say 20:400, which is far below the normal 20:20 eyesight—reported significant improvement when these aberrations were corrected. One patient’s vision became 24 times better.

With MAOP, clinicians can train their staffs to operate a single instrument with multiple functions and applications. The system can also collect and store patient information—before and after the correction is applied and the patient’s input is received—to provide an eyesight history for help with later diagnosis. A MAOP system outfitted with retinal imaging could be used to test new therapeutics in clinical trials and provide objective measurements of a therapy’s effectiveness.

MAOP is the first system to measure higher-order aberrations in the human eye, apply corrections, and immediately allow the patient to see the results. It’s an innovative technology for early detection and treatment of retinal diseases that cause vision loss and blindness. And it will improve optical treatment for the millions of people who depend on vision correction just to make it through the day.

—Sharon Emery

Key Words: eyesight correction, microelectromechanical systems– (MEMS-) based adaptive optics phoropter (MAOP), R&D 100 Award, retinal disease.

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We all know diamonds, or we think we do. Diamonds are a girl’s best friend, sang Marilyn Monroe in the movie *Some Like it Hot*. They appear on many a third finger, brilliantly faceted and sparkling. On a more practical note, because diamonds are one of the hardest substances on Earth, the industrial sector makes extensive use of them.

Who would suspect then that the most miniscule bit of diamond, just a few hundred atoms, would take on the exotic shape of a fullerene or buckyball at the surface? At the nanoscale—a nanometer is a billionth of a meter or 1,000 times smaller than the diameter of a human hair—materials behave differently than they do in their larger, bulk form. In this size regime, the laws of quantum mechanics predominate.

Yet the recent revelation that the outer surface of a molecule of diamond, a nanodiamond, is shaped like a soccer ball came as a real surprise. The discovery was made by a Livermore team that for the first time computationally modeled nanodiamonds to determine their optical properties. They had previously modeled two similar semiconductor materials, silicon and germanium, and expected about the same results.

Physicist Giulia Galli, who leads Livermore’s Quantum Simulations Group,
says, “At the nanoscale, the surface of silicon and germanium rearranges its atomic geometry in a way that somehow compresses the core of the nanostructure.” To their amazement, the team found that nanodiamond expands, with a crystalline diamondlike core and a fullerene-like structure around it at the surface.

The first fullerene was a 60-atom carbon buckyball. Livermore’s simulations are the first to reveal bucky diamonds, a new family of carbon clusters. The discovery of the bucky diamond was just one recent finding by a research team led by Galli and Tony van Buuren, an experimental physicist. The team performs quantum molecular simulations and scrutinizes materials experimentally as they seek to better understand the properties of the semiconductor materials silicon, germanium, and diamond at the nanoscale. As part of the Group IV series of elements on the periodic table, these three materials share some interesting properties, as described in the box on p. 10.

According to physical chemist Lou Terminello, materials program leader for the Defense and Nuclear Technologies Directorate, Livermore research on semiconductor nanostructures—also known as nanodots or quantum dots—is aimed primarily at using them in detectors to reveal the presence of biological or chemical warfare agents. A protein added to the surface of one of these nanoparticles would change when exposed to a biological agent, serving as an indicator.

At the nanoscale, silicon and germanium emit light when stimulated. Nanodiamond, which has more recently come under the microscope, may also change its optical properties as a function of size. In bulk form, all three semiconductors are compatible with biological materials and so could easily be linked with a protein. Whether this biocompatibility still exists when the semiconductors are reduced to the nanoscale remains to be determined. If these nanosemiconductors are indeed biocompatible, their optical, or light-emitting, properties could be exploited to detect specific molecules.

Other uses for light-emitting semiconductor nanoparticles include photonic switches, tunable lasers, and nanocrystal solar cells. Terminello adds, “Quantum dots will likely be some of the next-generation materials for targets at the National Ignition Facility.” By starting with nanostructures, scientists could dictate the target’s precise design. Atom by atom, they could gradually build up the targets in size from the nanoscale to macroscopic structures.

Nanoscience—the study of the very small—is fundamental to U.S. research. Funding by the U.S. government for nanoscience and nanotechnology is higher than ever, just behind defense spending and funding for biological research. Before tiny bits of any material can be put to use, their unique properties must be better understood. As the recent discovery of the bucky diamond illustrates, the world of Group IV semiconductor nanostructures is still a mystery.

Small Size, Big Change

Reducing any piece of material from a chunk that we might recognize to the nanometer scale changes virtually all of its most basic properties in a fundamental way. Its shape and crystalline structure change, as do its melting and boiling temperatures. Its magnetic properties may be different at the nanoscale. Its optical and electronic properties also change.

In a nanosemiconductor, an effect known as quantum confinement occurs when electrons and “holes” in the material are confined. (A hole is the absence of an electron; the hole behaves as though...
it were a positively charged particle.) Typically, quantum confinement causes the material’s optical gap—the energy difference between filled states and empty states—to widen. A larger optical gap prompts dramatic changes in electronic and optical properties. Bulk silicon when stimulated does not emit visible light, but in 1990, researchers found that nanoparticles of silicon do.

Livermore researchers and others have since determined that silicon nanoparticles emit different colors of light depending on their diameter. In 1997, germanium nanoparticles were found to emit light. In the last two years, other Livermore scientists have discovered that the optical gap of nanodiamond does not change until its size is reduced to less than 2 nanometers.

Nanoparticles are also different from the bulk form of the material in that the percentage of atoms at or near the surface of the particle is far greater. The surface of nanoparticles thus plays a large role in determining the particle’s electronic and optical properties.

**It Started with Silicon**

Livermore’s first work with Group IV semiconductor nanostructures took place in the mid-1990s. The photoluminescence of silicon had only recently been discovered, indicating that this element might be a promising material for optical applications.

Livermore researchers used a gas-phase vaporization process, in which melted silicon was heated and vaporized in the presence of a buffer gas, to synthesize silicon particles ranging from 1 to 6 nanometers. Numerous production techniques exist, but most of them allow only limited size control of the resulting particles. They also produce particles with a specific surface chemistry that is less useful for investigations of precise electronic structure.

Either hydrogen or oxygen was then bonded to the surface of the tiny molecules to “passivate” the dangling bonds of highly reactive silicon. Using spectroscopic and x-ray absorption techniques to probe the particles’ characteristics, the Livermore team was the first to measure the band edges of the optical gap of silicon and to determine that the gap changes as the nanoclusters become smaller. These findings clearly indicated the importance of the quantum confinement effect on the optical properties of silicon nanoclusters.

Subsequent fine-tuning of the synthesizing process made it possible to produce silicon nanoclusters in an even narrower distribution of sizes (±7 percent of average size) as measured using an atomic force microscope. Work in the late 1990s definitively correlated quantum confinement changes as a function of the size of silicon nanoparticles, in agreement with quantum confinement theory.

As Livermore and other research institutions worldwide experimented further with semiconductor nanoclusters, their potential uses as biological markers and nanostructure lasers became more evident. With increased concerns about bioterrorism, van Buuren and Galli obtained funding from the Laboratory Directed Research and Development Program to develop atomically controlled nanostructures for biowarfare detectors. Their team, composed of researchers from the Physics and Advanced Technologies and the Chemistry and Materials Science directorates, is relatively large. As interest in all things nano has burgeoned, the number of nanoscience experts at Livermore has grown.

**Simulations Verify and Surprise**

The traditional purpose of computerized simulations of physical phenomena is to verify experimental findings. But simulations can also go where an experiment cannot. This is especially true for examining the surface of nanoclusters. The effects of quantum confinement on semiconductor nanodots can be obtained experimentally; however, the changes in the properties of the comparatively large surface area of a nanostructure are difficult to determine in experiments. First-principles simulations, which do not contain any input from experimental data, are a valuable tool for discovering the dependence of a nanostructure’s optical and mechanical properties on its surface structure.

Using Livermore’s massively parallel supercomputers, Galli’s group has undertaken several computational studies of the surface chemistry of Group IV semiconductor nanoclusters. An early
Lawrence Livermore National Laboratory

study used density functional theory and quantum Monte Carlo codes to perform first-principles calculations of the surfaces of silicon nanoclusters. The group examined the effect of replacing one or more atoms of a hydrogen-passivated silicon nanocluster with other passivants. A remarkable change results when just two hydrogen atoms are replaced by more reactive oxygen atoms. The electron charge cloud is drawn toward the oxygen atom, dramatically changing the optical properties of the silicon dot.

From these and many similar calculations, the group has concluded that quantum confinement is only one mechanism responsible for a semiconductor’s light-emitting properties. For example, they have confirmed experimental findings by researchers outside the Laboratory that oxygen passivation of silicon dots reduces their optical gap while hydrogen passivation increases it.

A recent study modeled spherical silicon clusters ranging from 53 to 331 atoms (0.7 to 2.0 nanometers), the largest nanoparticles ever studied with the highly accurate quantum Monte Carlo technique. A team examined the process of surface reconstruction—in which unstable dangling bonds on a nanoparticle’s surface spontaneously rearrange themselves—and its effects on the particle’s optical properties. In this study, the team found that reconstruction of the surface of silicon nanostructures could have the effect of compressing the nanoparticle. “Time and again, we have found that the specific surface chemistry must be taken into account if we want to quantitatively explain the optical properties of semiconductor nanoparticles,” says Galli.

Germanium Joins the Fray

Although germanium was used extensively in early semiconductor devices, it has since been displaced by silicon as the substrate for most devices. But the 1997 discovery that nanodots of germanium emit light sparked a new interest in this element.

While he was at Livermore as a graduate student of the University of Hamburg, Germany, physicist Christoph Bostedt improved Livermore’s earlier vaporization chamber for synthesizing semiconductor nanoparticles. Among the many modifications he made, the chamber can now synthesize nanoparticles composed of virtually any element. Using this chamber, Bostedt found that by varying preparation parameters, he could dictate the size of the resulting germanium particles.

Now a Livermore postdoctoral fellow, Bostedt is using synchrotron radiation at Lawrence Berkeley National Laboratory’s Advanced Light Source (ALS) for photoemission spectroscopy and x-ray absorption studies of the electronic microstructure of germanium nanocrystal films. “Using ALS, we have produced spectra for germanium that are some of the best obtained anywhere,” he says.
Most recently, his team has shown in experiments with ALS that quantum confinement effects are greater in germanium nanocrystals than in silicon nanocrystals for particles smaller than 2 nanometers. The strong confinement they observed and the fast opening of the optical gap—which translate into a highly “tunable” material—indicate germanium nanocrystals would be especially useful in detectors and optoelectronic applications that require extreme sensitivity.

In the theoretical community, others have made similar predictions about the quantum confinement of germanium versus silicon, although considerable controversy exists. The Livermore team is the first to make this discovery experimentally using thin films of germanium nanocrystal, finding that the behavior of germanium nanocrystals is as sensitive to changes at the surface as silicon. “We believe that disagreements between our experimental results and some theoretical predictions are due to the structural details of the nanocrystals,” says Bostedt. “The structure, especially at the surface, of nanocrystals cannot be ignored.”

Theoretical models that do not use sophisticated quantum simulations typically use idealized nanocrystals isolated in space and not resting on any surface. The nanodot’s atomic structure is almost always ignored as well. In contrast, a quantum Monte Carlo investigation at Livermore into the structure and stability of germanium nanoparticles revealed the key role that structure plays. The simulations team found that the surface of germanium nanodots reconstructs when their diameters are smaller than 2.5 to 3 nanometers, a geometric rearrangement that agrees with the Laboratory’s photoemission experiments at ALS.

The Surprising Nanodiamond

Nanodiamond, the most recent Group IV semiconductor to be examined at Livermore, offers plenty of surprises. Livermore is one of the few research groups in the world to perform quantum simulations of nanodiamond behavior.

Livermore data show that the size of nanodiamond must be reduced to less than 2 nanometers before its optical gap increases beyond that of the bulk form. This behavior differs dramatically from that of silicon and germanium where quantum-confinement effects persist in particles of up to 6 and 7 nanometers. These results came from both computer simulations and x-ray absorption and emission experiments using ALS and the Stanford Synchrotron Radiation Laboratory. Both studies aimed to derive a structural model for nanodiamond.

The bucky diamond appeared during calculations of surface reconstruction of 1.4-nanometer diamond particles, which Galli performed with physicist Jean-Yves Raty of Livermore and the University of Liege, Belgium. These simulations started with bare, unpassivated nanodiamond. At low temperature, the bucky diamond reconstruction occurred spontaneously. The first faceted layer took on the properties of graphite, which was followed by the formation of pentagons linking the graphene fragments with atoms underneath. This change made the surface increasingly curved, eventually resulting in an arrangement like half of...
a 60-atom carbon molecule, the classic buckyball. Simulations showed similar results for surface reconstructions of 2- and 3-nanometer clusters.

These results point yet again to the importance of nanoparticle surfaces. “When the calculations and measured spectra of nanodiamonds are compared,” says van Buuren, “it becomes clear that the surface reconstruction identified by computer simulations is consistent with the features observed in absorption spectra.” Nanodiamond is interesting because it has been found in meteorites, interstellar dusts, and protoplanetary nebulae, and it appears in residues of detonation. (Nanoparticles of diamond for Livermore experiments are obtained through synthesis from detonation.) And regardless of whether they come from meteorites or detonation, most nanodiamond particles fall in the 2- to 5-nanometer range. Other nanomaterials display a much wider range of sizes even at this small scale.

Raty and Galli used computational methods to explore the causes for this size limitation. The team found that at about 3 nanometers—and for a broad range of pressure and temperature conditions—particles with bare, reconstructed surfaces become thermodynamically more stable than those with hydrogenated surfaces, and hydrogenation prevents the formation of larger grains.

**Prediction Is the Goal**

“Understanding how size and surface affect optical and electronic properties is what our research is all about,” says van Buuren. Experimentalists and quantum simulation experts are working together to establish a basic knowledge of the structure and optical properties of semiconductor nanostructures. Their goal is to match these two sets of data and form an ability to predict the characteristics of nanoparticles. Someday, a scientist will know exactly how to produce a nanowidget to detect a deadly pathogen. Perhaps the widget must emit blue light, and the scientist will know that using a nanoparticle of a given size and density produces the desired wavelength.

In the meantime, moving toward that goal, Livermore researchers are beginning to observe the interaction among nanostructures. One team recently performed quantum simulations of the interplay of silicon quantum dots, an inorganic material, and organic molecules, which will be essential in a semiconductor biodetector. In particular, investigators simulated what occurs when organic molecules are attached to silicon quantum dots. They found that the probability of attaching an organic molecule to a nanodot is greatly increased if light shines on the nanodot, a result that agrees with recent experimental findings by others. Their simulations also indicated a way to select silicon quantum dots with a specific optical gap at the same time that organic molecules are being attached.

Next on Bostedt’s agenda is to make thick films on which germanium particles are closer together and touching, which is how they will be in real-world applications. Unfortunately, when they touch, nanosemiconductor particles tend to lose some of their special electronic properties. Bostedt has developed a surface passivation technique that keeps the particles isolated, reducing the effect of touching. Further experiments will examine the interface where interactions occur between passivated layers to determine what happens to the electronic properties of the entire device.

Others on the team are starting simulations and experiments to explore the structural and optical properties of silicon and germanium nanoparticles in solution. A new two-step cluster aggregation source is under development that will allow for wet chemical modification of the surface of crystalline (a) Simulation of a silicon nanostructure in water. (b) and (c) Monte Carlo simulations from first principles of nanodiamond precursors in water. Both (b) methane and (c) silane are forms of carbon and are hydrophobic; that is, they repel water, just as oil repels water. Although the methane and silane are similar structurally, they interact with water quite differently.
A semiconductor is a crystalline solid that in its pure form exhibits a conductivity midway between that of metals and insulators. The three semiconductor materials that Livermore is studying for possible use as sensors and detectors are silicon, germanium, and diamond. Silicon accounts for almost 99 percent of all commercial semiconductor products. Germanium became famous when the transistor was invented but has since been replaced largely by silicon. Diamond, a monocystal of carbon, has the physical properties of a wide-optical gap semiconductor, but current technologies do not allow its use as a semiconductor.

These three materials comprise some of the Group IV elements on the periodic table, as shown below. Tin, the fourth potential semiconductor material in this group, has the physical properties of a semiconductor at low temperatures but at room temperature behaves like a metal. These four materials are elemental semiconductors.

Elements in Groups II and VI and in Groups III and V are often combined to form compound semiconductors. Gallium–arsenide is a typical Group III/V compound semiconductor often used in microwave devices and optoelectronics. Most experiments designed to explore the optical properties of semiconductor nanoclusters have focused on such Group II/VI compound semiconductors as cadmium–selenium.

In contrast, the synthesis of covalently bonded nanoparticles such as silicon has proven to be much more challenging. Silicon and other Group IV semiconductor elements are thus much less well characterized than Group II/VI compounds, and the interplay of quantum confinement and surface properties is less clear. Yet silicon is the preferred material for biomarkers because of its compatibility—at least in its bulk form—with biological materials. Silicon nanoclusters could also be integrated with existing silicon technologies to create nanoscale optoelectronic devices. Germanium and nanodiamond have been studied much less than silicon, but their intriguing characteristics inspire hope that they may be useful as well.

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**Key Words:** biodetector, buckyball, germanium, nanocluster, nanocrystal, nanodiamond, nanoparticle, nanoscale, nanoscience, nanotechnology, quantum dot, quantum molecular simulations, semiconductor, silicon.

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Livermore researchers are part of the design team for the first large-scale x-ray laser. The goal of the new fourth-generation light source is to image single molecules. Shown here are (foreground) the lethal-factor protein of an anthrax spore and (background) a simulation of its diffraction pattern.
Bright Idea

ITS short, intense pulses of x rays will reveal for the first time the structure and dynamic behavior of many proteins and viruses at atomic resolution and in three dimensions. It will unlock the secrets of high-energy-density plasmas, which are of interest to the nation’s Stockpile Stewardship Program. And it will create the hot, dense matter believed to exist in the center of large planets.

It’s the Linac Coherent Light Source (LCLS), the world’s first large-scale x-ray laser, being designed for installation at the Stanford Linear Accelerator Center (SLAC). “The immense power of its short-pulse, laserlike x rays will create a revolution in science,” says Alan Wootton, chief scientist for Livermore’s Physics and Advanced Technologies Directorate.

The heart of the LCLS is a free-electron laser that produces beams of coherent, high-energy x rays. Coherence—the phenomenon of all photons in a beam acting together in perfect lockstep—makes laser light far brighter than ordinary light. Think of a 10-watt night light; then compare its brightness with that from a 10-watt laser—a beam so bright it can cut metal. Because x-ray photons at the LCLS will be coherent, the resulting beam of light will be as much as 10 billion times brighter than any other x-ray light source available today.

The LCLS, and a cousin planned in Germany, will improve on so-called third-generation light sources. The third-generation sources are circular, stadium-size synchrotrons, and they produce streams of incoherent x-ray photons. Because their pulses are long compared to the motion of electrons around an atom, synchrotron light sources cannot begin to explore the dynamic motion of molecules.

The light from the fourth-generation LCLS will last for quadrillionths of a second, allowing its beam to capture such dynamic behavior.

Even determining the static structure of proteins and molecules will be easier and faster with the LCLS. Today, proteins and other macromolecules must be crystallized before their structure can be probed with synchrotron radiation. But not all proteins can be crystallized, and the crystallization process is long and involved. With the LCLS, a single powerful pulse will image one molecule with no prior crystallization required.

Lawrence Livermore is part of a SLAC-led consortium to plan, design, and build the LCLS. Other partners include the University of California at Los Angeles (UCLA) and Los Alamos, Brookhaven, and Argonne national laboratories.

Livermore’s primary responsibility, under physicist Richard Bionta, is to design and fabricate the optics that will transport the x-ray beam to experimental chambers and to measure, or diagnose, the beam’s condition. The extreme brilliance and ultrashort duration of the beam’s pulses will give the beam a peak power of as much as 10 gigawatts. These features make designing optics a challenge because, says Bionta, “The energy of the beam can melt many materials in a single pulse.”

Meanwhile, physicist Henry Chapman and other Livermore scientists are planning the first experiments at the LCLS and

![The Linac Coherent Light Source will use the linear accelerator (linac) at the Stanford Linear Accelerator Center to create very bright, ultrashort pulses of laser radiation.](Image)
establishing the x-ray pulse parameters that are needed for various measurements.

"At the LCLS, we’ll use lens-less imaging to determine the three-dimensional arrangement of atoms in a molecule,” Chapman says. “We’ll detect x rays scattered by a sample when the beam hits it and then examine the diffraction pattern.” Radiation from the powerful beam will destroy each sample, but the beam’s ultrashort pulse will generate diffraction data before that happens.

“Every molecule has a unique diffraction pattern,” says Chapman, “and that pattern depends on the molecule’s structure.”

Experiments at the LCLS will reveal protein structure, which determines protein function. Hence, the LCLS is expected to profoundly benefit structural biology and medical research. It could eventually help scientists solve the proteome—the entire system of proteins in the human genome.

A Single Straight Shot

When the LCLS becomes operational, sometime in 2008, the free-electron laser’s photoinjector will shoot electrons down part of the SLAC linear accelerator, or linac. The photoinjector will produce tiny bunches of electrons that travel in a narrow, bright beam at almost the speed of light. After the electrons enter the kilometer-long linac, compressors along the accelerator path reduce the length of each bunch by a factor of 30, which increases their peak current. Their energies may be pushed as high as 14 gigaelectronvolts, a value that will be adjusted from experiment to experiment to produce the desired range of x-ray frequencies.

The electrons then enter an undulator—a vacuum chamber just 5 millimeters across and about 125 meters long and lined with 7,000 magnets arranged in alternating poles. As the electron bunches move down this narrow channel, the magnetic fields push and pull on them, causing the bunches to emit x rays. The LCLS undulator is so tightly focused that x rays emitted by one electron interact with the electrons in front of it. This interaction causes the electrons to bunch more tightly, which generates more x rays.

As the process repeats, the bunches become smaller and smaller. This chain reaction is called self-amplification of spontaneous emission, or SASE (pronounced “sassy”). SASE eventually saturates the x-ray beam, producing a narrow, coherent beam of light—a laser.

Broadband spontaneous (not coherent) radiation about 10,000 times brighter than that from any other light source emerges from the undulator as well.

Livermore-designed optical devices, placed beyond the undulator, will manipulate the direction, size, energy spread, and duration of the x-ray beam. They also will diagnose the beam and direct x rays to one of two halls for use in experiments.

The experimental halls, A and B, are located 50 and 400 meters downstream from the end of the undulator. Experiments requiring a very narrow, high-energy-density beam will use facilities in Hall A, while Hall B will house experiments that require lower energy densities.

Optics Bear the Brunt

All the diagnostic equipment on the LCLS is designed to minimize interference with the beam. “Because the beam is so...

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Layout of the Linac Coherent Light Source at the Stanford Linear Accelerator Center. Experimental halls A and B will be to the left, beyond the photon beam lines.
powerful,” says Bionta, “our goal is to not put anything in its path, except a gas attenuator.”

A mask, valves, and movable jawlike slits just beyond the undulator intercept most of the spontaneous radiation that accompanies the beam. These devices are designed so that they do not block the narrow, intensely coherent x-ray beam.

Livermore researchers have been working for several years to understand the damage that occurs when an LCLS beam encounters optics, diagnostics, and targets. Several types of simulations, including Monte Carlo and wave models, helped them fully characterize the x-ray beam. Armed with these data, Wootton, Bionta, and others began to develop schemes for imaging such a bright beam.

The concept they selected uses a camera that will be one of the first diagnostic devices beyond the undulator. In this setup, a small fraction of the beam’s light is directly reflected off a thin, polished beryllium foil. Beryllium was chosen for the foil because it has a low electron density and tends to absorb few x rays. Beryllium also will be used for many of the reflective optics at the front end of the system where photon densities are highest.

When the beam reflects off the foil, it strikes the surface of a 100-micrometer-thick lutetium oxyorthosilicate (LSO) crystal doped with a 5-micrometer-thick scintillating layer of cerium. “The LSO crystal is designed to reflect just one-millionth of the total light from the beam,” says Bionta. Reflected visible light is collected by a microscope lens and forms a magnified image on a charge-coupled device (CCD) camera. The images of a beryllium–aluminum disk shown below demonstrate the fine resolution of the camera.

Using the CCD camera, the team has studied how photons from short-pulse lasers at various wavelengths interact with different materials. For example, silicon was irreversibly damaged even at low energy densities using a laser in the visible wavelength and pulse lengths similar to those of the LCLS.

Focusing the LCLS’s high-energy beam will be a challenge. The Livermore researchers are developing a new class of tubular optical devices in which the x-ray beam reflects off the inside wall. The slight grazing incidence of the beam on the wall of the lens reduces the absorbed energy considerably. X rays enter the tube at one end and are reflected once by the highly reflective interior surface. They then exit from the other end of the tube, but now the

Livermore’s novel charge-coupled device camera was designed so that its images would show features as small as one pixel across. (a–c) These images of a beryllium–aluminum disk demonstrate the camera’s resolution. (d, e) In these images, x-ray resolution is less than or equal to one pixel, as models predicted.
x rays are traveling in a slightly different direction.

A special focusing element has also been designed for the warm, dense matter experiments that will take place in Hall A. Warm, dense matter is an energetic plasma whose density is almost that of a solid, but it may be as hot as 10,000 kelvins. Scientists believe this matter may exist in the centers of large planets, such as Jupiter, and its properties are important to astrophysics and relevant to the production of inertially confined fusion reactions. Warm, dense matter will be created in the laboratory by focusing the x-ray laser’s beam to a 2-micrometer spot in the center of a sample of solid matter.

The focusing element will be a blazed phase lens, as shown in the top image below. The lens is made of carbon, which has low x-ray absorption characteristics. Although carbon is not as resistant as beryllium is to the intense power of the LCLS, it has a higher refractive power and is easier to machine precisely, allowing more interesting optical designs. To test the lens design, the research team had a prototype machined at Livermore’s Large Optics Diamond Turning Machine (LODTM).

The prototype lens is made from a thin disk of aluminum, which has the same optical properties as carbon. The aluminum lens was tested at the Stanford Synchrotron Radiation Laboratory. Although lens performance was limited by the material chosen and the geometry of the experiment was not ideal, the measured performance closely matched predictions from simulations.

Precision machinists at the LODTM are trying to make lenses from blocks of pure beryllium. Beryllium is a challenge to machine because of its grain structure and because it’s a hazardous material. In fact, Livermore’s LODTM is one of the few facilities in the nation authorized to work with it.

Perhaps the most challenging LCLS diagnostic will be measuring the 230-femtosecond pulse length. Streak cameras are not an option because they measure down only to 500 femtoseconds. One potential device is a fiber-optic interferometer developed by Livermore photonics experts. The interferometer uses the beam from a continuous-wave laser to monitor the electronic state of a tiny waveguide inserted across its measurement arm.

“When we tested the interferometer at Stanford’s synchrotron,” says Bionta, “it was sensitive to x rays perturbing the waveguide. In fact, its response was faster than we could measure with the synchrotron beam.” Further experiments will be conducted with shorter-pulse x-ray sources at Livermore and SLAC, to determine if the device is really fast enough to measure the 230-femtosecond LCLS pulse.

Technologies for Experiments

Two general classes of experiments have been proposed for the LCLS. In the first class, the x-ray beam will be used to probe the sample without modifying it, which is the current practice for most experiments with synchrotron sources. For example, scientists can use the x-ray laser to determine the dynamic behavior of chemical interactions, essentially by watching the interaction occur on a femtosecond scale, which has never been possible before.

In the second class of experiments, the LCLS beam will induce nonlinear
photoprocesses, or it will create matter in extreme conditions. These experiments include creating warm, condensed matter, as previously described, and determining the structure of macromolecules, by recording crucial information about a molecule before it is vaporized.

It is in biology that the hard x rays of the free-electron laser are expected to have the biggest effect. No technique available today can image the interior of micrometer-size particles in three dimensions at high resolution. With the LCLS, scientists will be able to analyze very small samples, from tens of micrometers down to single molecules.

With third-generation synchrotrons, the low-intensity x rays can diffract to atomic resolution only when a molecule has been crystallized. Once a protein has been crystallized, scientists can’t study its interactions with other biological molecules. Nuclear magnetic resonance spectroscopy is used to overcome these shortcomings of x-ray crystallography, but it does not work for larger proteins. With the LCLS, researchers can study proteins that can’t be crystallized, such as proteins linked to lipids (fats) and embedded in cell membranes. The short pulses of the LCLS will also reveal how some molecules change shape in just a few femtoseconds.

Recording the diffraction pattern before the molecules blow up is critical. X-ray pulses are diffracted by electrons orbiting the atoms in molecules. By studying the patterns made by these diffracted rays, biologists can deduce the structure of the molecule under analysis. Team members have developed a hydrodynamic model to understand the various interactions between the x-ray beam and the sample and to verify that the beam’s pulse will end before the sample begins to be torn apart. The figure to the right shows results from simulations of a 20-nanometer protein molecule when it’s hit by an x-ray free-electron laser. Models also indicate that a water tamper will suppress the explosion, extending the time range of the diffraction process. Researchers have used simulations to establish the minimum photon density required to classify diffraction and have determined that the necessary pulse durations range from 10 to 30 femtoseconds.

Experiments to verify the timing of the explosion will be performed at the Tesla Test Facility (TTF), the proving ground for the TESLA x-ray free-electron laser that is being designed in Germany. “The TTF is the only place we have now for testing any of these simulations experimentally,” says Chapman. “Its wavelength is longer than the LCLS’s will be, so we can’t get to atomic resolution. But we can begin to understand how and when damage occurs.”

The team is also exploring ways to get samples into the beam’s path. “Molecules will be just a few billionths of a meter wide,” says Wootton. “Somehow, we have to get them lined up with a beam that’s only slightly larger, a few millionths of a meter wide and running at the speed of light.”

Each pulse of the x-ray beam can hit just one sample in its path. Complete three-dimensional information about a molecule will then be collected by examining multiple, identical samples, one by one. One method for acquiring such data is to use some kind of “molecule gun” to feed samples into the beam path.

An alternative method is to tether several protein molecules to a membrane positioned in the beam’s path. This option, in which the molecules are oriented the same way, requires a lower photon density. Says Chapman, “Because in this case we can now use a lower photon density, which will cause overall less damage, models show we can use longer pulses where the rate of damage is reduced.” The team is
exploring whether dip-pen nanolithography can be used to produce this carefully oriented pattern of molecules. In dip-pen nanolithography, molecules of a protein or other organic material are deposited on a substrate in a regular pattern.

The Livermore researchers who are developing the algorithms to reconstruct diffraction patterns have been aided by experiments at the Advanced Light Source, a third-generation synchrotron at Lawrence Berkeley National Laboratory. One recent experiment, in collaboration with colleagues from Berkeley and Arizona State University, used a silicon nitride pyramid decorated with 50-nanometer gold spheres. These spheres were chosen because they could be well characterized by other, independent means. As shown below, a reconstructed image of gold ball clusters compares extremely well with an image obtained using a scanning electron microscope. “This reconstructed image is the first true lens-less x-ray image,” says Chapman.

Beyond the Tip of the Iceberg

Chapman’s team will also conduct experiments at the TTF in Germany. Those single-shot diffraction experiments will use samples mounted on a substrate and samples shot across the beam. Samples will include lithographic test patterns, diatoms, and wet cells.

“With these experiments, we’ll be able to achieve the long-sought goal of x-ray imaging at resolutions beyond the radiation-damage limit,” says Chapman. “We hope to get spectacular images. But they will be just the tip of the iceberg compared to what we will be able to achieve at the LCLS.”

—Katie Walter

Key Words: free-electron laser; Linac Coherent Light Source (LCLS); linear accelerator (linac); protein structure; Stanford Linear Accelerator Center (SLAC); x-ray laser; warm, condensed matter.

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Using Proton Beams to Create and Probe Plasmas

Proton beams generated by ultrashort-pulse lasers will help advance our understanding of plasmas.

PROTONS, the positively charged, subatomic particles discovered by Lord Rutherford nearly 100 years ago, are still surprising scientists. Lawrence Livermore researchers are discovering that proton beams created by powerful, ultrashort pulses of laser light can be used to create and even diagnose plasmas, the superhot state of matter that exists in the cores of stars and in detonating nuclear weapons. The proton-beam experiments promise new techniques for maintaining the nation’s nuclear arsenal and for better understanding how stars function.

The proton beams used in the Laboratory’s experiments are produced by pulses of laser light lasting only about 100 femtoseconds (a femtosecond is $10^{-15}$ seconds, or one-quadrillionth of a second) and having a brightness, or irradiance, up to $5 \times 10^{20}$ watts per square centimeter. When such fleeting pulses are focused onto thin foil targets, as many as 100 billion protons are emitted, with energies up to 25 megaelectronvolts. The protons come from a spot on the foil about 200 micrometers in diameter, and the beam’s duration is a few times longer than the laser pulse. The highest-energy protons diverge 1 to 2 degrees from the perpendicular, while the lowest-energy protons form a cone about 20 degrees from perpendicular.

Funded by the Laboratory Directed Research and Development Program, the Livermore experiments are led by physicists Pravesh Patel and Andrew Mackinnon. Patel, who works in the Laboratory’s Physics and Advanced
Technologies Directorate, is researching new ways to create and better understand plasmas. Mackinnon, from Livermore’s National Ignition Facility (NIF) Programs Directorate, is developing new ways to measure the plasmas created in NIF experiments. Both physicists are collaborating with colleagues from Queen’s University in Belfast, Northern Ireland; Heinrich-Heine-Universität in Düsseldorf, Germany; the LULI laser facility at l’Ecole Polytechnique in France; Rutherford Appleton Laboratory in the United Kingdom; and the University of California (UC) at Davis.

“Plasmas are often referred to as the fourth state of matter,” says Patel. “They are abundant in the universe but relatively uncommon on Earth. Plasmas are extremely hot, highly transient objects and thus are difficult to control or to accurately probe.”

The team wants to develop new methods for creating plasmas in the laboratory, so they can study them at temperatures ranging from a few electronvolts to hundreds of electronvolts and at the high energy densities (more than 100,000 joules per gram) that exist in stars. The current generation of high-power lasers makes such studies possible because they can compress and heat matter to these extreme states.

Ideally, scientists want to measure plasmas in a uniform-density, single-temperature state. As a material is heated to several electronvolts, the pressure in it increases to more than a million times atmospheric pressure. This increased pressure causes the plasma to expand hydrodynamically, as in a violent explosion. Under these conditions, measuring plasma properties is extremely difficult.

One way to overcome these problems is to use what scientists call isochoric heating—heating at constant volume. With isochoric heating, plasmas don’t expand during the time they are heated, and their energy can be relatively uniform. Established methods of isochoric heating, such as laser-driven shock heating, x-ray heating, and ion heating, are relatively fast ($10^{-6}$ to $10^{-9}$ seconds), but these timescales are still longer than those during which significant hydrodynamic expansion can occur ($10^{-11}$ to $10^{-12}$ seconds).

Another method, direct heating with intense subpicosecond ($10^{-12}$ seconds) laser pulses, creates a highly nonuniform heating pattern. The laser energy is absorbed within less than 100 nanometers of material, and the heat localization creates a large temperature and density gradient.

A novel approach to isochoric heating, discovered at Livermore, uses laser-produced proton beams to generate fleeting, dense plasma states at constant volume and density. The heating period is shorter than the time needed for significant hydrodynamic expansion to occur, so the material is heated to a plasma state in a few picoseconds. In effect, says Patel, the proton beam dumps a huge amount of energy almost instantaneously and suddenly increases a target’s temperature to millions of degrees.

### JanUSP Makes It Possible

In their experiments, the researchers rely on Livermore’s Janus ultrashort-pulse (JanUSP) laser, one of the brightest lasers in the world. (See *S&TR*, May 2000, pp. 25–27.) JanUSP produces a beam with an average intensity of $5 \times 10^{20}$ watts per square centimeter that lasts about 100 femtoseconds. The laser operates at a wavelength of 800 nanometers and delivers 10 joules of energy.

In one set of experiments, the laser pulse produced a proton beam from a 10-micrometer-thick sheet of aluminum foil. The proton beam then heated a second 10-micrometer-thick aluminum foil that was placed 250 micrometers directly behind the first. Within a few picoseconds, the heating created a 4-electronvolt plasma almost 200 micrometers in diameter—too short for much hydrodynamic expansion to occur.

The discovery that intense, highly directional proton beams could be generated from an ultrashort laser pulse heating a solid target was made by Livermore researchers several years ago while conducting experiments with the Laboratory’s Petawatt laser. The Petawatt laser operated on 1 of the 10 beam lines...
of Livermore’s Nova laser, which was decommissioned in 1999. (See S&T, March 2000, pp. 4–12.) Experiments by Livermore physicist Richard Snavely and others to characterize the proton beams revealed a unique combination of properties, including peak proton energies of 55 mega-electronvolts and conversion efficiencies (of laser energy to proton energy) up to 7 percent.

The scientists also discovered that the protons in the beam originated in hydrocarbons found in surface contamination on the foil’s back surface. Livermore theoretical physicists, led by Steve Hatchett and Scott Wilks, used computer simulations to study this behavior. They found that the pulse from an ultrashort laser accelerates electrons from the interaction region at the front of the target with relativistic energies; that is, the electrons travel close to the speed of light. The electrons emerging at the foil’s rear surface induce a large electrostatic charge field, which in turn accelerates protons from hydrocarbon contaminants on the rear surface. The protons accelerate from 0 to 20 mega-electronvolts at 20 percent the speed of light and travel in a well-defined, highly directional beam perpendicular to the target. X rays, in contrast, are emitted at random angles.

Simulations by Wilks showed that by curving the laser target’s rear surface, the proton beam could be focused to a far higher state of energy density. To test this design, the team asked General Atomics in San Diego, California, to manufacture aluminum hemispheres that are 10 micrometers thick, 320 micrometers in diameter, and almost perfectly smooth on the inside to ensure a high-quality proton beam. With the shaped targets, the proton beam was almost 10 times more powerful than the beam produced from flat targets. The proton beam was focused on a 50-micrometer-diameter area of a foil placed behind the target, which was then heated to 23 electronvolts.

“For the first time, the experiments showed that we can focus proton beams,” says Patel. He notes that when the
techniques of proton heating and focusing can be applied with more powerful lasers, scientists may be able to isochorically heat plasmas to much higher temperatures and pressures. This advance would provide many opportunities in high-energy-density physics and fusion energy research.

**Using Protons for Radiography**

The team is also using proton beams for radiographic applications to diagnose plasma conditions generated by high-power lasers at picosecond timescales. The first proton probing experiments of a laser-driven implosion were conducted by Mackinnon in 2002 using the 100-terawatt Vulcan laser at Rutherford Appleton Laboratory. This experiment was conducted in collaboration with scientists at Queen’s University and UC Davis.

“We wanted to investigate the suitability of proton radiographs to diagnose an implosion capsule in inertial confinement fusion experiments,” says Mackinnon.

Plastic microballoons, 500 micrometers in diameter—or about one-fourth the size of the targets planned for NIF—were used as targets. Each of the Vulcan laser’s six long-pulse beams was fired for 1 nanosecond at a wavelength of 1 micrometer and an irradiance of 10 terawatts per centimeter. Each beam’s energy was 100 to 150 joules, so the maximum energy on the target was up to 900 joules. The six laser beams illuminating the target arrived from six orthogonal directions, a setup designed to provide the best symmetry for this number of beams.

In addition, an ultrashort laser beam was used to make either a diagnostic proton beam of about 7 megaelectronvolts or a diagnostic x-ray beam of about 4.5 kiloelectronvolts. The proton beam was obtained by focusing a 100-joule laser pulse with an irradiance of about $5 \times 10^{19}$ watts per square centimeter for 1 picosecond onto a tungsten foil 25 micrometers thick. To image the implosion, the team used a multilayer pack of dosimetry film in which each piece of film was filtered by the preceding piece. In this way, the film pack gave a series of images from each shot with an energy ranging from 3 to 15 megaelectronvolts.
The team took radiographs of microballoons both before and during implosion. One image, of a 500-micrometer-diameter microballoon with a 7-micrometer wall thickness, showed good contrast at a resolution of 5 to 10 micrometers. A series of radiographs (shown on p. 14), which were taken by varying the delay between the implosion beams and the beam used to produce the proton or x-ray beam, revealed how the implosion process evolved.

In one experiment, the beams were set to converge on the target asymmetrically—that is, the six beams arrived at the target at slightly different times. The laser beams on the left-hand side arrived 1 to 2 nanoseconds before the laser beams on the right-hand side. This asymmetry led to significant distortions. For example, the shell traveled much farther inward on the left-hand side than it did on the right.

Under more symmetric drive conditions, the target remained nearly spherical during the implosion. However, even when the beams arrived at the same time, the proton radiographs revealed some plasma asymmetries. For example, in one experiment, the upper part of the shell traveled almost twice the distance traveled by the lower part of the shell.

These proton radiographs were the first taken of a laser-driven implosion with picosecond resolution. The team found that the temporal and spatial resolution remained high throughout all stages of the implosion.

“The images show the promise of proton radiography for diagnosing early time distortions in the implosion process with high resolution and very good image contrast,” says Mackinnon. “The x-radiographs also had good resolution, but the image contrast was high only when the density was high.”

According to Mackinnon, proton beams with energies from 50 to 100 mega-electron-volts, produced by an ultrashort-pulse laser, could one day be used to probe the cores of NIF targets as they are compressed by laser light. Lower-energy protons also could be useful, for example, to diagnose electric and magnetic fields inside hohlraums, the metal cases that enclose many NIF targets. More experimental and theoretical work is under way to fully investigate this promising technique.

Mackinnon notes that another kind of proton radiography is being studied by researchers at Lawrence Livermore and Los Alamos national laboratories. But the protons created in those studies are much more energetic—about 800 mega-electron-volts. (See S&TR, November 2000, pp. 12–18.) That research centers on beams of extremely high-energy protons focused with magnetic lenses and is designed to image deep inside larger exploding objects.

Livermore physicists Mike Key and Richard Town are also studying whether proton beams, instead of electron beams, can be used to drive fast ignition on NIF. (See S&TR, March 2000, p. 4–12.) In fast ignition, at the moment of maximum compression, a laser pulse plows through the plasma to make a path for another very short, high-intensity pulse (presumably, of electrons) to ignite the compressed fuel. In theory, fast ignition reduces both the laser energy and the precision requirements for achieving ignition.

**Field Strength and Geometry**

In collaboration with Marco Borghesi from Queen’s University and Oswald Willi and G. Pretzler from Heinrich-Heine-Universität, the Livermore team is investigating another aspect of proton radiography: diagnosing the transient electric and magnetic fields directly through particle-deflection measurements. Unlike x rays, protons are electrically charged, so they interact with electric and magnetic fields in plasmas. Proton probing would provide a new method to visualize and measure fields in laser plasma experiments, which are not well understood.

(a) In one particle-deflection technique for diagnosing the transient electric and magnetic fields, a proton beam passes through two identical gratings. The gratings are separated by a small distance, and their rulings are rotated at slight angles to each other. (b) The proton beam is imprinted with a grating pattern called proton moiré. A proton beam passing through the plasma causes a shift in the moiré pattern, which can be used to infer the strength of the electric and magnetic fields. (c) Proton moiré is similar to (d) the more common optical moiré.
For these experiments, the researchers are using the JanUSP, Vulcan, and LULI lasers. Developing such proton radiography diagnostics supports the Laboratory’s stockpile stewardship mission by helping scientists better understand hot, dense plasmas.

In one technique, the proton beam passes through two identical gratings. The gratings are separated by a small distance, and their rulings are rotated at slight angles to each other. In effect, the proton beam is imprinted with a pattern of the gratings, called proton moiré. When the beam passes through the plasma, the electric and magnetic fields can cause shifts in the moiré pattern. The change in pattern can then be used to infer the strength of the electric and magnetic fields.

A related technique uses a single, two-dimensional grid to subdivide protons into hundreds of small proton beamlets. A hybrid code that simulated proton propagation through a plasma containing a radial electric field essentially reproduced the main features of the experimental observations.

The Livermore team expects protons to complement x rays as a diagnostics tool, not replace them. The team is confident that its pioneering use of protons to create and diagnose plasmas will advance a host of research projects, both at Livermore and at plasma research centers worldwide.

—Arnie Heller

**Key Words:** Janus ultrashort-pulse (JanUSP) laser, National Ignition Facility (NIF), Petawatt laser, plasma, protons.

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Small Particle May Answer Large Physics Questions

Scientists go underground at Livermore to search out evidence of the elusive axion particle.
In one of those interesting intersections of particle physics, astrophysics, and cosmology, scientists from Lawrence Livermore National Laboratory, the University of California at Berkeley (UCB), the University of Florida (UF), and the National Radio Astronomy Observatory (NRAO) have joined together to try to pin down an elusive particle. This particle, called the axion, if it is found to exist and is not just a hypothesis, would be a long-sought relic from the first fractional second of the birth of the universe and one of the most weakly interacting particles known. Experimental verification of the existence of the axion would not only help “balance the budget” for the missing mass of the universe but also clear up one of the thorniest issues in particle physics.

Betting on a Dark Horse

The overall makeup of the universe is well agreed upon among physicists, astronomers, and astrophysicists. Luminous matter—stars and galaxies—is a mere fraction of 1 percent. Other nonluminous matter, such as intergalactic gas, neutrinos, and so on, accounts for not quite 4 percent. The remaining mass and energy of the universe is divided between dark matter (about 23 percent) and dark energy (about 73 percent). What makes up these dark components is unknown. Most of the theories and some observations point to dark matter being predominantly a remnant—perhaps a new and unknown elementary particle—from the very beginnings of the universe, a time known as the big bang.

As to what these particles are, ideas tend to fall into one of two camps: cold dark matter or extremely massive neutrinos—neutrinos much more massive than the three ordinary ones we know. Cold dark matter would be some kind of particle that did not acquire much velocity when it was created in the early universe. Nearby cold dark matter particles are expected to move at about the speed of the stars in our galaxy—velocities that are slow compared with the speed of light.

Massive neutrinos, however, would have been moving extremely fast at their birth in the early universe, and they would probably still have velocities close to that of light. Enormous masses of neutrinos whizzing about seem unlikely, because the density needed to make up a significant portion of dark matter would have smoothed irregularities and prevented the formation of structures that evolved into galaxies in the first few billion years of the universe.

The predominant form of dark matter, most researchers agree, must be some kind of cold dark matter. But which kind, exactly? Two hypothetical elementary particles are the main candidates: a stable weakly interacting massive particle (WIMP) that is about 10 to 100 billion electronvolts in mass, and an axion—a very light particle with neither electric charge nor spin so it interacts hardly at all.

The axion’s extreme lightness (trillions would occupy a sugar-cube volume of space yet weigh less than does half of a proton) and nearly nonexistent coupling to radiation conspire to make the particle incredibly long-lived, perhaps as long as $10^{50}$ seconds. The universe itself is estimated to be only $10^{18}$ seconds, or 100 billion years, old. The axion’s longevity would make it a stable particle for all intents and purposes. If axions exist, they could make up the bulk of dark matter. With an estimated 10 trillion of them packed into every cubic centimeter of space in our galaxy, what they lack in mass...
individually, they would make up for in sheer numbers.

In addition to answering the dark matter question, axions would also handily resolve a difficult issue in the Standard Model, which is the current theory that explains fundamental particles and how they interact. (See the box below.)

Whereas many experiments worldwide are dedicated to the WIMP search, only two are attempting to track down the axion: one in Japan (CARRACK2 at Kyoto University’s Institute for Chemical Research), and the other at Lawrence Livermore under the leadership of physicists Leslie Rosenberg and Karl van Bibber. This team consists of researchers from Livermore, UF, UCB, and NRAO.

“All in all,” says Rosenberg, “observing axions would help solve one of the eleven most important science questions of the new century, as set forth by the National Academy of Sciences two years ago. That question is: ‘What is the dark matter?’ At Livermore, we are seeking the answer and, if successful, we will be at the forefront of the most basic of basic science.” (See the box on p. 11.)

**Hunting the Elusive Axion**

The Livermore experiment is the only one in progress that can challenge recent theoretical estimates of axion mass and coupling. Laboratory physicists Rosenberg, van Bibber, Darin Kinion, Christian Hagmann, Stephen Asztalos (project

**Axions to the Rescue**

The fact is, no one knows if the axion exists. But through observations and calculations, both astrophysical and quantum mechanical, researchers have determined that many pieces in the puzzle would support the existence of this most elusive particle; they have even narrowed the estimates for its mass.

The axion was first proposed as a way to explain a particularly thorny problem in particle physics, that is, the absence of charge-parity (CP) violation in strong nuclear interactions. In physics, if two systems are mirror images of each other but are otherwise identical, and if parity is conserved, all subsequent evolution of these two systems should remain identical except for the mirror difference.

Nature, scientists have come to believe, generally prefers symmetry to nonsymmetry. That is, nature has no preference for right-handed versus left-handed behavior, at least as far as particle physics is concerned. In 1956, physicists Chen Ning Yang and Tsung Dao Lee realized that although many experiments had been conducted to show that mirror symmetry was true for the strong interaction (which holds the nucleus together) and for the electromagnetic interaction (which occurs between electrically charged bodies), no experiments had been conducted for the weak interaction (which is responsible for radioactive beta decay).

Experiments by physicist Chieng-Shiung Wu shortly thereafter showed that, contrary to what was expected, weak interactions did show a preference or “handedness” in cobalt-60. Wu observed the radioactive decay of cobalt-60 in a strong magnetic field. Her experiments proved that there was a preferred direction for emitting beta particles in a decay—in other words, the weak interaction violated the conservation of parity. The violation of parity conservation ran counter to all expectations.

In the 1970s, quantum chromodynamics (QCD) was developed. QCD is the theory of the strong interactions that hold the nucleus together. This theory required that QCD have large amounts of CP violation, yet no such violations have ever been observed even in exquisitely sensitive experiments. However, a completely different source of CP violation, stemming from the weak interaction mentioned above, was discovered first in kaons and recently in mesons produced at the B Factory. (See S&TR, January 1999, pp. 12–14.) Whereas the relatively large effects from the weak interaction are measurable, the analogous CP-violating effects from QCD are somehow suppressed. In an effort to explain this phenomenon, Stanford University physicists Roberto Peccei and Helen Quinn proposed a new symmetry of nature that resulted in a particle dubbed the axion. Early estimates predicted an axion mass of 100 kiloelectronvolts. However, searches for this particle in high-energy and nuclear physics experiments ruled out axions heavier than about 50 kiloelectronvolts.

Astrophysical observations then led scientists to believe that axion mass must be no more than $10^{-3}$ electronvolts—nearly nine orders of magnitude less than originally predicted. Among those observations were the data gathered from a supernova explosion in 1987. By looking at the signals recorded from neutrinos detected on Earth from this particular explosion, astrophysicists concluded that if the axion mass was above $10^{-3}$ electronvolts, the supernova core would have been cooled not just by emitted neutrinos but by axions as well. If this was the case, the length of the neutrino burst associated with the supernova would have been far shorter than that observed.

Axions lighter than a microelectronvolt, however, would have been overproduced in the big bang, resulting in the universe being much more massive than it is. This would be at variance with current observations, where dark matter is at most a quarter of the closure, or critical density of the universe.

Refined calculations have led scientists to believe that the axion must lie in a mass window of approximately $10^{-6}$ to $10^{-3}$ electronvolts.
manager), graduate student Danny Yu, and others are preparing for the next phase of this experiment to track down and identify cosmically generated axions.

The experiment is based on the theory that an axion, when it does interact, decays into two photons with frequencies in the microwave range of the electromagnetic spectrum. UF professor Pierre Sikivie and others formed the idea that an axion could be stimulated to decay into a single photon in the presence of a large magnetic field threading a microwave cavity. The experimental setup, which contains a sensitive radio receiver, requires a tunable microwave cavity permeated by a strong magnetic field and ultralow-noise microwave amplifiers.

The microwave cavity is slowly tuned over a range of frequencies. When the proper frequency of the axion-emitted photon is reached, the axion signal should appear as a narrow line in the spectrum. This experiment sounds simple, but there are some hidden “gotchas.” For instance, the expected signal, corresponding to only a few hundred axion decays per second, would be extremely faint. Rosenberg explains, “For an idea of how small of a signal we’re looking for, consider the signals received on Earth from the Pioneer 10 spacecraft’s transmitter. When Pioneer 10 was at the periphery of our solar system, its signal was $10^{-17}$ watts. The axion signal will be considerably weaker than that—optimistically, $10^{-22}$ watts. And with Pioneer 10, we knew what frequency to look for, a luxury we don’t have with the axion search.”

The Livermore axion experiment began in 1995 with funding from the Department of Energy’s Office of Science, which supports basic science in the public interest. Livermore’s Laboratory Directed Research and Development (LDRD) Program had supported the work that laid the groundwork for the experiment. The goal for the experiment was to extend LDRD efforts on one major front: increased power sensitivity. Livermore’s
plan to do this was to increase the sensitivity of the amplifiers and increase the size and magnetic-field strength of the cavity volume.

The initial proof-of-principle experiments, conducted in the late 1980s at Brookhaven National Laboratory and UF, validated the technology and strategy of the microwave cavity approach. However, they lacked the power sensitivity by two or three orders of magnitude to actually detect an axion. The experiment at Livermore has a much higher total magnetic-field energy, which increases the power conversion and allows the experimenters to edge into the sensitivities theoretically needed to detect cosmic axions from the galactic halo.

Models have predicted a density of about 10 trillion axions per cubic centimeter in Earth’s galactic neighborhood.

Whereas the first experiments had microwave cavities the size of a small coffee can, the Livermore cavity—a copper-plated stainless-steel cylinder—is closer in size to an oil drum (1 meter tall and 0.5 meter in diameter). A powerful 8-tesla superconducting electromagnet is wound around the outside of the cavity. The coil itself weighs 6 tons, and the remaining cryostat weighs another 6 tons.

The magnet’s static magnetic field, which is used to coax axions into decaying, is about 200,000 times more powerful than Earth’s magnetic field. Because the precise frequency of the axion decay is not known, the team has to be able to tune the cavity resonance over the range of possible frequencies, from 0.3 to 3 gigahertz. To do this, a set of tuning rods—metal ones for increasing the frequency of the cavity and ceramic ones for decreasing it—are inserted into the cavity. The rods are moved by stepper motors in tiny, incremental steps of a few hundred nanometers every minute. The lowest frequency occurs when both rods are nearest the wall of the cylinder. The frequency increases (for metal) or decreases (for ceramic) as one or the other approaches the center of the cavity.

The Livermore experiment incorporates the latest available technology for “hearing” any axion signals and separating them from the noise. A very small excess of microwave photons above thermal and electronic noise levels would signal the decay of an axion. Because the expected signal from the decay of an axion is so faint, sensitive amplifiers are needed to boost the signal to detectable levels. The amplifiers used were built by the NRAO and are based on the heterostructure field-effect transistor (HFET)—an exotic semiconductor device developed for military communications and now widely used by radio astronomers to amplify weak radio signals.

The first amplifiers had a noise temperature (which is the figure-of-merit for microwave amplifiers) of about 4.3 kelvins.
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The first amplifiers had a noise temperature (which is the figure-of-merit for microwave amplifiers) of about 4.3 kelvins (4.3°C above absolute zero). More recent NRAO amplifiers reach down to 1.5 kelvins. By comparison, the microwave amplifier in a home satellite TV receiver has a noise temperature of approximately 100 kelvins. In the experimental cavity, the signal output is amplified by low-noise, room-temperature amplifiers and transmitted to a receiver. The receiver then cleans up the signal so that only the portion of bandwidth that might contain a signal is recorded. (This is the same process that happens inside a radio: the receiver selects, amplifies, and converts into audio the music at a particular station’s frequency and eliminates everything else.) The lower the noise the better. Lower noise allows detection of weaker signals, or in this case, weaker-coupled axions.

By early 1996, the Livermore axion experiment was running and producing data. The research team continues to explore the region from 0.3 to 3 gigahertz, which corresponds to an axion mass of 1.2 to 12.4 microelectronvolts. This experiment has increased power sensitivity by two orders of magnitude over the previous experiments and is the first such search to probe realistic axion models. Although no axion decays have yet been detected, these results better refine the upper-limit estimates of axion densities in Earth’s galaxy.

Finding the Answer

The third-generation of axion experiments will require new technologies and techniques to further increase power sensitivity. These experiments will be able to detect axions even with the most pessimistic estimates of coupling and reach other parts of the frequency range not attainable with the current configuration. Rosenberg believes that these future experiments, once in place, will definitively answer whether axions exist.

For this search, HFETs would not be sensitive enough, so the team is turning to a new type of radio-frequency amplifier based on a superconducting quantum interference device (SQUID) developed by a research group under the direction of UCB physics professor John Clarke. Kinion is collaborating with Clarke’s team to develop the new amplifier, which uses a direct-current SQUID made from superconducting niobium and can operate at frequencies well above 3 gigahertz—with record-low noise temperatures of 0.005 kelvin. Once this radio-frequency amplifier and its niobium SQUID are part of the experiment, the signal-to-noise ratio from axion decay will get a much-needed boost, which should make it possible to detect even the most elusive axion.

“What this means,” says Rosenberg, “is that, for the first time, the experiment will be sensitive to weakly coupled axions, even if axions are a minority contribution to the local dark matter halo. These are the axions considered to be the most promising of the axion-based dark matter models. Once we have commissioned this upgrade, we will go back over the ground we have already covered and look for axions with greater power sensitivity. The new upgrade will be sensitive enough to detect even the weakest signals. In other words, this upgraded search will likely be the definitive search.”

Livermore team members (from left) Karl van Bibber, Stephen Asztalos, and Danny Yu work on the axion experimental apparatus. Leslie Rosenberg and Darin Kinion man the control room where signal data are recorded.
The plan for the proposed upgrade has been favorably received by the scientific community and the funding agencies, notes Asztalos. But until the fate of funding for the upgrade is known, the team will continue with the present experimental setup. “We are taking data with the current cavity through the first of 2004,” says Asztalos. “By then, we’ll have searched all the frequencies the present configuration can reach. At that point, we’ll change out the tuning rods to access a different frequency range.”

In addition, graduate student Yu and the team will be injecting a pseudo-axion signal into the cavity. As Yu explains, “Our numerous simulations indicate we should be able to detect these very small signals under the present conditions. But to confirm these findings, we will inject a synthetic signal of the same strength and shape directly into the cavity and see whether we find it in our data analysis.” This plan requires that the noise be well characterized, and Yu notes that the team has done its homework in this regard. “The noise output from the amplifiers is the biggest current uncertainty,” Yu adds.

(a) The current experimental setup is just sensitive enough to detect the strongest of axion signals in a narrow band of possible mass for the axion. Using conventional amplifiers based on conventional heterojunction technology, the lowest decade of the axion mass range can be scanned in 8 years. (b) With the superconducting quantum interference device amplifiers in place for the Phase I upgrade, the team will be able to scan at the current sensitivity more than four times faster and can scan more of the mass range supported by theoretical axion models. (c) In the Phase II upgrade, a dilution refrigerator will lower the system noise temperature from 1.5 kelvins to about 0.002 kelvin, making the experiment sensitive enough to detect the weakest of signals. The Phase II experiment will be the definitive search for the axion.
Is It Here or There or Anywhere?

The team will be on a five-year timeline once the upgrade is funded. The first two years will be devoted to the commission and construction phase. The upgrade will not be an easy one, notes Rosenberg. Azstalos concurs. “It’s somewhat like building a dark room and then crawling around to search out those pinholes that tiny amounts of light leak through,” says Azstalos. “Those leaks then need to be patched. Because the axion signals are so weak and the SQUIDs are so sensitive, there can be no stray electromagnetic signals. So we must be sure there are no electromagnetic leaks.”

This is a tall order when the entire experimental setup is experiencing a magnetic field of 8 tesla and the detectors are the most sensitive in the world to magnetic flux. Good shielding, says Asztalos, is key to the upgrade. “Although the SQUIDs will be some distance from the cavity, we nonetheless need to use a compensating magnet and layers of superconducting and iron shields, similar to those installed around computer screens. Once we have the SQUIDs functioning correctly, we’ll be ready to start operation."

The ensuing series of experiments will then stand to answer these questions once and for all: Does the axion exist? Does it constitute the dark matter that we know is there but cannot see?

“Livermore is poised to answer these fundamental and important questions,” says Rosenberg. “These questions unite the grandest scale (the universe) to the smallest scale (particle physics). And no matter what we discover, it will be illuminating. Either we will find the axion, proving that it exists and is part of the cosmological evolution of the universe, or we won’t. If we don’t find the axion, then something else—perhaps another particle, or symmetry, or path—makes up dark matter. Failure to find the axion would signify that an argument somewhere in the chain of theory is broken. But where? And how far back in the chain do scientists look for the faulty link? If there is no axion, there must be entirely new physics—some strange, new physics that we cannot as yet fathom. And that, too, would be very interesting indeed.”

—Ann Parker

Quarks to Cosmos: Connecting the Smallest to the Largest

In 2002, the National Research Council released a report entitled Connecting Quarks with the Cosmos: Eleven Science Questions for the New Century. The council’s eleven key questions, listed below, focus on the intersection of the universe at its two extremes—the very large and the very small.

What is the dark matter?
What is the nature of the dark energy?
How did the universe begin?
Did Einstein have the last word on gravity?
What are the masses of the neutrinos, and how have they shaped the evolution of the universe?
How do cosmic accelerators work, and what are they accelerating?
Are protons unstable?
Are there new states of matter at exceedingly high density and temperature?
Are there additional space–time dimensions?
How were the elements from iron to uranium made?
Is a new theory of matter and light needed at the highest energies?

Livermore’s search for the axion particle would help scientists determine the makeup of dark matter. Other efforts at Livermore, ongoing or planned, would help answer five others, indicated in red.

Key Words: axion, charge-parity (CP) violation, dark matter, heterostructure field-effect transistor (HFET), microwave photons, particle physics, superconducting quantum interference device (SQUID).

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Each year, some 48 million cargo containers move between the world’s ports. More than 6 million of these enter the U.S., but only about 2 percent are opened and inspected when they arrive at U.S. seaports. The West Coast ports of Los Angeles–Long Beach, Oakland, and Seattle alone process 11,000 containers per day, or about 8 containers per minute.

Because of this high traffic volume, U.S. seaports are especially vulnerable to a terrorist attack. Illicit radioactive materials could be hidden in any one of the cargo-filled containers that arrive at U.S. ports. Yet, searching every shipment would bring legitimate commercial activities to a halt. Improving security at U.S. ports is thus one of the nation’s most difficult technical and practical challenges because the systems developed for screening cargo must operate in concert with ongoing seaport activities.

Working at this intersection of commerce and national security, Lawrence Livermore researchers are applying their expertise in radiation science and detection to develop improved technologies for detecting hidden radioactive materials. One new technology being designed and tested at the Laboratory is a neutron interrogation system for cargo containers. This system will quickly screen incoming shipments to ensure that nuclear materials such as plutonium and highly enriched uranium (HEU) are not smuggled into the U.S.

Balancing Security and Commerce

The Livermore system would bathe suspicious containers in neutrons to actively search for nuclear materials. A truck carrying a container laden with suspicious cargo would be towed over a generator that would bombard the container with neutrons. It would then be towed through an array of detectors, much like driving through a car wash. If the
to Remove a Terrorist Threat

neutrons encountered any fissile material shielded and hidden among the container’s contents—whether produce, clothing, electronics, lumber, automotive parts, or other consumer goods—the interaction would induce tiny fission reactions. These reactions would produce the telltale delayed gamma rays of nuclear materials, which would be picked up by the detectors.

The Livermore system is not intended to screen every container entering a U.S. seaport. Instead, it will be used on the suspect cargo identified by screening procedures, such as radiography or passive radiation inspection, that show some of a container’s contents.

The 19-member project team draws on the talents of personnel from Livermore’s Engineering Directorate as well as the Physics and Advanced Technologies; Chemistry and Materials Science; Safety and Environmental Protection; Nonproliferation, Arms Control, and International Security (NAI); and Computation directorates. “To some approximation, we work like a soccer team of 8-year-olds,” says project leader Dennis Slaughter, technical director of Livermore’s 100-megaelectronvolt (MeV) electron linear accelerator (linac). “By that, I mean we all follow the ball. There are no established positions. Everyone ‘turns to’ the urgent task, and we all help each other without disciplinary distinctions.”

Originally funded by Livermore’s Laboratory Directed Research and Development effort, the detection project was picked up by the Department of Energy (DOE) in 2003 and is now supported by the Department of Homeland Security (DHS). The Livermore team is focused on developing a system that is not only reliable but also commerce-friendly.

“We want a system that can detect small targets of nuclear material—about 5 kilograms of HEU and 1 kilogram of plutonium—with low error rates of about 1 percent false positive and false negative,” Slaughter says. “This system would permit rapid scanning so it wouldn’t disrupt commerce. Our goal is to complete the scan and report in about a minute.”

An Active Interrogation System

Slaughter and his colleagues consider active interrogation to be the most promising option for detecting HEU in containers. Even moderate amounts of shielding make it difficult to passively detect radiation emanating from hidden sources. The high-energy, gamma-ray signature produced when neutrons interact with nuclear material is unique, so the liquid scintillation detectors can readily distinguish it from the signature for normal background radiation.

The neutron scan would pose few risks to cargo. Most residual radioactivity would dissipate within seconds after the scan. In the team’s experiments, radiation dose rates were low.

The team is also working to minimize potential risks to the people who will operate the equipment. The project goal is to limit radiation exposure to the normal allowable doses specified in federal standards for the general public. “Because people might be inside a container during irradiation,” says Slaughter, “we want the radiation dose to be too small to cause harm.”

Slaughter hopes to see such a system as a regular part of cargo container security at U.S. ports. Eventually, it might also be used at foreign ports to scan containers before they are loaded aboard U.S.-bound ships. Since 2002, the Livermore team has done considerable work related to basic science and engineering of the system, developing the detector and establishing requirements for the neutron generator. Research has been conducted at Livermore and at the 88-inch cyclotron at Lawrence Berkeley National Laboratory (LBNL). The team’s timetable is to build a research prototype and evaluate it in a laboratory setting during 2005 and field a vendor prototype at a container port in 2006.

Detecting the Gamma-Ray Signature

Use of a high-energy, gamma-ray signature to detect nuclear materials in containers was proposed by Stanley Prussin, a professor of nuclear engineering at the University of California (UC) at Berkeley, and Eric Norman of LBNL. Prussin, now the chief scientist for the cargo container project, has long consulted with the Laboratory’s NAI Directorate. He became involved with the cargo container effort in the summer of 2002 while on sabbatical at Livermore to work on an unrelated project.

Prussin was familiar with Slaughter’s work and attended a meeting at which modelers discussed the container effort. He says, “It didn’t take too long for me to become convinced that, under their defined worse-case condition, we ought to take another look at the technique they were modeling.”

Rather than high-energy gamma rays, the Livermore team originally considered a system that counted delayed neutrons emitted by neutron-induced fission. Delayed neutrons are emitted from a fraction of a second to a few minutes after fission and have lower energies than the fast prompt fission neutrons. Although delayed neutrons can be a reliable indication of nuclear materials, their yield is low.

Prussin noted a difficulty with using delayed neutrons: Hydrogenous cargo—fruits and vegetables, canned meats, wood, plastics—can absorb the short-lived...
neutrons and thus might interfere with the delayed neutron count.

"Any system we develop must look for fissionable materials that will be well shielded," says Prussin. "If the material is shielded by hydrogenous material, the probability for the delayed neutrons to actually escape from the container into an external detector is very small. In the U.S., we import almost everything under the sun, and many of those imports are hydrogenous."

Instead of the delayed neutron count, Prussin suggested the team measure the gamma rays emitted. Fission products make numerous gamma rays that have comparable decay characteristics of delayed neutrons. Yet, says Prussin, the probability of the neutron-induced gamma rays escaping from the container through hydrogenous material is about 1,000 times greater than it is for delayed neutrons.

In 2003, Prussin and Slaughter worked with Norman to arrange for a series of experiments, funded by DOE’s Office of Science, at LBNL’s 88-inch cyclotron. The first experiment was conducted using a deuteron beam on a beryllium target. The researchers also bombarded well-shielded sample targets of uranium-235 and plutonium-239, irradiating each sample for 30 seconds, going back and forth to get enough statistics for a relevant evaluation.

"The high-energy gamma rays essentially represent a unique signature that fission has occurred," says Prussin, "both because of their energies, which are above 3 MeV, and because of their temporal behaviors."

Researchers followed up the LBNL measurements with signature verification experiments at a new laboratory commissioned at Livermore for scanning cargo containers. The laboratory houses a 6-meter container provided by APL, one of the world’s largest container transportation companies, and gives the researchers a realistic testing environment. In these experiments, they irradiated a 22-kilogram target of natural uranium with a beam from a 14-MeV neutron source. Their results confirmed the intensity of the signature in a realistic cargo-scanning configuration using 150 grams of HEU and a low-intensity source.

Good Results with Simulated Cargo

In studies using simulated cargo stacked around the target, the gamma rays produced were very intense, between 2.5 and 4 MeV. The neutron beam energy must be high enough to penetrate the cargo but low enough to avoid interfering activation. (The research indicates the neutron source should be between 5 and 8 MeV.) Although gamma radiation is 10 times stronger than delayed neutrons, it is weak but detectable, and high-resolution detectors are not required to measure it. Large arrays of low-resolution detectors, such as liquid scintillators, can be cheaply produced and easily deployed.

One question the team must resolve is what accelerator characteristics are required for practical field applications. "Accelerators that can give the appropriate deuteron beam energy intensity on the appropriate target can, in principle, be manufactured commercially and for a reasonable amount of funding," Prussin says. "We don’t know that one has been constructed for the exact conditions we’ll specify, and we may have some technical issues to address. But our requirement is not for a scientific system. What we will want is a much simpler device."

Meanwhile, the team wants to resolve some problems found when using Monte Carlo codes to mock up experiments and test them on the computer. "We are developing a method that seems likely to serve our purpose," says Prussin. Experiments on irradiation of uranium, which will be conducted at LBNL, are being designed to help the researchers understand how well the computational procedures represent the experimental data.

Simultaneously, efforts are moving forward to develop a large array of liquid scintillators that are sensitive to both neutron and gamma rays. As currently envisioned, the design includes a bank of 20 liquid scintillator–filled tubes spanning each side of the car wash.

Benefits of Liquid Scintillator

Liquid scintillator is a good candidate material for the cargo interrogation problem. It has a fast response time, and it can be inexpensively instrumented to scan a large volume of material, which helps to ensure that a large fraction of the particle flux emitted by the neutron-irradiated nuclear material will be detected. Livermore physicist Adam Bernstein, who leads the detector design team, says, "Neutrons and gamma rays create a 20-nanosecond pulse of blue light when they scatter in the medium, and this
fluorescent pulse can be detected in photomultiplier tubes.” Such detectors can be used in various cargo detection and interrogation scenarios. For example, even with the neutron source off, the detector array may still be sensitive enough to scan cargo for some types of radioactive materials of concern.

The segmented array, which has a response time of about 100 nanoseconds or better, would indicate the location or spatial extent of radioactive material hidden in the cargo. “By establishing the geometric extent of the radioactive material,” says Slaughter, “we can better differentiate cargo with small amounts of uranium distributed throughout from normal cargo with a small component of nuclear material hidden in it.”

“The liquid scintillator project dovetails nicely with the Laboratory’s mission,” says Bernstein. “Livermore in general is a center for radiation detection because of nuclear weapons and other nuclear physics research.” He adds that the liquid scintillator work is building on a detection technology that has been used for years in high-energy physics. “These types of detectors are often used in fundamental physics research, where we engage in neutrino physics and dark-matter searches, but not for practical applications such as fissile material detection. In this project, we’re taking a technology that’s a workhorse in high-energy physics and applying it in the real world.”

Using liquid scintillators in such applications brings its own challenges for detector designers. “We have a lot of work to do in developing the algorithms for the gamma-ray signal that comes out of cargo containers,” says Bernstein. “We want to process the signal in a different way than we do in a physics experiment where we don’t have any time constraints and we can wait to obtain data. In this application, we have about a minute to decide whether the cargo container is suspicious or not.”

Keeping the false-positive and false-negative rates low is another technical issue facing the designers. “We want to optimize the signal-to-background ratio as best we can,” says Bernstein, “and we’ll have to establish the number of false positives that are acceptable. For example, if a few hundred cargo containers go through the car wash each day, a false-positive rate of 1 percent might be unacceptable because that could mean you stop the chain once a day to remove a container for closer inspection.”

Another challenge is to develop a robust system, one that can work continually for months or years and that can be operated by people who are not experts in radiation detection. “People frequently underestimate that aspect of the development process,” Bernstein says. Members of the team built a small prototype of a 0.6-meter-tall detector, which they successfully tested. This spring, they are working with an array of four detectors, each 2 meters tall and 20 centimeters in diameter, and according to Bernstein, the team expects this testing to result in some iterations of the design. By the end of 2004, the team hopes to be working on a larger array that would cover one side of the car wash.

“We most likely will build it at Livermore. While we’re designing the prototype, we’ll also try to make the system portable, so we can take it into the field—and possibly test it at a port.”

Slaughter is hopeful that by 2005 the Laboratory team will add a commercial partner to develop a system that could eventually be deployed in the fight against global terrorism.

—Dale Sprouse

Key Words: cargo containers, gamma rays, highly enriched uranium (HEU), homeland security, liquid scintillator, nuclear materials, neutron generator, plutonium, terrorism, weapons of mass destruction.

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Radiant space heater, people near the heater begin to feel warmer before the heater has had a chance to raise the temperature of the entire room.

Since the early days of modeling, thermal radiation transport codes have been used at Livermore to simulate how thermally generated photons interact with material. To set up a calculation using these codes, computer scientists divide a material into chunks called zones. Then they incorporate such data as the material’s properties and the photons’ initial energies, frequencies, and directions of travel. Time is also chopped into discrete steps. Once the problem is set up, the computer grinds through its calculations—step by step, photon by photon, zone by zone—to model how the photons, which transport the thermal energy, move through the material.

Modeling this thermal radiation phenomenon has always been difficult, Brooks notes. For example, a photon’s mean free path—the average distance it travels before colliding with another photon—may be shorter than the length of the zone, or its mean free time may be shorter than the time step. These problems are frequently encountered in opaque systems such as the interior of stars. Scientists have developed several mathematical methods to solve such problems, including Monte Carlo radiation transport.

**Tweaking for Results**

Until 1970, the Monte Carlo method used to solve thermal radiation problems was very unstable, Brooks says. “In solving the equations over and over, proceeding through each time step, the numerical solutions had errors that grew over time. It wasn’t a physical phenomenon, but a mathematical artifact that popped up in solving the problem on the computer.”

In 1971, Joe Fleck and J. D. Cummings worked out an innovative method to dampen this mathematical instability, a scheme they called implicit Monte Carlo (IMC). In essence, they introduced the concept of effective scattering, wherein a fraction of the radiative energy absorbed during a time step is instantly reemitted in all directions before the next time step. Once the problem is set up, the computer grinds through its calculations—step by step, photon by photon, zone by zone—to model how the photons, which transport the thermal energy, move through the material.

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**Monte Carlo Not Just for Gamblers**

Radiation is energy on the move in the form of light rays or particles such as electrons. Thermal radiation consists of photons, which display characteristics of both high-speed particles and electromagnetic waves. The study of radiation transport deals with predicting and measuring how these photons move through matter. Put simply, thermal radiation transport is a calculational method that examines how heat moves around.

Such calculations are an important part of models that, for example, simulate stellar evolution or inertial confinement fusion experiments. For a mundane example of radiation transport in action, consider a radiant space heater such as those commonly found in homes and garages. Radiant heaters generate invisible infrared radiation that transfers heat not to the air—as convection heaters do—but directly to objects and people themselves. With a radiant space heater, people near the heater begin to feel warmer before the heater has had a chance to raise the temperature of the entire room.
In the late 1980s, Fleck hired Brooks as a postdoctoral fellow to extend the IMC method so that it would be useful for lasers. Brooks developed a technique called symbolic IMC. “This technique removed the scattering problem,” he says, “and, instead, it gave us a system of nonlinear mathematical equations, or a matrix, to solve.”

Although the symbolic IMC method was faster and cleaner than the original IMC method, its nonlinear system still caused a problem: The noise in opaque materials required large numbers of Monte Carlo particles. Brooks and Szöke returned to this problem in 2003, to try to speed up the calculations. They found that the mathematical noise in the Monte Carlo system corresponds to what happens when a photon is absorbed in the zone in which it originates. This quick absorption of photons happens frequently in opaque materials. “As a result,” says Brooks, “when we’re modeling an opaque material, we often end up wasting a lot of time using computational power to solve a part of the problem that can easily be done with a pencil and paper.”

The breakthrough came when the scientists realized that calculations aren’t needed for all of the photons—only for the ones that escape one zone and are transported to the next. Szöke suggested subtracting the calculations of the photons being emitted and reabsorbed—a mathematical construct they called the difference formulation. “So far,” Brooks says, “the difference formulation is working very well.”

The initial test problem was a one-dimensional simulation of a thick material slab. The simulated slab was divided into many zones with various opacities and time steps. Using the difference formulation increased the algorithm processing speed by factors of up to 1 million, whereas using the older formulation on the massively parallel supercomputers improved speed by factors of 1,000 or so. The makers of supercomputers need not worry, however, because the difference formulation can be adapted to parallel computing, and, says Brooks, the demands of computer users for increased speed are insatiable.

### Algorithms in Nanoscience

Mathematical improvements to Monte Carlo methods benefit other Livermore research areas besides astrophysics, including nanoscience. Williamson, Hood, and Grossman, who all work in PAT’s Quantum Simulations Group, model systems with only 100 to 200 atoms to better determine their material properties. “At these sizes, quantum mechanical effects can change a material’s properties,” says Grossman. “For instance, shining laser light at a palm-size piece of silicon will cause the silicon to emit photons at a wavelength not visible to the human eye. If we shine the same laser light on a silicon quantum dot of 100 atoms (about 2 nanometers square), the dot emits visible light. What’s more, the color of the emitted light—whether blue, red, or something in between—will depend on the size of the silicon chunk.” (See S&TR, November 2003, pp. 4–10.)

Why do materials behave so oddly in such small quantities? The answer can be found in a solution of Schrödinger’s equation, which describes the properties of an electron’s wave function. In this world of the very small, the electron is treated as a wave, not as a particle. Solving Schrödinger’s equation for one particle is simple enough to be done by hand. But as the number of electrons or particles grows, the calculation’s complexity increases exponentially, so computers—and lots of computational time—are required to solve the problem.

One approach to these calculations is called the Quantum Monte Carlo (QMC) method. The QMC method uses random numbers to generate an approximate answer with an error bar that indicates the accuracy of the approximation. The smaller the error bar, the more accurate the approximation. To shrink the error bar, the code must choose more random numbers, which increases the program’s processing time because the code runs more iterations. Ideally, the

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**Graph:**

A material’s temperature is increased by the transport process of a thermal wave, which is propagating from left to right. The material was initially at 0.01 temperature units. At the start of the simulation, it was abruptly heated on the left side at a temperature of 1 unit. The black curve shows the results from a simulation using the standard formulation. The curve’s jagged appearance is caused by the mathematical noise in the calculations. The red curve shows the results from a simulation using the difference formulation. This calculation was performed using the same run time on the same computer as the standard formulation. The Monte Carlo noise in the difference formulation is too small to be shown.
Monte Carlo Primer

In 1946, mathematician Stanislaw Ulam named a set of statistical problem-solving methods “Monte Carlo.” The code itself was created at Los Alamos National Laboratory during the Manhattan Project, and the first Monte Carlo calculations were performed in 1948 on the ENIAC, the world’s first electronic digital computer. Monte Carlo methods use sequences of random numbers to perform computer simulations. Every simulation is based on events that happen randomly, so the outcome of a calculation is not always absolutely predictable—much like the throw of a dice or turn of a card. Monte Carlo is used routinely in diverse fields, including simulations of radiation transport in Earth’s atmosphere and esoteric subnuclear processes in high-energy physics experiments. The difference between Monte Carlo, the method, and Monte Carlo, the gaming capital, is that the method’s “game” involves a physical system rather than a game of chance, and its outcome is not a pot of money or stack of chips, but rather the solution to a problem.

Simple Monte Carlo at Work

A simple example of the Monte Carlo method is shown in the figure at right, where random numbers are used to calculate the area under a curve as a fraction of the rectangular box encompassing the curve. The original curve is enclosed within a rectangle, and points within the rectangle are chosen at random. The number of points under the curve is then determined as a fraction of the total points chosen. Because the total area of the enclosing rectangle is known, the ratio of the points under the curve to the total points approximates the fraction of the area lying under the curve. As more points are chosen, the approximation becomes more exact.

For example, when only 500 points are chosen, the calculation estimates the area under the curve as 69.6 percent of the total area within the rectangle. But the accuracy of this estimate may be off by as much as 6 percent. Accuracy improves when more random numbers are chosen. With 5,000 points, the area under the curve is estimated to be 63.96 percent, and the error shrinks to 0.29 percent. With 500,000 points, the area is 63.53 percent with an error of 0.13 percent.

A computer code using Monte Carlo calculations can estimate the area under a curve as a fraction of the rectangular box that encompasses the curve. (a) When the code generates 500 random points, the area under the curve is estimated to be 69.6 percent of the rectangle, but the error is 5.9 percent. (b) With 5,000 points, the area is estimated to be 63.96 percent, and the error shrinks to 0.29 percent. (c) With 500,000 points, the area is 63.53 percent with an error of 0.13 percent.
error bar should be smaller than the differences being measured in the calculation. For example, if scientists want to determine whether the light emitted by a particular quantum dot will be blue or red, they set the code to calculate an answer that’s accurate enough—that has an error bar small enough—to differentiate between the opposite ends of the visible spectrum.

In determining whether an answer can be trusted, scientists can either run the simulation until the error bar is small enough or compare the results with accuracy benchmarks established in physical experiments. “In nanoscience, experiments are difficult to do because of the extremely small scales,” says Grossman, “so the ability to use highly accurate benchmark methods such as QMC are quite valuable.”

Until recently, however, QMC was only practical when looking at systems composed of small numbers of atoms. “It was a scaling issue,” says Grossman. “For instance, if it took 10 minutes for QMC to run a problem with 10 atoms, then running that same problem with 100 atoms required 10,000 minutes—or nearly a week of computational time.”

To solve the scaling problem, Grossman, Williamson, and Hood applied a novel mathematical approach called the Wannier basis to the QMC algorithm. Essentially, they performed a mathematical transformation, taking a problem that was difficult to solve and transforming it into a domain where it was easier to solve. For example, one common mathematical transformation is using logarithms, a method for converting difficult multiplication problems into simpler addition problems. Another is performing a Fourier transform, to change the wave of a complex electrical signal into simpler sine and cosine waves.

In the original QMC algorithm, the time needed to solve a problem scaled as the cube of the number of atoms involved. Applying the Wannier transformation to QMC produces an algorithm that scales linearly. As a result, the 100-atom system, which previously took a week to process, now requires only 100 minutes.

Williamson is working with Livermore physicist Fernando Reboredo to optimize these Wannier transformations. “We’re using nonorthogonal basis functions, which speed up the code another five times,” says Williamson. “That increase reduces the run time for the 100-atom system to only 20 minutes. The code also uses eight times less memory, so we can study much larger nanoscience problems.”

Math That Makes a Difference

Even as supercomputing hardware improves, computational scientists, physicists, and others look for better ways to increase the speed of their calculations. Each advance in trimming the time to run a code opens the possibility for simulating a process in more detail and for running multiple simulations in the same amount of time—or even less time—than had been required to process only one.

“Each step forward,” says Brooks, “is based on the work that was done before. The advances often happen when people have the opportunity to come together and think differently. It’s the collision of people and ideas—through hard work and sudden insights—that leads to these new mathematical constructs, which, in turn, yield faster and in some cases more accurate predictions of phenomenon. In a way, these innovations owe much to serendipity, a lucky roll of the dice—it’s Monte Carlo in the scientific realm.”

—Ann Parker

Key Words: algorithm, difference formulation, implicit Monte Carlo (IMC) method, Monte Carlo, nanoscience, quantum dots, Quantum Monte Carlo (QMC) method, thermal radiation transport, Wannier basis.

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Shocking Plutonium to Reveal Its Secrets
A new two-stage gas gun at the Nevada Test Site is helping scientists better understand the behavior of plutonium.

One of the most daunting scientific and engineering challenges today is ensuring the safety and reliability of the nation’s nuclear arsenal. To effectively meet that challenge, scientists need better data showing how plutonium, a key component of nuclear warheads, behaves under extreme pressures and temperatures. On July 8, 2003, Lawrence Livermore researchers performed the inaugural experiment of a 30-meter-long, two-stage gas gun designed to obtain those data. The results from a continuing stream of successful experiments on the gas gun are strengthening scientists’ ability to ensure that the nation’s nuclear stockpile is safe and reliable.

The JASPER (Joint Actinide Shock Physics Experimental Research) Facility at the Department of Energy’s (DOE’s) Nevada Test Site (NTS) is home to the two-stage gas gun. In the gun’s first test, an unqualified success, Livermore scientists fired a projectile weighing 28.6 grams and traveling about 5.21 kilometers per second when it impacted an extremely small (about 30-gram) plutonium target. This experiment marked the culmination of years of effort in facility construction, gun installation, system integration, design reviews, and federal authorizations required to bring the experimental facility online.

Ongoing experiments have drawn enthusiastic praise from throughout DOE, the National Nuclear Security Administration (NNSA), and the scientific community. NNSA Administrator Linton Brooks said, “Our national laboratories now have at their disposal a valuable asset that enhances our due diligence to certify the nuclear weapons stockpile in the absence of underground nuclear weapons testing.”

Bruce Goodwin, associate director of Livermore’s Defense and Nuclear Technologies Directorate, said, “I am proud of the team effort that has produced the successful JASPER shots. I have personal appreciation for the extraordinarily challenging nature of plutonium. The precise data generated by these gas-gun experiments will open up our scientific understanding of plutonium.”

Mark Martinez, Livermore’s JASPER test director, notes that the experimental results have been so good they are generating significant interest in accelerating the test schedule. “The JASPER data are demonstrating superb quality and indicate that JASPER will meet its intended goal of generating high-precision plutonium data,” he says. JASPER was built at a total cost of about $20 million and sited in existing aboveground buildings at NTS. The facility was developed by personnel from Lawrence Livermore, Los Alamos, and Sandia.
national laboratories and Bechtel Nevada, the NTS prime contractor.

Gas Guns Well Established

A well-established experimental technique for determining the properties of materials at high pressures, temperatures, and strain rates is to use a gas gun to shock a small sample of material with a projectile traveling at high velocity and then diagnose the material’s response. Lawrence Livermore’s three two-stage gas guns have made important contributions to solving scientific puzzles in condensed-matter physics, geophysics, and planetary science. For example, in 1996, Livermore’s largest two-stage gas gun produced metallic hydrogen for the first time. Recently, with experimental techniques that will be used at JASPER, this gas gun was also used to determine the melting point of iron at Earth’s core.

Neil Holmes, chief JASPER scientist and head of Livermore’s shock physics program, says that two advantages of a gas gun are its proven dependability and scientists’ extensive experience with it. Lawrence Livermore has more than 40 years experience shocking materials with gas guns. “When the projectile hits the target, the pressure wave is as steady as it can be,” says Holmes. “As a result, researchers can focus on the target and diagnostics rather than the gun’s performance.”

Scientists fire projectiles from the JASPER gas gun into plutonium targets equipped with instruments for measuring and recording data. The projectile’s impact produces a shock wave that passes through the target in a millionth of a second or less, creating pressures of more than 600 gigapascals (6 million times the pressure of air at Earth’s surface), temperatures to thousands of kelvins, and densities several times that of plutonium’s original solid state.

The JASPER team’s role in the Stockpile Stewardship Program is to measure the fundamental properties of plutonium. Data from the experiments are used to determine material equations of state, which express the relationship between pressure, density, and temperature. The equation of state is essential for generating reliable computational models of plutonium’s behavior under weapons-related conditions. Knowledge of these properties is required to assess, without nuclear testing, the performance, safety, and reliability of nuclear weapons.

Long Qualification Phase

Prior to the construction of JASPER, the only facility available for performing shock tests on plutonium was the 40-millimeter, single-stage gas gun built at Livermore and currently located at Los Alamos. This gun can achieve a maximum projectile velocity of about 2 kilometers per second and up to 30 gigapascals of pressure.

Researchers determined that much higher projectile velocities were needed to achieve the desired conditions for plutonium research. Two-stage, light gas guns similar to the JASPER gun have been operational at Lawrence Livermore, Los Alamos, and Sandia national laboratories for many years, but they are not licensed to perform experiments on plutonium.

In the late 1990s, it was recognized that a new two-stage gas-gun facility dedicated to plutonium research, and located in a remote location, could provide valuable data on plutonium’s equations of state. Ideally, the facility would operate with a short turnaround time between shots and at a modest cost per shot. In early 1998, a study conducted by a team of scientists and engineers from several national laboratories identified the Able Site at NTS as the best location. The site’s three main buildings had previously been used by Los Alamos’s nuclear test program.

Construction and facility modifications at the Able Site started in April 1999 and were completed in September 1999. The JASPER gas gun was installed in early 2000, and the first system-integration demonstrations were completed in September 2000. From February 2001 to April 2003, Livermore staff verified the gun performance and containment systems, validated the diagnostics and operating procedures,
JASPER Gun Matches Livermore’s

The JASPER gas gun was designed to match the internal dimensions of the large two-stage gas gun at Livermore, which has been operational since 1972. By copying that design, researchers took advantage of the extensive database and experience that exists from using the Livermore gun, thereby minimizing the effort required to characterize the JASPER gun at start-up. Although the internal dimensions are the same, JASPER’s containment system is significantly more complex because the Laboratory’s gas gun is not used with hazardous materials such as plutonium and, hence, does not require a special material-confinement system. (See the box on p. 8.) The Livermore gas gun serves as a test bed for developing techniques and training personnel for future experiments at JASPER. “We work out JASPER experiments first on our two-stage gun at Livermore with nonnuclear materials,” says Martinez.

JASPER’s gas gun is driven first with gunpowder and then with a light gas. In the first stage, hot gases from the gunpowder propellant drive a 4.5-kilogram plastic deformable piston down a pump tube. The piston compresses a light gas, typically hydrogen, as it travels down the narrowing tube. This gas, which is the second-stage driving medium, is compressed until it builds up enough pressure to burst a valve. The explosive gas accelerates a 15- to 30-gram projectile down the launch tube toward the target at a velocity of up to 8 kilometers per second. (See the figure on p. 9.)

The projectile is made of plastic with a flat, metal plate embedded in its face to directly impact the plutonium target. Depending on the desired shock pressure, the metal plate is made of aluminum, tantalum, or copper. A typical projectile measures 28 millimeters in diameter and weighs 25 grams.

The speeding projectile enters the primary target chamber (PTC), which houses the plutonium target. Just prior to entering the PTC, the passing projectile is sensed by a continuous x-ray source and detector, which

The two-stage gas gun at the JASPER Facility in Nevada fired its first shot in July 2003. Livermore operates the facility for the National Nuclear Security Administration. Bechtel Nevada supplies resources for facility maintenance and operation, and diagnostic design and operation.

Electronics project engineer John Warhus monitors preparations for a gas-gun experiment from the JASPER control room.
trips a switch that triggers the detonation of the ultrafast closure valve. This valve effectively traps radioactive debris within the PTC following the projectile’s impact on the plutonium target.

When the projectile hits the plutonium target, the impact produces a high-pressure shock wave of about 600 gigapascals. The temperature, a critical variable in a material’s equation of state, can reach as high as 7,000 kelvins. By comparison, the surface of the Sun is about 5,800 kelvins. The destroyed plutonium target is contained within the PTC. Following the experiment, the PTC is discarded and sent to the federal Waste Isolation Pilot Plant in New Mexico.

Projectile velocities are precisely determined by experimental parameters such as the type and amount of gunpowder, the driving gas, the diameter of the barrel, and the mass of the projectile. JASPER facility manager Ben Garcia notes that as a precaution, all shots are first simulated using gun performance codes on computers. “We want to make sure we don’t produce any pressures that could exceed the design limits of the gun,” he says.

Livermore engineers adopted a dual-layered approach for JASPER’s two-stage gas gun to ensure that plutonium dust or fragments are not released into the building or the environment after each experiment. The two layers are the primary target chamber (PTC) and the secondary confinement chamber. The PTC, which houses the plutonium target, is designed to contain target material under worst-case conditions following impact with the speeding projectile. The PTC is discarded after every shot and shipped to the federal Waste Isolation Pilot Plant in New Mexico.

Lead PTC engineer Matt Cowan notes that designing the PTC has been a challenge because of the dynamic loading of the PTC during a shot. “We anticipated two potential failure modes in the PTC: loads that cause a rupture in the pressure vessel and loads that cause a dynamic gap at the sealing surfaces.”

The primary target chamber, which houses the plutonium target, is designed to contain target material under worst-case conditions. It is located inside the secondary confinement chamber. Other key features inside the secondary confinement chamber include the flash x ray for measuring projectile velocity, the continuous x ray for tripping the ultrafast closure valve, and the high-explosive gas accumulator for trapping gases after the ultrafast closure valve has been tripped.

The engineers conducted extensive modeling to determine where plutonium debris would be distributed inside the PTC following impact with a projectile. In addition, experiments using plutonium surrogates provided valuable experience in refining the design of the PTC. For example, researchers applied a layer of phosphorous-32, which has a two-week half-life, to a gold target because radioactive materials are easier to detect if they escape from the PTC. Debris shields were added to absorb some of the momentum of high-velocity impacts and to protect critical O-rings that seal the PTC’s interior. “JASPER experiments cause particulates to fly everywhere at extremely high speeds, so we need to protect O-rings from the sandblasting effect,” explains Cowan. Engineers also expanded the volume of space around the target impact plane.

Livermore’s High Explosives Applications Facility (HEAF) was used to demonstrate the PTC’s design limits. The testing at HEAF created explosive forces about 150 percent of the predicted dynamic loads that the PTC would experience with plutonium targets. The data from HEAF agreed with results from simulations and strengthened the engineers’ confidence that plutonium would be contained.

The PTC’s ultrafast closure-valve system at the chamber’s entrance was designed and manufactured by Ktech Inc. (Albuquerque, New Mexico), and adapted for use on JASPER by Livermore engineers. The valve closes a 1.3-centimeter-diameter aluminum tube in about 60 microseconds by detonating 90 grams of high explosives wrapped around the tube. The valve then traps plutonium debris within the PTC. “A splash-back of plutonium travels at the same speed as the projectile, so we need to close the tube extremely quickly,” says Cowan.

The PTC is located in the secondary confinement chamber, which has a large circular door to access the PTC. The secondary chamber ensures that any material that might escape from the PTC will not migrate into the building. “The secondary chamber is not expended after a test,” says Cowan, “and it is not significantly challenged during a shot.”

As a final precaution, radiation-control technicians, fully suited with respirators and radiation detectors, enter the gas-gun building following every shot to make sure the plutonium debris has been fully contained within the PTC.
Currently, the major diagnostic instruments are two flash x-ray units, which measure projectile velocity to within 0.1 percent accuracy, and electrical pins, which measure the speed of the shock wave from the impact of the projectile. The facility also has the capability to use a Velocity Interferometer System for Any Reflector (VISAR), a tool that measures the velocity of the exploding target by recording Doppler-shifted reflected light. These data are essential to understanding plutonium’s material properties. Additional diagnostic instruments are planned that will measure the temperature, electrical conductivity, and other characteristics of the target after impact.

**Targets Made at Livermore**

The first series of JASPER experiments used plutonium targets nicknamed “top hats,” which consist of a plutonium disk the size of a half dollar bonded to a smaller, nickel-size disk of plutonium. The top hat design was first proven on Livermore’s two-stage gas gun with copper, aluminum, and tantalum disks.

Engineer Randy Thomas, who is responsible for the production and machining of JASPER targets at Livermore, notes the top hat targets must meet extremely precise requirements: flat to within 2.5-millionths of a meter with the two faces of each disk parallel to each other within 2.5-millionths of a meter. Meeting such tight tolerances requires a complex and time-consuming production and machining process. Plutonium is first cast into a cylinder using a graphite mold. The resulting cylinder is sliced into disks and then heated to eliminate internal stress. The disks are rolled with specific orientations to obtain correct metallurgical properties, heated again, and machined until they are within less than 1 percent of their final dimensions. Then the disks are checked for the correct density and radiographed to detect any voids and inclusions. Even slight imperfections result in the plutonium target being unusable. The disks undergo final machining and inspection to ensure they are flat and parallel. Then they are bonded together.

After final measurement and characterization, the plutonium is loaded into the target assembly. The assembly is aligned beforehand so that the projectile will impact the target at its exact center. The target assembly is leak tested, backfilled with an inert atmosphere, placed in a federally approved shipping container, and trucked to NTS. Holmes describes the final product as, “The highest quality plutonium samples we’ve ever seen. That quality reflects the superb plutonium fabrication and machining capabilities at Livermore.”

The top hat plutonium target uses 13 diagnostic electrical-shorting pins mounted on its surface: 6 on the large disk, 6 on the small disk, and 1 that fits through a hole in the middle of the smaller disk. On impact from the projectile, a shock wave travels through the base plate and electrically shorts the pins. The velocity of the shock front passing through the target is calculated using the measured shock arrival times from the shorting pins and the known target thickness. The pins’ orientations allow for correcting the effects of projectile tilt during target impact.

**Data for Equations of State**

Livermore scientists are excited about the experimental results. “The JASPER gas gun
has validated itself as an important tool for plutonium shock physics. Everything has worked as planned,” says Holmes. “We’re thrilled with the quality of data. These experiments have never before been done on plutonium with this accuracy.”

Each JASPER experiment provides one data point on plutonium’s Hugoniot curve. The Hugoniot is derived from conservation of mass, momentum, and energy equations using experimental values of projectile velocity (flash x-ray data) and shock velocity (electrical pin data). Hugoniot curves are then used to develop material equation-of-state models used in weapon performance calculations.

“Equation of state is one of the most important elements in building a robust capability for predicting weapon performance,” says Holmes. “We mainly use theoretical equations of state for our simulations. That’s not sufficiently accurate for stockpile stewardship purposes. We need data that will either validate our theories or force changes in them.”

JASPER experiments complement the subcritical nuclear materials experiments that Livermore scientists have conducted underground at NTS since 1997. (See S&TR, July/August 2000, pp. 4-11.) Those experiments use high explosives to blow apart tiny amounts of plutonium but stop short of nuclear chain reactions. These complex hydrodynamic experiments provide vital information on the behavior and performance of aging nuclear materials.

The gas gun allows scientists to study plutonium over a broader range of conditions than is the case with subcritical experiments. Moreover, gas-gun technology eliminates uncertainties introduced by high-explosive-driven experiments. Holmes points out that gas-gun experiments can generate distortions in projectiles, but the distortions are always the same shape and are readily accounted for.

**Future Directions**

The early experimental successes have generated significant discussion regarding how to schedule more experiments and how to extract more data from each experiment.

To meet the increasing demand for experiments, the JASPER team is exploring ways to increase the number of experiments scheduled from the current 12 per year. For example, a glove box (required for safe handling of plutonium) has been commissioned at the Device Assembly Facility (DAF) at NTS, located about 15 kilometers from JASPER. Livermore managers are planning to ship plutonium samples from Livermore to DAF for final bonding and placement in the target assembly to support a busier schedule. Using DAF would also decrease the risk of damage from transporting finished plutonium targets and diagnostics over a long distance.

New diagnostics are being considered to generate additional information about the physical processes occurring in shocked plutonium. For example, plans are under way to measure electrical and thermal conductivity as well as sound...
speeds of shocked plutonium targets. The optical properties of the shocked target—the light emitted during an experiment—will also be studied using lasers.

Another set of experiments being planned would test aged plutonium to determine if its shocked properties are different from newly cast material. At the same time, physicists and engineers are looking at new projectile designs, such as those made of different densities, to obtain specific shock pressures. Martinez recalls how Livermore personnel once predicted, “If we build it (JASPER), they will come.” He notes that physicists at Los Alamos are designing a series of experiments, as are colleagues from Britain’s Atomic Weapons Establishment. In fact, about 10 years of shots are already in the planning stages. Martinez says, “People are getting new ideas all the time to find out more about plutonium with JASPER.”

—Arnie Heller

Key Words: Device Assembly Facility, equation of state, gas gun, Hugoniot curve, Joint Actinide Shock Physics Experimental Research (JASPER) Facility, Nevada Test Site (NTS), plutonium, stockpile stewardship, Velocity Interferometer System for Any Reflector (VISAR).

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Seeing the Universe in a Grain of Dust

Imagine traveling halfway to Jupiter—3.2 billion kilometers—for a small handful of comet dust. That’s the mission for the National Aeronautics and Space Administration’s (NASA’s) Stardust spacecraft launched on February 7, 1999. This past January, Stardust flew by Comet Wild 2’s nucleus and through a halo of gases and dust at the comet’s head, collecting cometary dust particles released from the surface just hours before. In 2006, the spacecraft will deliver the less than 1 milligram of particles to Earth. A Lawrence Livermore team is perfecting ways to extract and analyze the tiny particles using its new focused-ion-beam instrument and SuperSTEM, a scanning transmission electron microscope.

Stardust is the first NASA space mission dedicated solely to collecting comet dust and will be the first to return material from a comet to Earth. Comets are the oldest and most primitive bodies in the solar system. They are formed from frozen gas, water, and interstellar dust and may have brought water to Earth, making life possible. Wild 2—pronounced “Vilt 2” after the name of its Swiss discoverer—was formed with the Sun and the rest of the solar system 4.5 billion years ago. For billions of years, it has circled the Sun in the Kuiper Belt, a region beyond the orbit of Neptune. Scientists think comets from this region have escaped the warming, vaporization, and collisions that have altered matter in the inner solar system.

Unlike Halley’s Comet, which has been altered as a result of orbiting the Sun for a long time, Wild 2’s pristine composition is expected to offer a rich source of information about the solar system’s potential building blocks.

As the 5-meter-long Stardust spacecraft traveled through Wild 2’s dust and gas cloud, to within about 100 kilometers of the comet’s nucleus, particles were captured in the spacecraft’s collector grid. The 1,000-square-centimeter grid is filled with the silica-based material aerogel, whose lightness minimizes damage to the grains as they encounter the spacecraft at a speed of about 21,000 kilometers per hour—or six times faster than a bullet. In the late 1980s, Livermore scientists developed an aerogel made up of 99 percent air, making it ideal for NASA projects. Mission planners expect to have collected more than 1,000 grains between 2 to 5 nanometers in diameter. Most of the grains will be heterogeneous aggregates of carbonaceous matter, glass, and crystals.

Livermore is part of the Bay Area Particle Analysis Consortium (BayPac) formed to develop regional expertise on interplanetary dust particles. BayPac’s members include University of California (UC) at Berkeley, UC Davis, Lawrence Berkeley National Laboratory, and Stanford University. Funding for SuperSTEM—the first of its kind in the world—comes from NASA and
Livermore’s Laboratory Directed Research and Development Program. John Bradley, director of the Laboratory’s Institute of Geophysics and Planetary Physics, says, “This consortium provides a unique opportunity for a collaboration between universities and national laboratories in the San Francisco Bay Area to work together on a NASA mission.”

Perfecting Extraction and Analysis Techniques

The particles collected by Stardust will be extremely small, so analytical instruments with a spatial resolution of approximately 2 nanometers or less will be needed to focus on the individual grains. Each member of BayPac works on particle manipulation and analysis using a variety of methods and instruments. To study the isotopic compositions of the dust particles, the Livermore team uses the 200-kiloelectronvolt SuperSTEM, which has a 10- to 100-fold resolution increase over other instruments, and its NanoSIMS (nano secondary-ion mass spectrometry), which is one of only two ion microprobes in the U.S. The team also uses a nuclear microprobe that radiates a sample with 3 megavolts of protons to measure its density.

Scientists in the consortium are studying interplanetary dust particles from Russia’s Mir Space Station and the International Space Station to refine the extraction techniques they will use on Wild 2 dust. “These particles are perfect analogs to study,” Bradley says, “because they were also collected in aerogel, although at a significantly higher speed (11 kilometers per second) than the Stardust collection speed.”

About three years ago, researchers from UC Berkeley’s Space Sciences Laboratory developed the “keystone” technique to remove a particle from a sample of aerogel. The term keystone is derived from the tiny wedge that contains the particle track and that is cut out of the aerogel. Detailed optical images of these impact tracks show evidence that particles fragment quite extensively as they project into the aerogel. With the development of the keystone technique, researchers have been able to further refine techniques to remove the fragmented particles. These fine-grained particles must be recovered for comprehensive analysis of cometary material.

Livermore researchers are determining which method will best remove micrometer- and submicrometer-size particle fragments from the tracks within keystones. Focused-ion-beam microscopy is one promising method being used to extract 0.1-micrometer-thick sections of a particle fragment. The thin sections are then examined using the transmission electron microscope, the NanoSIMS ion microprobe, and synchrotron infrared microscopy. Because the focused-ion-beam method destroys most of the particle fragment, only one or two sections can be harvested from each sample. The advantage of this method is that researchers can extract particles as small as 100 nanometers or less from targeted regions and cut them into thin sections. Livermore scientists take samples from specific...
isotopically anomalous hot spots, that is, areas where the highest concentration of a given isotope is found. Using this approach, researchers can correlate isotope measurements and mineralogy with nanoscale precision.

**Preparing for the Return**

Scientists worldwide will analyze Wild 2’s dust, and many of them will travel to Livermore to use the Laboratory’s SuperSTEM. Until then, Livermore will continue to refine extraction and specimen preparation techniques. Bradley notes, “For the first time in 30 years, we will be analyzing returned samples, and Livermore will be busy preparing a large quantity of specimens.” In addition to collecting particles, Stardust has an optical navigation camera that has captured images of Wild 2’s nucleus. Mission planners were surprised when the first pictures relayed back to Earth showed a large, circular nucleus rather than the expected potato shape seen in comets thus far.

In January 2006, Stardust is programmed to eject its reentry capsule, which will parachute to the Utah desert southwest of Salt Lake City. The much-anticipated return of the capsule will perhaps yield more surprises. Scientists are excited about what Wild 2’s dust may reveal about the origins of life on Earth.

—Gabriele Rennie

**Key Words:** Comet Wild 2, focused-ion-beam microscopy, interplanetary dust particles, nano secondary-ion mass spectrometry (nanoSIMS), Stardust, SuperSTEM (scanning transmission electron microscope).

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Livermore’s Radiation Detection Center is helping scientists conceive and develop innovative solutions to meet the nation’s radiation detection needs.
If you think a device that resembles a cellular phone but detects a potential nuclear threat and transmits a description of the nuclear material to every nearby crisis center sounds like something out of a James Bond movie, you are in for a surprise. Since the 1930s, when scientists first used the Geiger counter, radiation detection equipment has gone through an amazing evolution in size, sensitivity, deployability, and power.

Lawrence Livermore, which has been developing radiation-related technologies for decades, continues to adapt radiation detection devices for national security needs. In 1999, the Laboratory began forming its Radiation Detection Center (RDC), a multidisciplinary organization that centralizes Livermore’s radiation detection efforts. The RDC is supported through a memorandum of understanding between eight Laboratory directorates. Recently, several new radiation detection projects were funded by the Department of Homeland Security (DHS), which is expected to invest more than a billion dollars this year in science and technology across the nation to help the country detect and respond to terrorist threats.

The RDC helps to initiate and support many projects throughout the Laboratory that are developing new technology for national security and basic science programs within DHS, the Department of Energy (DOE), the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency, the National Institutes of Health, the National Aeronautics and Space Administration (NASA), and others. In addition, the center serves as an institutional resource for these organizations.

Many of today’s radiation detection tools were developed in the 1960s. For years, the Laboratory’s expertise in radiation detection resided mostly within its nuclear test program. When nuclear testing was halted in the 1990s, many of Livermore’s radiation detection experts were dispersed to other parts of the Laboratory, including the directorates of Chemistry and Materials Science (CMS); Physics and Advanced Technologies (PAT); Defense and Nuclear Technologies (DNT); and Nonproliferation, Arms Control, and International Security (NAI).

The RDC was formed to maximize the benefit of radiation detection technologies being developed in 15 to 20 research and development (R&D) programs. These efforts involve more than 200 Laboratory employees across eight directorates, in areas that range from electronics to computer simulations. The RDC’s primary focus is the detection, identification, and analysis of nuclear materials and weapons. A newly formed outreach program within the RDC is responsible for conducting radiation detection workshops and seminars across the country and for coordinating university student internships.

Simon Labov, director of the RDC, says, “Virtually all of the Laboratory’s programs use radiation detection devices in some way. For example, DNT uses radiation detection to create radiographs for their work in stockpile stewardship and in diagnosing explosives; CMS uses it to develop technology for advancing the detection, diagnosis, and treatment of cancer; and the Energy and Environment Directorate uses radiation detection in the Marshall Islands to monitor the aftermath of nuclear testing in the Pacific. In the future, the National Ignition Facility will use radiation detection to probe laser targets and study shock dynamics.”

RadNet is a low-cost radiation detector that includes a cellular telephone, a personal digital assistant with Internet access, and a Global Positioning System locator.
Sorting the Signals

One of the challenges facing nuclear researchers today is developing “smarter” detection systems that distinguish between radiation emissions from legitimate sources (for example, medical isotopes) and those from threatening sources. Nuclear materials, whether used in weapons or cancer therapy, typically emit gamma radiation. Many radioactive isotopes emit a unique spectrum of gamma rays that can penetrate substantial amounts of ordinary matter without being scattered or absorbed as visible light would be. These gamma rays can be analyzed to indicate the specific type of nuclear material.

The problem with early radiation detection systems is that they detected gamma rays from all radioactive material and could not distinguish between isotopes. Radioactive material is everywhere—from the concrete in our streets to the food we eat. Americium-241 is used in smoke detectors; cobalt-60 is used in medical treatment equipment; and potassium-40, a naturally occurring isotope in soil, is found in fruits and vegetables. (See the box below.)

Livermore scientists and engineers have made significant advancements in radiation detection equipment. Isotopes are now more easily distinguishable, reducing the confusion between threatening and nonthreatening sources. “We don’t know exactly how a terrorist will build a device,” says Labov. “But now we have more sophisticated instruments that have better spectral resolution. These instruments help us to identify common and legitimate radioactive materials, which increases our sensitivity to possible threats.” Specialized integrated circuits and microelectronics, improved computer codes, and advancements in detector materials have made these instruments possible.

How many types of detection devices are needed? Labov says, “Several types are necessary because the needs vary depending on the field. A customs agent at a U.S. maritime port will benefit from cargo interrogation systems as well as radiation detectors placed in buoys, while a firefighter responding to a potential dirty bomb threat might benefit from a high-resolution, handheld detector. If smuggled nuclear material is intercepted, an ultrahigh-resolution gamma-ray spectrometer may help identify the origin of the material.” (See S&T, January/February 2004, pp. 19–22; May 2004, pp. 12–15.)

Detection devices also vary in cost. The price tag for a large, laboratory-type spectrometer is $50,000 to $80,000, whereas a handheld detector may cost as little as $2,000. In some cases, the low-cost detector may be more appropriate for a particular task. “For example,” says physicist Bill Craig, who leads the Advanced Detector Group in PAT, “when you don’t know the location of a threat, the dispersion of many cheaper detectors may be more efficient so that first responders can cover more area.”

Radiation All around Us

Radiant energy exists in two forms—ionizing and nonionizing. Ionizing radiation has sufficient energy to remove electrons from neighboring atoms, thereby creating charged particles (ions or radicals) in materials it strikes. An effect from such ionization can be biological damage at the molecular and cellular level. Nonionizing radiation, such as laser light and microwaves, does not have enough energy to remove electrons from neighboring atoms. The only observed biological effects of nonionizing radiation are heating effects.

The common types of ionizing radiation are alpha, beta, gamma, neutron, and x radiation. Some atoms, for example uranium and thorium, are naturally radioactive. Other radioactive isotopes, for example tritium and iodine-131, are made in reactors or accelerators.

Radiation deposited in a material, such as may occur in an experiment, is called a radiation dose. Dose equivalent is the term used when determining the effect on humans. Dose equivalent is measured in rems or sieverts. The total number is based on the radiation dose and type and whether the exposure was internal or external. Because the majority of radiation exposures is small, the unit of one-thousandth of a rem, or 1 millirem, is commonly used.

Background ionizing radiation (that is, radiation from natural sources) measures about 300 millirem per year in the U.S. The radiation comes from cosmic rays, radioactive material in the earth, naturally occurring radionuclides, such as potassium-40 in food, and radon gas present in the air we breathe. Sources of human-caused ionizing radiation contribute an additional dose of approximately 70 millirem per year and include medical procedures, consumer products, and fallout radiation from the era of aboveground nuclear testing.

Exposure to large amounts of ionizing radiation (on the order of hundreds of times the natural exposure levels) increases the risk of cancer and genetic mutations that can be passed on to future generations. The extent of cell damage depends on the total amount of energy absorbed, the time period and dose rate of exposure, and the organs exposed.

In 1928, the International Commission on Radiological Protection—an independent, nongovernmental expert body—was established to recommend the maximum radiation dose to which people could be exposed. The commission set the level to not exceed 5 rem (5,000 millirem) per year. That limit is still used for radiation workers.

Most of the exposure associated with human activity is low-dose radiation. Although low-dose radiation does result in some damage to living tissue, the body can repair the damage. Recent research has indicated that low-dose ionizing radiation may activate protective and repair mechanisms and offer protection to the cells from a subsequent high dose of ionizing radiation. (See S&T, July/August 2003, pp. 12–19.) The model used for setting radiation protection limits is based on the risk being proportional to any radiation exposure above zero and is thus called the linear, no-threshold model.
Detector Makes Phone Calls

The recently developed RadNet detector is both inexpensive (about $2,000) and easily dispersed. This handheld instrument combines a cellular telephone, a personal digital assistant with Internet access, and a global positioning system locator with a radiation sensor. A number of RadNet units could be deployed as part of a wide-area network. Data collected by the units could be transmitted and plotted to a geographic map. In this way, law enforcement or other personnel could find the exact location of high-radiation signals from possible clandestine nuclear materials or devices.

In addition to being lightweight and able to operate at low power, each RadNet unit has sufficient energy resolution to eliminate alarms from background radiation emitted by such sources as food, medical devices, and soil. When it is not measuring specific radioactive samples, a RadNet unit monitors the ambient radiation field and communicates with a central processing system in real time. "RadNet is a detection device that first responders, customs agents, and border inspectors can carry and use routinely because of its other features, such as a cellular phone," notes Labov.

The RDC is using a RadNet prototype in demonstrations to customs officials, fire departments, and other first responders. "Customs officials," says Craig, "have had radiation pagers for some time. However, those pagers cannot identify the radiation source or send information back to someone who can analyze the data."

The RadNet project combined resources from directorates across the Laboratory, which is what the RDC management likes to see. "RadNet’s detector technology came from the astrophysics program in PAT," says Labov. "Engineering supplied electronics expertise for processing the detector’s signals. CMS lent its expertise in detector material, and NAI and Engineering provided expertise in analyzing gamma-ray signatures to identify nuclear isotopes."

Leave No Gamma Ray Behind

Researchers have also made advances in semiconductor-based, gamma-ray imaging detectors. These imagers use increased sensitivity and spatial resolution to detect weak radioactive sources that would otherwise be masked by background gamma-ray emissions. Gamma-ray imagers are particularly useful when searching for lost, stolen, or hidden nuclear material in a large area. DOE, DHS, and DTRA are interested in Livermore’s research on gamma-ray imaging because they are the agencies likely to be called if such a search is necessary.

Livermore is developing several gamma-ray imagers, each having different capabilities. One imager, called the gamma-ray imaging spectrometer (GRIS), can take gamma-ray "pictures" of the high-energy radiation emitted by nuclear materials. (See S&TR, October 1995, pp. 14–26.) This instrument is useful for a variety of applications, including treaty inspections, mapping radioactive contamination, and determining what is inside a suspect object. Because gamma radiation is so difficult to focus, the instrument uses an imaging technique originally developed for high-energy
astrophysics. The images are encoded on the detector by placing a sheet of material opaque to the radiation in front of the detector. The sheet is pierced with a carefully selected hole pattern that allows researchers to mathematically recover the image with a simple computer program. The system is about half the size of a personal computer.

GRIS was first developed for use in treaty inspections to monitor the location of nuclear missile warheads in a nonintrusive manner. In addition to its use in counterterrorism applications, GRIS is also expected to be useful in space to search for distant black holes and in hospitals to better detect, diagnose, and treat cancer.

Another version of GRIS being developed, the large-area imager, will be suited for longer-range searches. The large-area imager—approximately the size of a sofa—will be mounted in a small truck and capable of picking out weak radioactive sources from as far away as 100 meters.

The Compton camera is yet another type of gamma-ray imager under development. In addition to taking gamma-ray pictures, this imager should be able to identify very weak and typically invisible gamma-ray sources. The Compton camera operates without a mask or collimator, which can block many of the gamma rays emitted from a source. Instead, gamma rays coming from all directions at once are tracked as they scatter inside the detector. The camera’s omnidirectional sensitivity is significantly higher than that of other imaging systems. Mathematical algorithms are used to retrace the paths of the gamma rays within the detector, and the results reveal the direction of the source.

Livermore’s work on the Compton camera was originally funded through the Laboratory Directed Research and Development Program and later by DOE. Today, DHS is funding a Livermore effort to develop a compact, potentially portable Compton camera. The main goal for the camera is to detect clandestine nuclear materials. However, the instrument could also be used to detect cancer early by using radiolabeled tracers to target unique molecular characteristics of the disease. A field-deployable prototype of the Compton camera is still a few years away. Laboratory researchers continue to test detector materials and determine the best size for the instrument.

Livermore physicist Kai Vetter says, “We are developing various types of gamma-ray imaging systems. Individuals who work in the field, searching for nuclear materials or carrying out stockpile stewardship activities, will tell us which system best suits their needs.”

Uncovering Hidden Elements

Another radiation detection instrument is a spectrometer that can detect light elements, such as oxygen, within a heavy matrix, such as plutonium. While gamma-ray spectrometers are ideal for certain applications, in many situations, they cannot detect the presence of oxygen because oxygen is stable and does not usually emit gamma rays. Stockpile stewardship and radioactive waste characterization may benefit from this capability. For example, the neutron spectrometer could measure oxygen bound to plutonium, which may have resulted
from seepage through casks containing nuclear weapons or spent nuclear fuel. (See figure on p. 10.)

Physicist Stephan Friedrich of the Advanced Detector Group leads a team developing the ultrahigh-resolution neutron spectrometer. In addition to providing a spectral emission that distinguishes a light element within a heavy element matrix, neutron spectrometers can also detect nuclear material behind a shield and perhaps even determine the composition of the intervening material. If plutonium, for example, were concealed in a lead object, the lead, or any heavy metal shield, would absorb the gamma rays emitted from the plutonium, whereas neutrons would travel through the lead and scatter in ways that provide a signature.

The ultrahigh-resolution neutron spectrometer uses lithium fluoride to absorb incoming neutrons. It then measures the released energy from the neutrons interacting with the lithium fluoride combined with the energy of the neutrons as they enter the detector. The spectrometer will operate in laboratories where the units can be cooled to 0.1 kelvin, the temperature required to obtain ultrahigh-energy resolution.

“A prototype of the ultrahigh-resolution neutron spectrometer could be complete in a year,” says Friedrich. “Collaborations at workshops conducted by the RDC helped our team refine ideas for this necessary technology and also revealed potential applications for other areas.” The spectrometer is so sensitive that it will be able to detect the energy deposited by a single neutron.

A New Frontier: Sensor Fusion

Combining various types of radiation detection devices into a network that maximizes the benefits of each is the next frontier. Craig notes, “The first push was for radiation detectors. Now, there is the realization that a first responder called to check out a potential bomb threat on a bridge, for example, may not be in the best position to analyze the data.” This realization has launched the area of sensor fusion—taking information from an ensemble of detectors.

“Sensor fusion,” says Craig, “is a discipline that allows scientists to combine data and provide a sum greater than the parts. For example, information from a portable radiation detection system can be combined with that from handheld detectors and video cameras, and all of the data can be integrated to give a more complete report than one type of detector could provide.”

Labov says DHS is interested in adding wireless data transmission to radiation detectors, but no system is currently in place to collect and analyze the data. “We could use analyses from science applications at the Laboratory to integrate and interpret the data. With sensor fusion, information gathered from multiple gamma-ray detectors, neutron detectors, and detectors that take visual images, for example, could be combined and analyzed together. Combining the information is a discipline in computer science. We are strategizing on the most effective methods to accomplish this goal.”

Sharing Bright Ideas

Running analyses and interpreting the data from a network of different radiation detection equipment requires special skills in nuclear science. Yet despite the increasing demand for this expertise, the last two decades have seen a nationwide decline in the number of students pursuing careers in nuclear engineering, physics, and chemistry because of decreasing job prospects. For
example, it has been decades since a nuclear power plant was built in the U.S. As a result, many universities are closing their nuclear energy programs and shutting down their research reactors.

But changes are under way. DOE is investing millions of dollars in the Nuclear Energy Research Initiative Program to support nuclear R&D. The National Nuclear Security Administration (NNSA), the Department of Defense, and DHS also sponsor many R&D efforts and are turning to Livermore to provide technical expertise in radiation detection. Jeff Richardson, a division leader for NAI, notes, “These agencies are looking to Livermore for creative solutions to homeland security and general nonproliferation objectives.”

In 2000, the RDC formalized an outreach program to conduct workshops, coordinate technical discussion groups, and provide internships for university students interested in nuclear science. This year, the center hired an education coordinator to put together a plan for attracting new graduates to nuclear science. RDC members are working with students at universities, such as the University of California (UC) at Berkeley, which has a strong nuclear engineering program, and the University of Michigan, known for its nuclear science program. Graduate summer students work at Livermore’s Seaborg Institute for Transactinium Science, which was established in 1991 to foster research in fundamental and applied nuclear science and technology.

Christie Shannon, the RDC’s outreach coordinator, keeps a pulse on researchers’ needs so that the center can arrange for relevant seminars and workshops. “The seminars and workshops provide a forum for collaboration with radiation experts within the Laboratory and from other organizations, including other national laboratories, government agencies, universities, and industry personnel.”

To date, the RDC has hosted more than 80 seminars on such topics as detecting cosmic axions and the use of antineutrino detectors for reactor safeguards. In addition, technical discussion groups focus on brainstorming new approaches to radiation detection. For example, a group was formed to discuss using the air filters in police cars to examine air particles after a nuclear terrorist attack.

In a series of workshops held from December 2003 to February 2004, 60 Laboratory scientists and engineers met to identify critical needs in radiation detection and prioritize a list of potential solutions. The idea for a large-scale effort in sensor fusion came from these collaborations. A new effort to develop detectors based on nanomaterials also emerged. A directional neutron detector
and the ultrahigh-resolution neutron spectrometer are two other ideas that were refined at the workshops, enabling them to become fully funded R&D projects. Friedrich notes, “After the workshops, the ultrahigh-resolution neutron spectrometer became a prominent goal for the Laboratory, and it became clear where we needed to go to complete development.” The work on this spectrometer is now funded through NNSA’s Office of Nonproliferation Research and Engineering.

The RDC also hosts DOE workshops featuring speakers with innovative ideas for detecting nuclear materials. Workshop topics have included investigating alternative signatures for detecting fissile materials; improving tags, seals, and intrusion sensors for container shipping security; and remotely monitoring nuclear material using attended and autonomous intelligent-sensor systems.

Astrophysics: Past and Future

Many Livermore radiation detection advances have resulted from technical developments in astrophysics. For years, Livermore researchers have collaborated with scientists from the California Institute of Technology, NASA’s Goddard Space Flight Center, UC Berkeley, Columbia University, Massachusetts Institute of Technology, Harvard University, and other universities and government laboratories to develop the latest technologies for detecting and imaging space phenomena. “We are finding ways to combine better science with better security,” says Labov. “For example, astrophysicists at Harvard University approached Livermore for assistance on a satellite project in which the scientists needed an 8-square-meter area of crystal to operate as a detector. Some developments from that project resulted in technology later used for RadNet.”

The coded aperture system used in GRIS is another example of a technology invented by astrophysicists. And the technology used for the Compton camera came from the Imaging Compton Telescope, COMPTEL, which was built in 1989 at Goddard to study gamma-ray sources such as pulsars, supernova remnants, and molecular clouds.

Although some of Livermore’s radiation detection technology came from astrophysics, Craig hopes to see the reverse as well. “We’re hoping to help astrophysicists use RadNet-like detection systems for missions, such as probing for black holes.”

Detectors have come a long way over the last decade. From sensors on buoys to low-cost networks, today’s devices promise almost tailor-made solutions to meet the needs of first responders. Richardson notes, “We are continuing to push the envelope in all areas of radiation detection, particularly in the areas of high sensitivity and selectivity.”

As new tools for radiation detection and networking of systems develop, the RDC will continue to pilot efforts to realize the Laboratory’s goals. Perhaps there may even be a new gadget for James Bond to take on his next mission.

—Gabriele Rennie

Key Words: Compton camera, gamma-ray imaging spectrometer (GRIS), large-area imager, Radiation Detection Center (RDC), RadNet, Seaborg Institute for Transactinium Science, sensor fusion, ultrahigh-resolution neutron spectrometer.

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Solid-State Technology Meets Collider Challenge

PROBING the frontiers of particle physics and delving into the mysteries of the universe and its beginnings require machines that can accelerate beams of fundamental particles to very high energies and then collide those beams together, producing a multitude of exotic subatomic particles.

The proposed Next Linear Collider (NLC), being developed by Stanford Linear Accelerator Center (SLAC), Lawrence Livermore and Lawrence Berkeley national laboratories, and Fermi National Accelerator Laboratory (Fermilab), is such a machine. The NLC is expected to produce a variety of subatomic particles by smashing together electrons and their antimatter counterparts (positrons) at nearly the speed of light with energies in the teraelectronvolt (TeV) range.

Plans are that the NLC will initially operate at 0.5 TeV and ultimately be scaled up to 1.5 TeV. (See S&TR, April 2000, pp. 12–16.) Work at the facility will complement the research to be conducted at another high-energy particle accelerator, the 14-TeV Large Hadron Collider at the European Laboratory for Particle Physics (commonly known by the acronym CERN from its former name) in Geneva, which is scheduled for completion in 2007.

Achieving beam energy levels in the TeV range requires modulator systems that can convert ac line power—the same type of power one gets from the wall plug—into dc pulses. Ultimately, these pulses are transformed into radiofrequency (rf) pulses that “kick” the particles up to the required energy levels. Livermore scientists and engineers have designed a solid-state modulator to replace old-style modulators based on vacuum-tube technology. These new modulators promise to be far more efficient, reliable, and serviceable than the previous components. Livermore’s Laboratory Directed Research and Development Program supported the basic research and development on the solid-state modulator technology, and SLAC supported the systems integration.

A conceptual drawing of the Next Linear Collider, housed in a tunnel approximately 30 kilometers long, inside of which are two opposing linear accelerators (linacs). Within each linac, the electrons (or positrons) are accelerated inside thousands of copper accelerator structures, each made up of more than 200 precision-machined copper cells (see inset).
Start of the Power Train

The NLC will accelerate a beam of electrons and a beam of positrons down two opposing 15-kilometer linear accelerators, or linacs. Each linac is a repetitive system with pulses identical in energy level and wave shape generated at the rate of 120 pulses per second.

The basic linac consists of a modulator to convert ac line power into dc pulses and klystrons (oscillators) that are driven by the dc pulses to produce 75 megawatts of peak rf power at 11.4 gigahertz. The linac also includes pulse compressors that reformat the rf output into 300-megawatt, 300-nanosecond-long pulses. These pulses are then delivered to accelerator structures constructed of copper disks. The electron and positron particle beams surf the pulses as they travel through these disks, gaining energy as they pass from one accelerator structure to the next. The NLC is an order of magnitude larger in size than any other linear accelerator yet designed and will have between 5,000 and 10,000 accelerator structures.

Modulating Power with Solid State

When Livermore engineers began the modulator design for the NLC, they revisited the possibility of creating a solid-state system. The old-style modulators based on hydrogen thyratron-fired pulse-forming networks (PFNs), a technology dating from the 1940s, have some definite drawbacks for a system the size of the NLC. For example, a thyratron-switched PFN can drive only a single 75-megawatt klystron and has an operational lifetime of 2 years or less before requiring replacement. Engineer Ed Cook notes that few vendors exist today who make thyratron switches. “Fabricating these switches is a bit of a black art. It requires a lot of manual expertise, and that expertise is disappearing. For a long time, we’ve wanted to replace these vacuum-tube switches with solid-state switches.”

The biggest obstacle has been that, until fairly recently, solid-state switches couldn’t handle high voltages. Thyratron switches can withstand the high voltages used in high-energy physics experiments and can easily reach 100 kilovolts. However, 6.5 kilovolts was the limit for a solid-state switch that could be turned on and off with a gate control signal, and the NLC requires a 500-kilovolt pulse. Livermore came up with a design capable of withstanding this voltage level using a series of solid-state switches buffered with a transformer.

The solid-state modulator’s efficiency is vastly improved over thyratron-based modulators. The shape of the modulator’s energy pulse largely determines its efficiency. The ideal pulse shape is rectangular because the energy in the pulse’s rise and fall time is not usable by the klystron to generate rf power. For the NLC, the goal is to have a rise and fall time of less than 200 nanoseconds, which is difficult to obtain with a PFN modulator using thyratrons. The performance of a solid-state modulator based on an inductive

(a) The Next Linear Collider being developed by the Stanford Linear Accelerator Center and other laboratories will consist of thousands of basic linear accelerator (linac) units. Each unit consists of modulators, klystrons, pulse compressors, and accelerator structures. (b) This schematic shows a four-cell stack of the Livermore-designed modulators based on solid-state switch technology. (c) A close-up view of the modulator shows a solid-state switch, a capacitor, and a transformer core.
Livermore physicist Jeff Gronberg, “We’re looking at nearly 30,000 boards in all, so reliability and ease of maintenance are very important.” The plan is to have redundant boards and then switch to the backup board if one goes bad, a much less painful process than replacing a failed thyratron. “When a thyratron fails, a section of the linac goes down with it,” says Gronberg. “It can take the better part of a day to replace it and have the system running again.”

Testing the System

Last year, Livermore delivered the first full-power prototype modulator consisting of 15 cells. The Livermore team and the Power Conversion Group at SLAC are conducting tests on the entire rf system using the solid-state modulators and a new 500-kilovolt, 75-megawatt klystron.

“We’re testing each component of the basic linac unit—modulator, klystron, pulse compressor, and accelerator structure—to demonstrate its reliability and performance,” says Gronberg. “Reliability is critical. Once the NLC is up and running, it will be on line 24 hours a day, 7 days a week, 9 months a year. Now, with the solid-state modulator, the loss of one or two boards in any given modulator will not affect the accelerator’s operation. Routine maintenance can be performed at scheduled down times. Previously, we would have had to maintain 2,000 vacuum-tube thyratron switches for the entire collider. Given the failure rate of the vacuum tubes, we would have been repairing on average one per day.”

The modulator prototype recently achieved its design parameters, producing 1.6-microsecond pulses of 500 kilovolts with a 120-hertz repetition rate. “The Laboratory’s investment in the modulator project is now paying off in dividends,” says Gronberg. “Using this technology will save about $200 million on the cost of the NLC. The benefits are also accruing in other accelerator projects and in pulse-power applications, such as Pockels cell drivers for high-power lasers. Once a new technology is demonstrated, people often find other applications where it can make a difference.”

—Ann Parker

Key Words: electron–positron linear collider, Next Linear Collider (NLC), klystron, particle accelerator, solid-state modulator, Stanford Linear Accelerator Center (SLAC), thyratron, vacuum-tube technology.

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Modulator efficiency is determined largely by the shape of the energy pulse produced. The new solid-state modulator yields more useful energy per pulse using either Mitsubishi (green and black waveforms) or Eupec (red waveform) insulated gate bipolar transistors (IGBTs), as shown by the far steeper rise and fall times, than the old-style modulator using hydrogen thyratron-fired pulse-forming networks (blue waveform).
Responding Rapidly, Reliably

One of the methods a terrorist might use to disperse a biowarfare agent is through an aerosol attack. In fact, the anthrax mail room release in 2001 and the ricin release in 2004 involved relatively small amounts of deadly material. Countering such threats in an effective manner requires an automated system that continuously monitors the air, quickly analyzes samples, and identifies a wide range of agents without false positives.

APDS is designed to meet that need. It monitors the air for the three types of biological threat agents: bacteria, viruses, and toxins. Because it operates continuously, the system can detect low concentrations of bioagents that might go undetected by a system that is triggered only when the overall number of particles in the air is high. APDS collects aerosol samples, prepares them for analysis, and tests for multiple biological agents simultaneously. This automation reduces the cost and staffing that would be required to manually analyze samples.

The current system is configured to test simultaneously for 11 agents and can be expanded to 100 agents without a change in instrumentation. “Given the number of pathogens potentially available to terrorists,” says Langlois, “the ability to detect and analyze large numbers is critical.” APDS also identifies particles within 1 hour—faster than comparable systems, which can take 4 to 20 hours. Having results promptly is crucial for emergency-response efforts, as is being certain that the results are real. “Our goal was to have two independent, autonomous, ‘gold-standard’ assays to provide the highest confidence in detection results in the shortest possible time,” says Langlois.

Checking It Twice

As APDS collects air samples, it first runs them through an immunoassay detector. If that detector returns a positive result, APDS performs a second assay based on nucleic-acid amplification and detection. Having two different assay systems increases system reliability and minimizes the possibility of false positives.

The immunoassay detector incorporates liquid arrays, a multiplexed assay that uses small-diameter polystyrene beads (microbeads) coated with thousands of antibodies. Each microbead is colored with a unique combination of red- and orange-emitting dyes. The number of agents that can be detected in a sample is limited only by the number of colored bead sets. When the sample is exposed to the beads, a bioagent, if present, binds to

The Autonomous Pathogen Detection System (APDS) monitors the air continuously for biological threat agents and uses two identification technologies to reduce the probability of false alarms. It can measure up to 100 different agents per sample and reports identified agents within an hour.
the bead with the appropriate antibody. A second fluorescently labeled antibody is then added to the sample, resulting in a highly fluorescent target for flow analysis. Preparing the sample and performing this first analysis takes less than 30 minutes.

System software compares the result with preset threshold criteria for a positive identification. A positive immunoassay result triggers the second test—a DNA analysis using the rapid polymerase chain reaction (PCR) technique. For this test, an archived sample is mixed with reagents for the target organism and introduced into the flow-through PCR system, which consists of a Livermore-designed, silicon machined thermocycler mounted in line with the sample preparation unit. Specific nucleic-acid signatures associated with the targeted bioagent are amplified up to a billionfold and detected as a change in fluorescence. The PCR analysis is completed within 30 minutes.

Results are transmitted every hour to a control center, where the instrument’s performance is monitored. “The architecture of wireless communication with a command center works well with existing building safety and security systems,” says Langlois. “Because malfunctions and failures are rare, a small command staff can easily oversee a network of 10 to 100 instruments and still provide maintenance, scientific interpretation of assay results, and communication with the appropriate authorities.”

Saving Time, Saving Lives

In September 2003, APDS passed a series of pathogen exposure tests at a high-containment laboratory at the Dugway Proving Ground in Utah. In these trials, the system clearly demonstrated that it could detect real pathogens and confirm the identifications with a fully automated second assay method. APDS units were also deployed at the Albuquerque Airport in New Mexico and at a Washington, DC, Metro station, where they provided continuous monitoring for up to seven days, unattended.

The system can be adapted for situations where environmental or clinical pathogens require monitoring. For example, APDS could test for mold or fungal spores in buildings or for the airborne spread of contagious materials in hospitals. It also could identify disease outbreaks in livestock transport centers or feedlots. “Basically, there are no fully integrated systems with the capabilities of APDS commercially available in the civilian or military market,” notes Langlois. “The system offers ongoing environmental monitoring and rapid detection of harmful pathogens, allowing emergency workers to respond immediately to decontaminate areas and, most importantly, save lives.”

—Ann Parker

Key Words: anthrax, Autonomous Pathogen Detection System (APDS), biological agents, bioterrorism, multiplex immunoassay, polymerase chain reaction (PCR), R&D 100 Award, ricin.

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