

About the Cover

Something like the small, tweezer-held capsule shown on the cover will be the focus of Lawrence Livermore's National Ignition Facility (NIF) laser. On completion, NIF will be the world's largest laser, covering an area as large as a sports stadium. But all its experimental work will depend on minuscule targets: 2-millimeter-diameter plastic spheres. The article beginning on p. 4 discusses the exacting design and fabrication of these targets used to achieve fusion ignition. Successful ignition—reproducing in miniature thermonuclear burning in a nuclear weapon—will be an important achievement supporting the Department of Energy's Stockpile Stewardship Program.



About the Review

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

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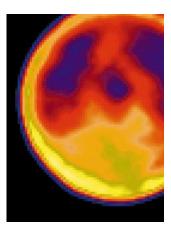
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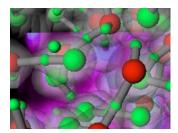
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The NIF target chamber is dedicated

At June 11, 1999, ceremonies at Lawrence Livermore, Secretary of Energy Bill Richardson was joined by Director Bruce Tarter and senior defense officials from the United Kingdom and France to dedicate the 130-ton target chamber built for the National Ignition Facility (NIF). All employees and their families were invited to the dedication.

NIF, the largest laser in the world, will be a cornerstone of the DOE Stockpile Stewardship Program, which will keep the U.S. nuclear arsenal safe and reliable without underground nuclear testing. Tarter stated his confidence in NIF to fulfill this purpose. "I am very optimistic about our ability in the long term to meet that challenge," he said. With both Britain and France collaborating on the project, Secretary Richardson pointed out that NIF is a model of true international cooperation.

The dedication of the target chamber marks the on-time completion of the first and largest piece of equipment for the laser's operation. It also marks the halfway point in construction. *Contact: Gordon Yano (925) 423-3117 (yano1@llnl.gov).*

Lab's new gas chromatograph works on the spot

Lawrence Livermore's miniature gas chromatograph is making it faster and easier to identify what's in samples of air and water. The device, weighing about 5 pounds and requiring just 2 minutes to analyze liquid and gas species to sensitivities of parts per billion, contrasts with previous chromatographs that have taken hours, even days, to process samples and were too large to be deployed where chemical weapons or poisonous gases were suspected of being released.

The new, portable device results from work in Livermore's Center for Microtechnology. Engineer Conrad Yu scaled down the chromatographs's column, where the various constituents of the sample are separated before being directed to a detector for counting. Previous attempts to scale down the column were unsuccessful because they could not keep the column perfectly circular, which is crucial for analytical accuracy.

Yu etched perfect half circles on two silicon wafers—similar to those used for computer chips—and then lined up the semicircles and bonded them together. He was thus able to make a circular column 100 micrometers wide and several

meters long. The chromatograph's smaller column allowed the associated detector and computer to be scaled down also.

The new chromatograph will have many potential applications in medicine, industry, law enforcement, and environmental cleanup. Yu and colleagues want to make this technology commercially feasible within several years. *Contact: Conrad Yu (925) 422-7356 (yu1@llnl.gov).*

Burst bubbles support astrophysicists' theory

Lawrence Livermore astrophysicist Richard I. Klein, UC Berkeley astronomy chair Jonathan Arons, and UC Berkeley Space Sciences Laboratory's J. Garrett Jernigan have found evidence to support a theory about powerful x-ray emissions from neutron stars—rotating, magnetized, collapsed stars that are some of the most violent objects in the universe. Ten years ago, Klein and Arons posited that when a neutron star pairs up with another star, its powerful gravitation siphons off material from the second star. That material is channeled to the neutron star's polar caps, where it creates an unusual field of radiation, or photon, bubbles. The bubbles merge and burst, releasing a shower of high-frequency x rays in a more or less regular fashion, causing the neutron star to flicker or oscillate.

Jernigan, involved in developing NASA's Rossi X-Ray Timing Explorer satellite since its inception, suggested using it to look for radiation bubbles. For the search, the scientists selected the neutron star Centaurus X-3, some 30,000 light years away in the Milky Way galaxy.

For three days, they took satellite measurements and obtained data whose analysis showed the x-ray emissions flickering at rates from 100 to 2,000 times per second, a range the scientists had earlier predicted. "This is the fastest known x-ray emission of any collapsed star in the universe, be it a white dwarf, black hole, or neutron star," Klein said. "The discovery lends strong support to our theory that the origin of these rapid x-ray fluctuations is the exotic photon bubbles we predicted."

Klein, Arons, and Jernigan reported their findings at a recent meeting of the High Energy Astrophysics Division of the American Astronomical Society in Charleston, South Carolina. *Contact: Richard I. Klein (925) 422-3548 (rklein@llnl.gov).*

(Continued on p. 26)



Fusion Ignition as an Integrated Test of Stockpile Stewardship

A new era of nuclear weapons policy, prohibiting testing and the development of new types of weapons, raises this challenge for the nation: ensuring that our current weapons stockpile remains safe, secure, and reliable into the indefinite future, regardless of aging. Confidence in the U.S. nuclear arsenal now must depend on our fundamental understanding of weapons science and technology, pursued without recourse to the detonation of full-scale nuclear devices.

Under the Department of Energy's Stockpile Stewardship Program, scientists at Lawrence Livermore are addressing the issues inherent in this challenge. They are developing advanced computer modeling and simulation to predict weapons performance and are establishing benchmarks against existing underground test data. However, the best gauge of this computer modeling capability is how well it predicts experimental results. Several experimental efforts are under way to enhance the accuracy of our computer modeling. They include advanced hydrotesting, subcritical experiments, and superlasers.

High-power lasers are unique in that they can produce energy density (energy per unit volume) approaching that of nuclear devices. The lasers can produce momentary, microscopic versions of some important aspects of nuclear detonations. The National Ignition Facility (NIF), now under construction at Livermore, will incorporate such a laser. Based on nearly 30 years of fusion laser development, NIF is being designed to deliver 1.8 million joules of energy with micrometer precision onto millimeter-size targets. (See the article beginning on p. 4 for a description of work on designing and fabricating fusion targets.) The intent is to produce thermonuclear burn that, for a few trillionths of a second, produces conditions found only in the center of the sun and in the core of a burning nuclear weapon. Achieving ignition outside a nuclear device will be a landmark achievement for stockpile stewardship.

More than four decades of dedicated work by weapons scientists has provided us with sophisticated scientific knowledge critical to understanding the design and performance of nuclear weapons. Fusion ignition is a complex physical process that will be a challenging integrated test of this knowledge and of our modeling and experimental capabilities. Before the actual ignition experiments, scientists will spend several years on simulations and preliminary experiments to calibrate the details of target physics that are impossible to model, even with modern supercomputers. Experiments preliminary to ignition can start early because the facility is being built so that some of the laser's 192 beams can be used to conduct target experimentation even as other parts are being constructed and installed. These preparatory results, along with decades of experimental data from smaller lasers and the powerful modeling and simulation capability developed by the Accelerated Strategic Computing Initiative—another arm of the Stockpile Stewardship Program—will be used to determine the final target and laser configuration used to drive ignition.

Once ignition is achieved, it can be used in several important ways. The Stockpile Stewardship Program can explore the physics of thermonuclear burn and its effects. The burning capsules can be used as sources of neutrons and x rays for studies on nuclear weapon effects. NIF also can be used for basic science applications and to develop nuclear fusion as an energy source.

NIF is the next step in laboratory thermonuclear fusion. It will provide a detailed, integrated test of our understanding of nuclear detonation processes. It will also further our understanding of the fundamental physics of nuclear weapons, thereby enhancing our ability to predict weapons performance and help to provide a sound basis for assuring the safety and reliability of the nuclear stockpile.

■ Mike Anastasio is Associate Director, Defense and Nuclear Technologies.

On Target Designing for Ignition

Guided by computer simulations and scientific collaborations, Department of Energy researchers at Livermore and Los Alamos are designing targets for the world's first laser ignition experiments.

OR more than 40 years, laser fusion researchers worldwide have worked to achieve a momentous event called ignition, the fusion of atomic nuclei and the liberation of more energy than the fusion fuel first absorbed. The \$1.2-billion National Ignition Facility (NIF), now under construction at Lawrence Livermore National Laboratory, promises to make that long-awaited event a reality.

NIF's 192 laser beams are designed to produce 1.8 megajoules of energy and 500 terawatts of power, more than enough to fuse the hydrogen isotopes of deuterium and tritium into helium nuclei (alpha particles) and yield considerably more energy in the process than was required to initiate the reaction.

By achieving ignition, NIF will allow weapons scientists to perform several kinds of experiments for the Department of Energy's Stockpile Stewardship Program to ensure that the U.S. nuclear arsenal remains safe and reliable. During ignition, NIF's targets will become miniature stars for about 10 trillionths of a second—a vanishingly short time, yet long enough to replicate aspects of physics at the energy densities and temperatures that occur during detonation of a nuclear device.

Of the 1.8 megajoules of energy produced by NIF, about 30 kilojoules is ultimately transferred into the deuterium-tritium fuel in the target. With ignition and successful burn, the fuel can produce some 600 to 1,000 times more energy than is put into it. That generous payback is not lost on energy scientists who will be using NIF to advance their understanding of how to deploy laser fusion as a cheap and safe civilian source of energy in the future.

The size of a covered sports stadium, NIF will house some three-quarters of an acre of highprecision optical instruments. And yet, the focus of its thousands of components will be a target of millimeter dimensions. The success of every NIF experiment will depend greatly on the ability to



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design and manufacture the intricate, tiny targets so that their structure, materials, and manufacturing tolerances match the giant laser's power and energy and meet the goals of each particular experiment.

The responsibility of designing the targets falls to researchers at Lawrence Livermore and Los Alamos national

laboratories. The work requires coordinated effort from physicists, materials scientists, chemists, computer scientists, and technicians.

Physicist Steve Haan leads the Livermore effort to design ignition targets. For more than 20 years, experts such as Haan have conducted research on the design, production, and performance of target capsules as an integral part of Livermore's Laser Programs. Although the first shots on NIF will not occur before about 2002, with the first ignition experiments several years later, the team must finalize many aspects of the target design and fabrication technology well before that.

Codes and Computers Lend a Guiding Hand

In designing NIF targets, Livermore researchers are guided by increasingly detailed modeling that uses the latest generation of supercomputers. The modeling must account for a variety of physical phenomena that occur during an implosion and resulting ignition.

The simulations study the physics of both laser-driven hohlraums and capsule implosions. The study of hohlraums includes the refraction, reflection, and absorption of laser light passing through the hohlraum's laser entrance holes, the interaction of the laser light with low-density plasma, the conversion of absorbed laser light into x rays, the flow of those x rays within the hohlraum, and their absorption onto the ablator layer.

Capsule physics encompasses the variation of the capsule ablation, implosion, and hydrodynamic instability growth and mixing within the capsule, and the thermonuclear burn of the deuterium–tritium fuel.

The simulations reflect certain experimental realities: implosion is an inherently unstable process, and ignition experiments on NIF will involve neither perfectly smooth and spherical capsules nor a perfectly uniform field of x rays to ablate the outer layer and compress the fuel inside.

Several Livermore-developed codes are used because no single code can simultaneously model all ignition phenomena. LASNEX

is a venerable two-dimensional radiation hydrodynamics code with very complete

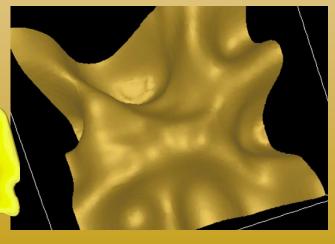
Researchers use
Livermore's LASNEX code
to model the target physics.
The code is used to produce
simulated data, such as this
neutron image, which will be
compared with data from
NIF experiments.

modeling of most relevant physical processes. Researchers use LASNEX to model the full geometry of the hohlraum and capsule as well as the incident laser beam. In these simulations, called integrated modeling, the capsule, hohlraum, and laser light are modeled simultaneously.

HYDRA is a three-dimensional radiation hydrodynamics code that contains all the physics necessary for imploding NIF ignition capsules. Additional features are being added that include hohlraum modeling and enable the code to run efficiently on massively parallel computers. In particular, HYDRA is used to study hydrodynamic instabilities in detail. Instead of simulating a hohlraum, the code models an x-ray flux to the exterior of the capsule.

Other codes model in detail the laser–plasma instabilities. A principal code for this application is F3D, which simulates the interactions of the laser light with the electrons and ions in the plasma.

Any one of these calculations can require days or even weeks of supercomputer time. As computers become faster, more and more detailed simulations can be done with acceptable turnaround time.



HYDRA 3D is a Livermore code used to model capsule implosions, including hydrodynamic instabilities, in detail.

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Nova Provided Experience

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The current Livermore effort builds upon a strong experimental program conducted on NIF's predecessor, the 10-beam Nova laser, which ceased operation in the spring of 1999. Many thousands of experiments on Nova led to an ever-increasing capability in target design and fabrication, diagnostic instrumentation, and computer simulation, as well as a firmer grasp of physics issues affecting ignition.

"Aside from giving us enormous experience with target design and fabrication," says Haan, "Nova showed us that NIF would be able to provide both the required hohlraum drive temperature and the laser symmetry to make ignition possible."

The team has also aggressively taken advantage of computer modeling. Livermore target designers use some of the most advanced computational facilities in the world to test target design options (see box on p. 5). The simulations give Livermore scientists good reason to believe ignition will be successful on NIF, says Haan. In fact, all indications are that NIF will provide a factor-of-2 performance margin above the ignition threshold.

The technical soundness of Livermore target designs has been validated by colleagues at other laser fusion research

centers, both in the United States-at Los Alamos and the University of Rochester—and in Britain and France. In particular, French scientists from the research agency Commissariat a l'Energie Atomique, which plans to build a laser fusion facility similar to NIF, are collaborating with Livermore ignition target designers.

Ignition on NIF targets will involve compressing a 2-millimeter-diameter capsule that contains enough deuteriumtritium (D-T) fuel to achieve ignition and sustain burn. At first glance, the design resembles a typical Nova target, but it will be some four times bigger and

will contain frozen D-T to help achieve conditions supporting ignition. The capsules will have a central volume of D-T gas, a frozen D-T solid-fuel layer, and an outer ablator layer.

For at least the first several years, ignition experiments will use indirect drive, in which laser light heats the inside of a gold cylinder called a hohlraum (Figure 1). The light is converted with close to 100 percent efficiency into an intense flux of x rays of almost 1,000 terawatts per square centimeter. The x rays will converge on the capsule's outer ablator layer, heating and expanding it. The

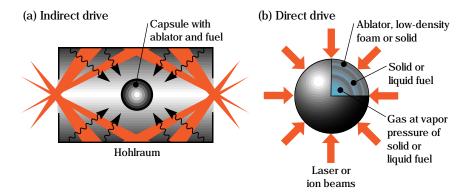
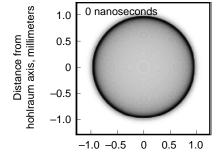
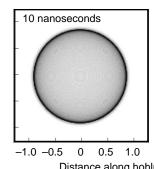
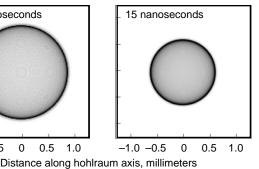


Figure 1. Ignition experiments on NIF will use indirect drive to heat the inside of a cylinder (hohlraum). The incident laser light will enter the cylinder through holes at its end caps and will be converted to x rays that will converge on a 2-millimeter-diameter capsule. NIF also has an option to conduct direct-drive experiments, with the laser light directly incident on a capsule.







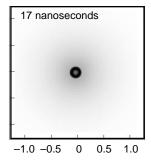


Figure 2. During implosion, x rays will converge on the NIF target capsule's outer ablator layer. The rocketlike blowoff of the ablator will then push the rest of the capsule inward, compressing the interior fuel to the extreme pressures and temperatures found in a star and a detonating nuclear warhead. The implosion can be backlit with x rays, producing data like the simulated images here, which show the implosion process from 0 to 17 nanoseconds. These images will be used to validate the timing and symmetry of the x rays driving the implosion.

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rocketlike blowoff of the ablator will then push the rest of the capsule inward, compressing the interior fuel to the extreme pressures and temperatures found in a star and a detonating nuclear warhead (Figure 2).

Haan notes that NIF will also have the option of doing direct-drive ignition targets with the laser light directly incident on a capsule, thereby eliminating the need for a hohlraum. Experiments required to prove the feasibility of direct drive will be conducted over the next few years at the Omega laser of the University of Rochester's Laboratory for Laser Energetics (see *S&TR*, June 1999,

pp. 19–21). Livermore researchers are participants in the Omega effort because direct drive on NIF has the potential to produce energy gains some three to eight times higher than indirect drive.

For the present, Livermore target designers are focusing on both the indirect-drive capsules and the hohlraums enclosing them. The baseline hohlraum measures about 10 millimeters long and 5.5 millimeters in diameter, with a 2.8-millimeter-diameter laser entrance hole on either end.

The hohlraum will be filled with an equal mixture of hydrogen and helium gas to minimize scattering of the laser light and to hold back the ionized gold. The gas will be contained within the hohlraum by 1-micrometer-thick polyimide foil windows that cover each hole. Before a shot, the hohlraum will

be maintained at a carefully chosen temperature—around 18 kelvins (-255°C)—to keep the D-T fuel frozen and the central gas core at the right temperature and density (Figure 3).

Haan points out that while the baseline design has been fixed for some time, variations might prove to be important. The ability to shoot different targets, varying in design details to adjust for physics uncertainties, is a vital part of NIF's experimental plan. For example, different ablator materials and drive temperatures will give the team options to cover possible errors in current computer modeling.

Other target configurations will also be explored. For example, the target designers are researching the feasibility of a spherical hohlraum with four laser entrance holes in a tetrahedral configuration. The unique geometry might provide a more even x-ray illumination of the capsule (Figure 4).

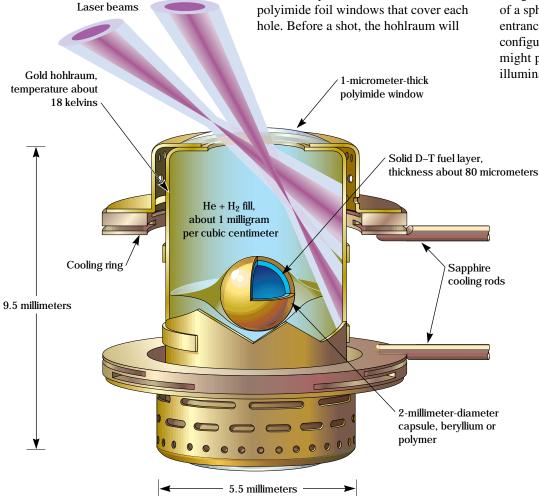


Figure 3. The hohlraum will be filled with hydrogen-helium gas (which will be contained inside polyimide windows) to minimize laser light scattering. The hohlraum will be maintained at 18 kelvins (see cooling ring) to keep the deuterium-tritium (D-T) fuel frozen and the central D-T gas core at the correct temperature and density.

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Forming Cones of Light

Laser light of 0.35-micrometer wavelength will enter the laser entrance holes to form two cones: an inner cone that illuminates the hohlraum wall near the equator of the capsule and an outer cone that illuminates an area of the wall closer to each hole. In turn, each inner and outer cone will be composed of two subcones (Figure 5).

NIF's 192 beams are clustered in 48 groups of 4 beams so that there will be 8 spots in each of the two inner cones and 16 in each of the two outer cones. The large number of NIF beams will allow the laser illumination to more closely approximate a uniform x-ray field than did Nova.

Nevertheless, a basic asymmetry will still exist because of hot spots heated directly by the laser beams and cold spots where heat is lost through the laser holes. Because ignition is dependent upon smooth x-ray illumination of the capsule, target designers intend to reduce asymmetries in the x-ray flux to less than 1 percent by properly locating the laser-heated hot spots, adjusting the exact length of the hohlraum, and modifying the laser pulse intensities.

Haan says that two key factors influence the choice of the critical x-ray temperature that drives the capsule implosion. The first is laser–plasma instability. For the best target performance, the laser light needs to be absorbed in the gold hohlraum wall. Many forms of laser-plasma instability can occur as the laser light crosses the plasma before it is absorbed. These instabilities can cause laser light to be scattered back out of the holes or redirected so that it hits the wall someplace other than where it was originally pointed. In either case the result can significantly degrade the planned symmetry of the capsule implosion.

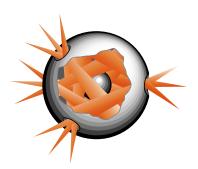
The second key factor affecting the choice of the x-ray temperature is Rayleigh–Taylor hydrodynamic instability (Figure 6). This instability magnifies small surface irregularities on the ice and ablator surfaces during the ablation phase of the implosion. Any perturbations can grow and eventually mix cold D–T fuel with the igniting hot D–T fuel. If the hot fuel is cooled too much by this mixing, it could fail to ignite.

The key to minimizing Rayleigh— Taylor instabilities is the x-ray flux onto the ablator surface. At higher fluxes, that is, at higher x-ray drive temperatures, the ablation of the material also carries off the growing perturbations. Initial perturbations are also minimized by making capsule layers as smooth as possible.

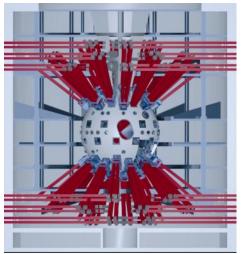
Laser-plasma and hydrodynamic instabilities are complementary threats to ignition, and the targets are



Cylindrical indirect drive



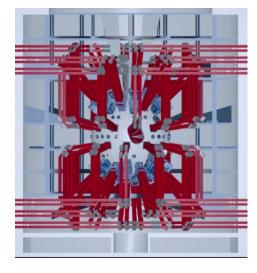
Tetrahedral indirect drive





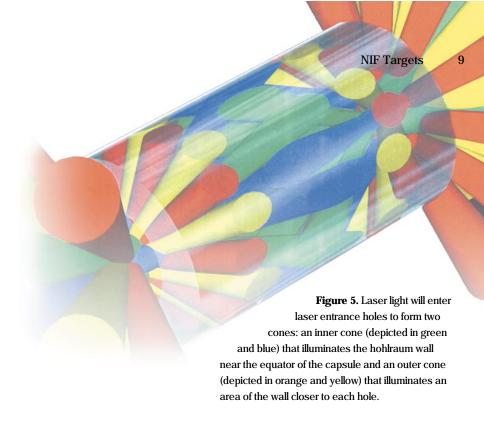
Direct drive

Figure 4. NIF can accommodate three different geometries for target laser illumination: cylindrical indirect drive, tetrahedral indirect drive in which the hohlraum has four laser entrance holes instead of two, and direct drive. The target area and beam-transport system relevant to cylindrical indirect drive and direct drive are shown at right.



intentionally designed so that the two threats are roughly balanced. Higher temperatures requiring higher laser intensities worsen laser–plasma instabilities but minimize hydrodynamic instabilities. In turn, low temperatures minimize laser–plasma instabilities but magnify hydrodynamic instabilities. As a result, designers have arrived at low and high x-ray temperature boundaries, about 250 electron volts and 350 electron volts, beyond which efficient implosion and ignition are difficult to attain.

For example, Haan and Livermore physicist Tom Dittrich designed and analyzed the simulated performance characteristics of a capsule to define a



Target Builders Aim for Tighter Tolerances

NIF ignition capsules will be similar to those used on Nova, but four times larger and with considerably tighter tolerances for smoothness and roundness. Capsules built for ignition experiments must be close to uniformly spherical, or they will not ignite.

Livermore researchers have decades of experience fabricating plastic capsules for use on Nova and its predecessors. However, because of their exacting tolerances and dimensions, NIF ignition capsules will require either improvements to previous fabrication techniques or entirely new methods. Livermore manufacturing experts are working with colleagues at Los Alamos National Laboratory and General Atomics in San Diego, California, to explore ways to meet the rigorous specifications.

Livermore experts are planning to build plastic spherical shells from a liquid solution of polymers and then applying a coating of polyimide. For capsules with outer beryllium layers, Livermore researchers have explored sputtering the beryllium atoms onto the plastic shell. Los Alamos scientists have developed a technique that machines two beryllium-coated capsule hemispheres and bonds them with a submicrometer-thick joint of copper atoms. Upon heating, the copper diffuses into the beryllium, providing a uniform copper doping throughout the beryllium.

The capsules are filled with a precise amount of deuterium—tritium (D–T) at high pressure and temperature. The D–T gas diffuses through the shell until the desired fill is reached at a pressure of about 500 atmospheres. When it is cooled to the operating temperature of 18 kelvins (–255°C), the gas naturally forms an outer layer of solid D–T.

A central issue for capsule fabrication is surface roughness and defects in both the ablator surface and D-T ice layer. The D-T ice

layer must be smooth enough so that it does not become too large a "seed" for hydrodynamic instabilities. Fortunately, in what Livermore target designer Steve Haan calls a "gift from nature," the D–T ice layer's natural radioactivity makes it smooth to within 1 micrometer, about what is required. Careful heating of the D–T with infrared light may allow even smoother ice surfaces. One advantage of beryllium ablator capsules is that they can tolerate a rougher D–T ice surface than polyimide capsules; a corresponding disadvantage is that the fuel cannot be smoothed beyond its natural roughness, because the beryllium is opaque to the infrared heating.

For either material, the ablator layer must be some 30 times smoother than the ice layer because it is more unstable during the implosion. Fortunately, the roughness of this surface can be controlled by the fabrication process or polishing.



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lower boundary on the successful implosion of an ignition capsule. The target requires only 900 kilojoules of laser energy and 250 terawatts of laser power from NIF, thereby lowering the hohlraum x-ray drive temperature from 300 electron volts to 250 electron volts. Because of the small size and low drive temperature characterizing this target, it is quite susceptible to Rayleigh–Taylor instabilities and would require very smooth surfaces. At the same time, laser–plasma instabilities would be expected to be minimal.

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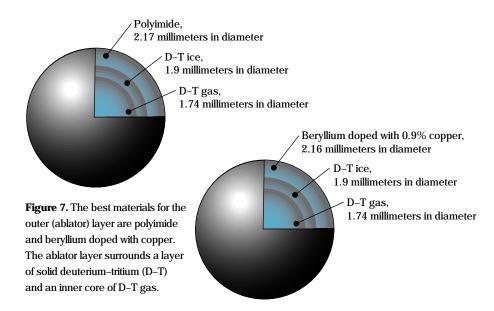
Ideal Is 300 Electron Volts

Haan says an x-ray-driven temperature of 300 electron volts seems to be an ideal

temperature for capsule compression. Most of the model simulations used to set specifications have been done at this temperature. The baseline target uses 1.4 megajoules and 400 terawatts of laser energy and power, well within NIF's 1.8-megajoule and 500-terawatt specifications.

The choice of the x-ray temperature is crucial because it dictates the material forming the capsule's outer ablator layer, key to the implosion and subsequent ignition reactions. If this layer is smooth enough and bathed uniformly in x rays, its ablation will efficiently force the capsule inward at a velocity of about 400 kilometers per second (more than one-thousandth of the speed

Figure 6. Rayleigh–Taylor hydrodynamic instability magnifies small surface irregularities on the capsule ice and ablator surfaces. If these irregularities grow large enough, they will prevent ignition.



of light) and create the pressure and temperature required for fusion reactions to begin.

Livermore and Los Alamos target designers have tested a number of ablator materials (Figure 7). Polyimide is likely to be the best ablator at higher temperatures (up to 350 electron volts), while beryllium is the best at low temperatures (down to 250 electron volts). Polyimides are plastic polymers that exhibit an exceptional combination of thermal stability and mechanical toughness at a wide range of temperatures. They are often used as a protective coat for semiconductors.

Beryllium is attractive at lower hohlraum temperatures (250 electron volts) because it absorbs more energy and at lower temperatures produces higher pressure than plastic. The use of beryllium as an ablator has been explored since the earliest days of the laser fusion program. Its properties have so impressed Los Alamos target designers that they have adopted it as their standard ablator material and are working hard to devise ingenious methods to manufacture beryllium capsules (see box on p. 9).

One drawback to beryllium is that it is opaque to visible light, preventing optical inspection of the fuel. Beryllium ablator capsules also require a dopant with a high atomic number, typically copper, to better absorb the x rays. (Polyimide layers generally need no dopant because their opacity to x rays is about right.)

Both capsule designs must be cooled to 18 kelvins, colder than liquid nitrogen. That temperature is chosen to maintain in equilibrium the central, relatively low-density D–T gas and the high-density, 80- to 100-micrometer-thick D–T ice layer.

The D-T ice layer, the main fuel for ignition, lies just inside the ablator layer. As the capsule is compressed, this dense layer serves to contain the central volume, called the hot spot, at the temperature required for fusion to occur (around

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10,000 electron volts, some 30 times hotter than the hohlraum). The burn from the hot spot eventually spreads into the surrounding dense D–T, which has been compressed during the implosion to a density of about 1,000 grams per cubic centimeter.

Performance Margin Tradeoffs

Haan says that NIF's performance margin should cover estimated uncertainties in the performance of the facility and the targets. Indeed, designers must be sufficiently conversant with the physics issues, targets, and specified tolerances of NIF optical components so they can systematically allocate various sources of asphericity. "Many factors contribute to making the capsule implosion not round," says Haan. "Most can be traded off against each other."

For example, capsules are manufactured to a certain degree of roundness, and laser beams will exhibit some deviations from their specified power rating. "All we care about is obtaining good spherical implosion," Haan says, "so we can tolerate poorer power balance if we manufacture more spherical capsules, or vice versa."

Haan emphasizes that ignition experiments will be preceded by a twoto three-year phase of experiments testing components, diagnostics, and various aspects of the hohlraum and target designs. The team plans to start out slowly, with noncryogenic and nonignition targets that are more forgiving of asymmetrical laser light. The team will not wait for all 192 beams to be up and running. Instead, target experiments will use four-beam clusters as soon as they are available.

"We want to proceed smoothly up the learning curve as we gain experience with the facility," says Haan. "The first couple of years will tell us exactly what we need to know to maintain the hohlraum at the desired temperature and achieve ignition."

With the aid of collaborations worldwide and rigorous computer simulations, the team—and the scientific community—is confident that NIF target designs will support ignition. Successful ignition will fulfill a dream of decades and usher in an era of experiments conducted at the extreme physical conditions found only in stars and detonating nuclear devices.

-Arnie Heller

Key Words: ablator, Commissariat a l'Energie Atomique, deuterium-tritium (D-T), F3D, hohlraum, HYDRA, Rayleigh-Taylor hydrodynamic instability, ignition, implosion, laser-plasma instability, LASNEX, Los Alamos National Laboratory, National Ignition Facility (NIF), polyimide, stockpile stewardship.

For further information contact Steve Haan (925) 422-4715 (haan1@llnl.gov).

About the Scientist



STEVE HAAN received a B.S. in physics from Calvin College in Grand Rapids, Michigan, and a Ph.D. in physics from the University of Maryland. He joined Lawrence Livermore in 1981, where he has concentrated on target design and modeling of inertial confinement fusion (ICF). He participated in the Halite–Centurion program of underground tests for ICF and currently is working on the theory and modeling of hydrodynamic instabilities in ICF targets, on the design

and modeling of Nova and Omega experiments, and on the design and modeling of targets for the National Ignition Facility. In 1994, he was designated a fellow of the American Physical Society (APS). Along with coworkers, he was awarded the 1995 APS Award for Excellence in Plasma Physics Research. He is a 1999 recipient of the Edward Teller Medal in Inertial Fusion.

A New View of the Universe

With Livermore's laser guide star and adaptive optics systems, the heavens are becoming clearer. Dim objects will become brighter, and some invisible ones will be visible.

STRONOMERS consider Earth's atmosphere a real nuisance. The very air we breathe distorts their view of the heavens and prevents a telescope from forming sharp images. But in recent years, scientists have found a way around this problem by using optical systems that correct incoming light, in effect getting rid of the turbulence in the atmosphere.

Known as adaptive optics, these systems for sensing and correcting atmospheric aberrations were first proposed in 1953. The first solution to be implemented was tilt-tip correction, the tilting of a secondary mirror several times a second to eliminate or reduce the dancing motion of an image. But that did not get rid of the blurring that the atmosphere produces. Sharpening the image required new technologies to split the incoming light beam into many small elements and correct each element separately, hundreds of times a second.

These technologies are available today because of research funded by the Departments of Energy and Defense into methods for imaging objects that are far away and for keeping a laser beam sharply focused in the atmosphere.

Right now, there are about 10 adaptive optics systems installed on astronomical telescopes. Adaptive optics correct incoming light from distant celestial bodies, which typically are very dim, by using a relatively bright, natural guide star as a reference. With adaptive optics, resolution of the dim objects improves dramatically—as long as they are close enough to a bright reference star.

When observing at visible wavelengths, astronomers using adaptive optics require a nearby fifthmagnitude star, one that is just bright enough to be seen unaided, as a natural guide star. For near-infrared observations, only a twelfth-magnitude star—a thousand times fainter—is needed. There are hundreds of thousands of these natural guide stars, but they are only enough to allow adaptive optics to function over about 1 percent of the sky.

Enter Lawrence Livermore's laser guide star and adaptive optics systems.

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They can be mounted on a telescope and directed into virtually any part of the heavens an astronomer wants to study. In 1995, Livermore installed a laser guide star on the 3-meter Shane telescope at the University of California's Lick Observatory on Mount Hamilton near San Jose, California. The Shane became the first major astronomical telescope to use an artificial guide star system with full adaptive optics.

Every telescope has a limit to its resolution, defined largely by the size of the telescope's mirror. With Livermore's laser guide star and adaptive optics, the images obtained from the Shane telescope are as close to perfect as possible. The telescope can now achieve diffraction-limited results, meaning that only diffraction effects limit its performance. Figure 1 demonstrates how adaptive optics is improving astronomical viewing for near-infrared light.

Physicist Scot Olivier, who is leading the adaptive optics work at Livermore, is clearly excited about the work. "Results to date at Lick are impressive, and now an adaptive optics system is also being installed at the Keck II telescope in Hawaii. The two Keck telescopes are the largest in the

world and are quickly becoming the preeminent tools in astronomy" (Figure 2).

The Lick Observatory system was the prototype for the one at the 10meter Keck II telescope atop Mauna Kea in Hawaii. The two Keck telescopes are owned jointly by the University of California, the California Institute of Technology, and the National Aeronautics and Space Administration. Livermore and Keck Observatory are collaborating on the installation of the adaptive optics system. Livermore is responsible for developing the laser and high-speed wavefront control systems, and Keck personnel are responsible for the optomechanical system, user interface, supervisory control, and project management. Testing is expected to be completed by this fall; fully functional adaptive optics should be available for scientific use in early 2000. A laser guide star system designed and built by Livermore will also be installed at Keck next year.

A Sodium Star Is Born

Since the 1980s, two types of laser guide stars have been developed at laboratories and universities around the world. One uses Rayleigh scattering of

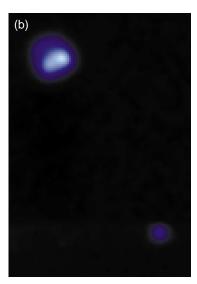
ultraviolet or visible light at a height of 5 to 15 kilometers in the atmosphere. The other uses resonant scattering of light from a layer of sodium atoms that sits in the upper mesosphere at about 90 to 100 kilometers in altitude. The second scheme has the advantage of putting the reference beacon higher, thus sampling a larger portion of the path of light from a celestial object in space to a telescope on Earth.

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The sodium guide star was an idea co-developed by Claire Max, currently Livermore's Director of University Relations, as part of a study for the Department of Defense in 1984. Max initiated Livermore work on laser guide stars and astronomical systems in the early 1990s, once laser technology had evolved to make these projects technically feasible. Engineer Herb Friedman led the development of the laser systems used in this work.

Livermore's guide star is created by a dye laser system, a cousin to the laser used for Livermore's Atomic Vapor Laser Isotope Separation (AVLIS) program. Green light from flashlamppumped, solid-state lasers beneath the main floor of the telescope dome travels through fiber-optic lines to a compact dye laser mounted on the side of the telescope. The dye laser converts





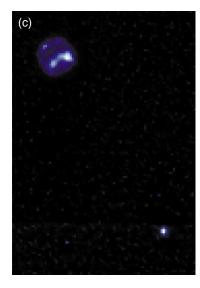


Figure 1. Three views of Neptune and its moon Triton: (a) a typical infrared image, (b) a better image taken from a better observation site, and (c) an image taken with adaptive optics, in which cloud bands are clearly visible. (Neptune and Triton are bright enough that a laser guide star is not needed to view them.)

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Figure 2. Keck I and Keck II telescopes atop the Mauna Kea volcano in Hawaii.



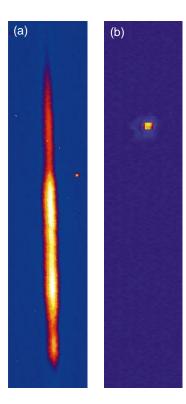
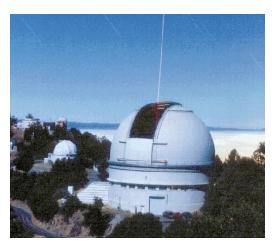


Figure 3. Views of the laser guide star at the Lick Observatory.

(a) From another telescope at Lick, the guide star appears as a streak.

(b) From the Shane telescope, the guide star looks like another star in the sky.



the light from green to yellow, the same color as sodium-vapor street lights. A beam projector then directs the yellow light up through the atmosphere.

For the first 30 or so kilometers, the light is visible because it is scattered by air molecules and dust in the atmosphere. For the next 60 kilometers, the light is invisible as it travels through the clearer stratosphere. Then at about 95 kilometers, the laser beam hits the layer of sodium atoms, the product of micrometeorites vaporizing as they enter the upper atmosphere. Tuned to 589 nanometers, sodium's resonant wavelength, the laser excites the atomic sodium, which emits the yellow light in all directions to create a glowing guide star (Figure 3).

As with any light source in the heavens, some of the light from this

artificial sodium star travels back through the atmosphere. At the telescope, the adaptive optics system measures and corrects the guide star image for atmospheric distortions caused by air turbulence and temperature changes. Any corrections made to the guide star's light affect all of the celestial objects in the same patch of sky, thus improving the view of the particular object the astronomer wants to see.

Several research institutions around the world have carried out sodium guide star experiments, but the only other sodium laser guide star currently in use is at the Calar Alto Observatory in Spain. Its laser is about one-fifth as powerful as the one that Livermore is using at the Lick Observatory.

Covering the Sky

A natural guide star travels through Earth's atmosphere only once, while the laser guide star must traverse it twice, up and back. Atmospheric effects cause the artificial guide star to appear larger than a comparable natural guide star, making it somewhat less accurate as a reference point. A natural guide star is about two times more effective as a wavefront reference than the laser guide star, although engineer Don Gavel and others at Livermore are working to make the laser spot smaller to improve its performance.

But the laser guide star makes up for its deficiencies by offering a significant improvement in sky coverage. This is because the laser can be pointed anywhere in the sky to make a bright artificial star.

Making Stars Bright

In the adaptive optics system, a wavefront sensor and a deformable mirror make corrections to light beaming into the telescope (Figure 4). The system must work quickly because the atmosphere between the telescope

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and the heavens typically blows by at about 10 meters per second, requiring a correction every few milliseconds.

A tilt-tip mirror, with its own sensor and camera, makes the initial correction to the incoming beam of light to stop it from dancing. Then the beam travels to a deformable mirror where the shape of the incoming wavefront is determined. A Shack-Hartmann wavefront sensor, which at Lick has 40 subapertures, examines part of the shape of the incoming wavefront. The sensor measures the difference between the actual shape and a perfect, flat wavefront. The measurements go into a computer that directs the activities of the deformable mirror. As the atmosphere blows by, the wavefront sensor and deformable mirror are in constant communication, searching for errors and correcting them.

The mirror at Lick has 127 electrostrictive actuators—each a tiny piston—arranged in a triangular pattern. Each

actuator can raise or lower a part of the mirror surface by as much as 4 micrometers to straighten out the incoming light and make it all travel in the same direction. (This mirror is much like other deformable mirrors that Livermore has developed to correct wavefront aberrations in laser light in the 192-beam National Ignition Facility.)

The goal for astronomical adaptive optics is to flatten the guide star's incoming wavefront to achieve as perfect and hence as bright an image as possible. Once the system operators are satisfied with the image they have achieved for the guide star, the imaging camera, also known as the science camera, is turned on to gather data on the celestial object of interest.

Keck has a larger adaptive optics system than Lick because its telescopes are much larger. At Keck, the wavefront sensor has 241 subapertures and the deformable mirror has 349 actuators arranged in a square pattern.

The View from Lick

With the laser guide star and adaptive optics mounted on Lick's Shane telescope (Figure 5), images of distant stars are smaller by a factor of almost 4. Figure 6 compares the view of a distant, dim star without adaptive optics in place and with laser guide star adaptive optics. This star is located in a part of the heavens where no bright natural guide star exists, so Livermore's laser system is the only method available for improving images.

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Livermore scientists have used Lick's adaptive optics to examine young stars to see whether they are actually binary stars (Figure 7). Disks of dust within which planets are forming may surround some of these bright stars. Some scientists believe that our solar system was formed that way, and a look at a similar solar system in the making would be exciting indeed.

Livermore astronomer Bruce Macintosh has scheduled five nights in

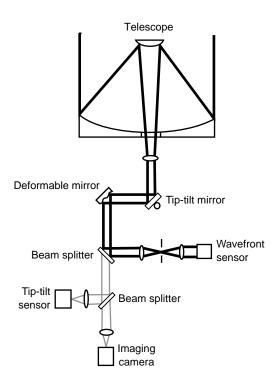


Figure 4. Schematic of adaptive optics system.

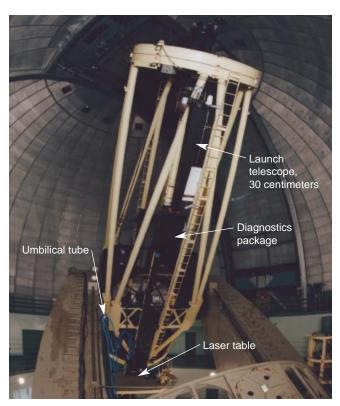


Figure 5. The Shane telescope at the Lick Observatory is mounted with the Livermore laser guide star and adaptive optics system.

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September on the Shane telescope to search for nearby brown dwarf stars. Brown dwarfs have a mass between that of a large planet and a small star, as much as 80 times the mass of Jupiter. Their mass is too small to sustain fusion, but they still glow from stored heat. Brown dwarfs are thought to be a contributor to the dark matter in the universe. According to Macintosh, "Brown dwarfs are rare, so it takes a long time to search for them. Five nights in a row will be enough to look at all the young, nearby stars in half the sky. I have another five nights reserved in the spring of 2000 to look at the other half. All told, we will look at about 200 of the closest stars to see if any of them are brown dwarfs."

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And the View from Keck

With the largest mirrors in the world, the Keck telescopes on Mauna Kea can produce the highest-resolution images available. With that capability, it is not surprising that demand is high for time at Keck. Even without an

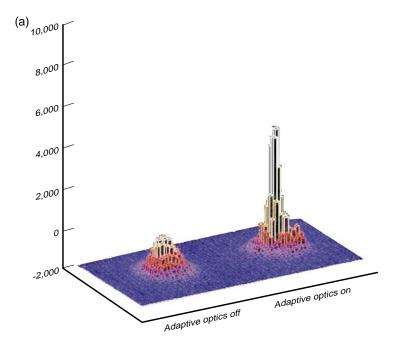
adaptive optics system, Keck's huge telescopes are bringing understanding to faint objects that until now have been difficult to see.

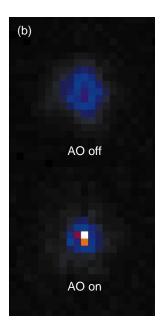
Saturn's moon Titan holds special interest for scientists because it is the only planetary moon that has a thick, nitrogen-dominated atmosphere. Although it is several hundreds of degrees colder than Earth and its atmosphere is rich in methane, in some ways its chemistry seems to be like that of Earth before life appeared. Titan's organic chemistry is also driven by sunlight, as Earth's is. On Titan, however, sunlight works to transform methane to ethane. Some scientists believe that Titan may have liquid seas formed by ethane that has "rained out" to produce reservoirs of liquid hydrocarbons. Titan's orange haze makes it impossible for Earth-bound scientists to see its surface in visible light, but in the near infrared, a few spectral "windows" allow surface features such as continents and potential hydrocarbon "oceans" to be detected.

Macintosh, scientist Seran Gibbard, and their colleagues from Livermore have been working at Keck with University of California–Berkeley professor Imke de Pater and her students to use speckle imaging to study Titan. With adaptive optics installed at only a few telescopes, speckle imaging has been the best way to learn more about many celestial objects. Traditional astronomical imaging uses long exposure times to gather as much light as possible and often results in a picture resembling a fuzzy blob. Speckle imaging involves taking several hundred pictures with short exposure times-snapshots to freeze atmospheric turbulence-and then reconstructing an image that is generally much sharper than otherwise available. But the method only works with bright objects.

Speckle images of Titan at Keck achieved higher contrast and spatial resolution than any previous images, including those from the Hubble Space Telescope. But speckle imaging is slow

Figure 6.
(a) Views of a star observed with and without laser guide star adaptive optics (AO) correction.
(b) The AO correction makes the star smaller and its peak intensity brighter.





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and inefficient. It requires taking many pictures, which means considerable time both on the telescope and on the computer to reconstruct a final image.

Recent tests of Keck's adaptive optics systems produced an even higher resolution image of Titan (Figure 8). Adaptive optics is much faster than speckle imaging, producing almost immediate results as well as better information about Titan's atmosphere and surface.

At Keck, Livermore astronomers also want to study binaries and other bright objects that do not need an artificial guide star. These include Neptune and Io, the innermost of Jupiter's moons. Io is the most volcanically active area in our solar system because of extreme tidal forces caused by the gravitational effects of nearby Jupiter.

Other Life out There?

In two years or so, when both adaptive optics and a laser guide star are available on the Keck II telescope, a whole new view of the universe will be possible. Once dim objects will look brighter, and some objects once invisible will become visible.

Just a few months ago, astronomers from San Francisco State University and Harvard made news yet again for discovering a star with a planetary system. This one appears to have three huge planets, the third and largest being four or more times the size of Jupiter. This marked the first discovery of another planetary system with more than two planets. Only the enormous mass of the third planet made it detectable.

Such discoveries come not from seeing the planets revolving around a star but from observing regular wobbles in the star's motion that result from the strong gravitational pull of nearby planets. Only very close and very large planets affect a star enough to induce the wobble. In fact, if

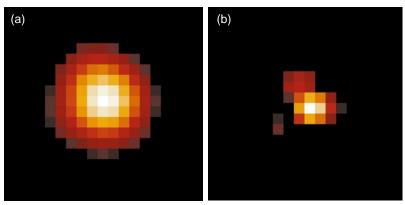


Figure 7.
Images of FS
Tau, a young
star, (a) without
adaptive optics
and (b) with
Lick laser guide
star adaptive
optics, in which
a faint binary
companion is
seen.

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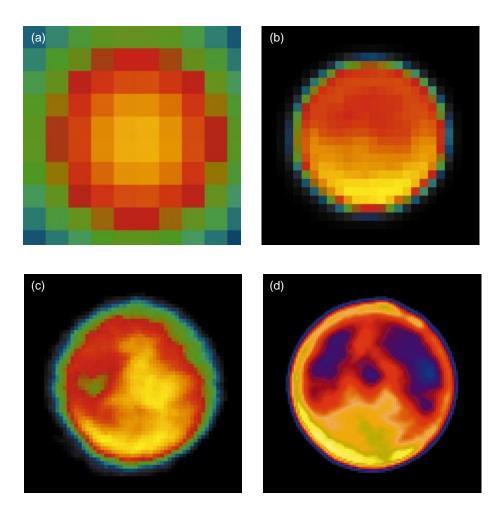


Figure 8. Four views of Titan obtained by different telescopes. (a) Image from a ground-based telescope without adaptive optics. (b) Image from the Hubble Space Telescope (diameter = 2.4 meters) at a wavelength of 0.8 micrometers. (c) Speckle image from the Keck 10-meter telescope in the near infrared. (d) Adaptive optics image from the Keck telescope in the near infrared, showing a different face of the moon than was imaged in (c).

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Trainees from Hawaii at Livermore

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Livermore has been home since March to two interns from Hawaii who may some day work on the Keck telescopes or at one of the other great observatories in Hawaii. After completing general training in a variety of technical fields, Kristian `Alohalani Keahi from the island of Kaua`i and Shordon Kanaiaupuni Lopes from the island of Oahu began working in Livermore's adaptive optics laboratory. There they are operating lasers as well as setting up experiments and gathering data using a variety of optomechanical, electrooptical, and electromechanical equipment. They also have been working at the Lick Observatory as part of the Livermore team.

Their stay is part of Livermore's National Security Field Experience Initiative (NSFEI), which provides hands-on experience and mentoring to individuals interested in becoming part of the scientific and technological work force. NSFEI focuses on locations that are of strategic importance to national security, such as Hawaii and Alaska. The purpose of the internship program is to prepare the participants for careers in existing and emerging technologies, especially those that contribute to addressing global issues. The first NSFEI partnership was established in 1996 with ALU LIKE, Inc., a nonprofit, native Hawaiian training and job placement center.

Kristian and Shordon are two of eight Hawaiian interns who completed eight weeks of training at Livermore in late April. They worked in a variety of technical fields, such as computer system administration and applications, vacuum technology, electronics, telecommunications, machining, adaptive optics, and more.

"The interns are immersed in technology and given the big picture," says Marjorie Gonzalez, the NSFEI program leader. "Many started with an interest in telecommunications, but after being introduced to vacuum technology and optics, most chose to redirect their focus." Kristian and Shordon elected to gain more experience in adaptive optics.

After completing their training, NSFEI interns return to Hawaii where they seek entry-level employment, participate in additional on-the-job-training internships, or continue their formal education. All interns who have completed the program in the



past are currently employed in Hawaii, several on defenserelated environmental remediation projects and in defense telecommunications.

Kristian Keahi and Shordon Lopes in the adaptive optics laboratory. someone on a planet somewhere else in the universe were observing our solar system with current detection techniques, the Earth and even Jupiter would not be detectable because the Earth is too small and Jupiter too far from the sun to impose much of a wobble.

The recently found planetary system may actually have more than three planets, but we cannot detect them yet. Astronomers hope that with adaptive optics, Keck will make that solar system or others like it not just detectable but actually visible in picturelike images.

Astronomers at Livermore also plan to study galaxies in the early universe to learn more about their structure. Located at the distant reaches of the universe, these dim galaxies require laser guide star adaptive optics to provide a clear view of the turbulent dynamic processes that led to their formation.

It's Not Over Yet

The success of the laser guide star and adaptive optics is enticing. If they work so well, what else can be added to give astronomers and astrophysicists even more information about the universe? Beginning next year, spectroscopic instruments will augment current adaptive optics imaging. Spectroscopy, long a part of the tool kit of those who study the sky, looks at the absorption and emission of light by matter. Each element gives off a different wavelength of light or signature spectrum.

Spectroscopic analysis has led to some remarkable astronomical discoveries. The study of spectral emissions of distant galaxies led to the revelation that the universe is expanding rapidly and in all directions. The finding was based on the observation of a Doppler shift of spectral lines. It was Edwin Hubble, after whom

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the Hubble Space Telescope is named, who discovered in the 1920s a roughly linear relationship between the distance of these galaxies from Earth and their Doppler shift. In any direction one looks, the farther away the galaxy appears, the faster it is receding from Earth.

Studying individual objects spectroscopically is more challenging than simply taking their pictures. Some objects in the sky are bright enough that scientists can apply spectroscopic analysis and determine their chemical makeup. But if the only image of an object is a poorly defined, faint blob, spectroscopic analysis is not always possible. Adaptive optics can solve that problem by replacing a blob with a much more clearly defined and brighter image. For example, we can now produce an image of Neptune clear enough for meaningful spectroscopic analysis of its clouds and its cloud-free regions (Figure 1c).

Research also continues on improving deformable mirrors. Work is under way on techniques that use liquid crystal and microelectromechanical devices to implement more phase control points. Thus far, Livermore has demonstrated a system with 1,800 liquid-crystal actuators. Mirrors as deformable as that could extend adaptive optics correction from near-infrared wavelengths into visible wavelengths for large astronomical telescopes.

As long as astronomers continue to study the skies from ground-based telescopes, our planet's atmosphere will be in the way. For us to be the living, breathing creatures we are, we wouldn't want it any other way. At least now there is a way to punch through the atmosphere and get a clear look at the entire sky.

-Katie Walter

Key Words: adaptive optics, astronomy, Keck Observatory, laser guide star, Lick Observatory.

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About the Scientist



SCOT OLIVIER is an optical physicist in Lawrence Livermore's Laser Programs Directorate and currently is adaptive optics group leader in the directorate's Information Science and Technology Program. He joined the Laboratory in 1991 as a postdoctoral researcher after receiving his Ph.D. in physics from the University of California at Santa Cruz. His B.S. from Princeton University is in electrical engineering and computer science as well as

engineering physics. He has specialized in optical science throughout his career and has published 29 papers on adaptive optics.

Quantum Molecular Virtual Laboratory

HAT happens to water under high pressures and temperatures? Why does silicon carbide break where it does when strained? How does DNA interact with water?

Complete, accurate answers to these deceptively simple questions—and others like them—require knowing what is going on at the atomic level. This means one must account for the behavior of individual atoms and electrons in an entire system: how they move, how they chemically bind, and how those bonds form and break. Not an easy proposition, once one moves beyond a small number of simple atoms.

Computers have long been used to model material behavior, both on the large and small scales. Macroscopicscale modeling applies statistical mechanics methods to the system as a whole, ignoring details about how each atom

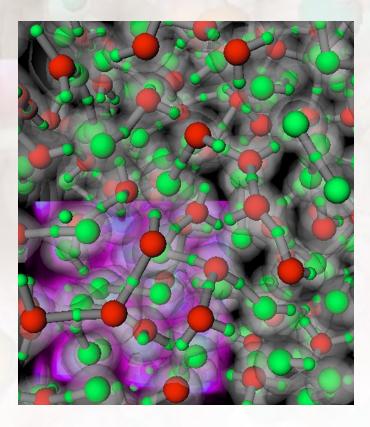


Figure 1. This quantum-level simulation of hydrogen fluoride–water mixtures at high temperatures and pressures took 15 days on the ASCI computer, on which trillions of operations per second were performed, to calculate one picosecond of the mixtures' atomic interactions.

responds. Atomic-scale modeling applies the laws of quantum mechanics—fundamental physics equations that describe electrons—but because of the complex nature of the equations, these models can handle only a few atoms at a time.

Lawrence Livermore physicists Francois Gygi and Giulia Galli and their collaborators are using the computer power of the Department of Energy's (DOE's) Accelerated Strategic Computing Initiative (ASCI) and Gygi's JEEP code to push the limits of atomic-scale modeling of complex systems. ASCI, guided by the Office of Strategic Computing and Simulation under the DOE Assistant Secretary for Defense Programs, is developing capabilities to simulate nuclear weapons performance in lieu of nuclear testing. To do so requires computers of unprecedented computational power and speed, as well as simulation codes such as JEEP.

JEEP, which Gygi began developing at the Swiss Federal Institute of Technology about five years ago, uses quantum molecular dynamics (QMD) methods to simulate the behavior of materials at the microscopic level. "Unlike the macroscopic-scale codes, we make no assumptions in using JEEP," explains Gygi. "Using QMD, we input only absolutely known quantities into the code—that is, the identities of the atoms and the laws of quantum mechanics. Combining this approach with ASCI's computational power, we can examine material systems of hundreds of atoms and thousands of electrons extremely accurately."

With JEEP, the ASCI computer becomes a virtual laboratory, where scientists can follow the trajectories of atoms and study the forming and breaking of chemical bonds. This powerful combination can be used to predict physical properties of various materials, investigate properties not directly accessible through physical experiments, and interpret and complement physical experiments.

QMD simulations have a number of applications, from deepening our understanding of materials under extreme conditions—a vital issue for DOE's Stockpile Stewardship Program—to forming a better understanding of complex biological systems.

Modeling the Impossible Experiment

The detonation of some high explosives produces hydrogen fluoride and water, both of which are hydrogen-bonded systems. Little is known about this mixture because hydrogen fluoride is toxic and corrosive, making experiments difficult.

Using the JEEP code on the ASCI computer, Galli, Gygi, and physicist Francis Ree conducted quantum-level simulations of hydrogen fluoride—water mixtures at high temperatures and pressures (Figure 1). These simulations were of unprecedented scale: a picosecond-long "peek" at the interactions of 600 atoms with 1,920 electrons required updating and computing 200 million unknowns. It took 15 days and the entire resources of ASCI's Sustained Stewardship Blue Pacific machine, with teraops (trillions of operations per second) calculational power, to simulate this one picosecond's worth of interactions.

The results provided a better understanding of high-explosive detonation products, revealing their molecular interactions and chemical reactions. The results also helped scientists better understand the equation of state of the mixture. The simulations indicated that hydronium fluoride and hydrogen difluoride anions are produced at high pressures, something that has been hypothesized but not yet observed.

Stretch and Break

In another numerical experiment, Gygi and Galli simulated what would happen when a microscopic chunk of amorphous semiconductor (silicon carbide) is stretched past its breaking point (Figure 2).

"One of the advantages of computational simulations over experiment, in general, is that we can define chemical purity at 100 percent," explains Galli. "We can create the configuration that we want, apply a strain to the system, and let the code run. We watch what happens, what bonds break and where, and how the resulting microfracture relates to the chemical properties of the material."

These quantum simulations provided numbers relating to the elasticity and hardness of the material that could then be compared to results gathered from physical experiments. Galli notes that this was the first time hardness had been computed from first principles for a disordered alloy. "In the past," says Gygi, "it's only been computed for crystal or ordered structures, because disordered systems are much more complex."

They also discovered that the simulated semiconductor material broke at a silicon-rich "island" and were able to define the surface where the material cleaved. "Most of the surface atoms were silicon," says Galli. "In laboratory experiments with this material, physicists find precisely that, so we were pleasantly surprised when we saw it in our numerical experiment as well."

Galli and Gygi plan to continue these studies by simulating atomic clusters residing on other types of semiconducting surfaces as well.

Delving into DNA

Their most recent work involves examining components of the familiar two-strand, double-helix DNA structure. Each strand of DNA consists of a "backbone" on which chemical bases attach. When the two strands are wound around each other in the familiar configuration, a base from one strand attaches to a base on the partner strand, forming base pairs that step up like ladder rungs (Figure 3).

Working in conjunction with Michael Levitt from Stanford University and Livermore's Eric Schwegler, Gygi and Galli are examining what happens to the DNA backbone in water, its natural medium. They plan to isolate a fragment of the DNA backbone and simulate how a molecule of dimethyl phosphate from that fragment interacts with water molecules. While the Livermore scientists use JEEP for the simulation, Levitt will be running a simulation code with his widely used model of this interaction. The numerical experiments at Livermore are expected to validate or invalidate some of the assumptions

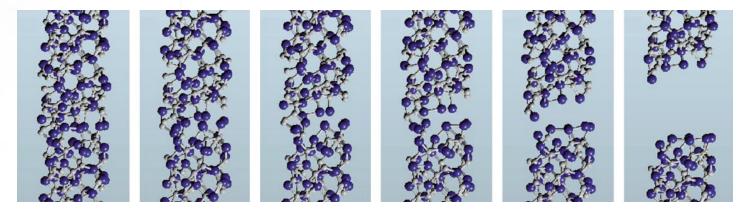
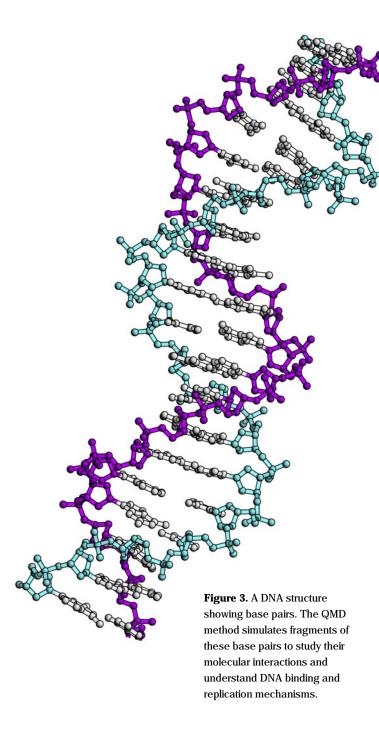


Figure 2. A chunk of silicon carbide, a disordered structure, was simulated being stretched to breaking to see which bonds break and how the resulting microfracture relates to its chemical properties.

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made in standard models and serve to improve them. The results will also deepen understanding of this complex biological system. The work is being carried out within a Laboratory Directed Research and Development strategic initiative on computational biology led by Mike Colvin.

In another DNA experiment, Gygi, Colvin, Raymond Fellers, and Daniel Barsky are extracting a single DNA base pair to see how the complementary bases interact. They expect to better understand what causes DNA to bind and which molecular interactions are key to binding. On a larger scale, they hope to find out how binding mechanisms affect the replication of DNA.

At stake is understanding the fidelity of DNA replication. Sometimes, because of damage or mutation, a different molecule replaces one of the bases. The question then is, will the DNA successfully replicate itself? "Understanding this issue is a very long-range goal," Gygi notes. "For the short term, we hope to calculate the energy needed to separate a base pair and, through the results, discount certain scenarios of DNA binding."

"One key thing to keep in mind about all this work," adds Gygi, "is that the JEEP simulations do not provide the full picture. But they do provide key pieces to a puzzle, which allow us to look at yet other pieces and say whether those are a part of the same puzzle."

Laboratory Is a Unique Environment

The Laboratory provides the requisite elements for performing QMD: top-notch physics, the biggest computational machines available, and state-of-the-art visualization tools to help view and interpret enormous amounts of data. "There are few places in the world where you can pull all this together," says Gygi. "We've been able to apply our methods to different problems and learn things that relate to other areas of research. The big machines with terascale computing power have made it possible to study more and more complex systems, more reliably and accurately. Finally, these big machines have made it possible to build a bridge between two worlds of simulation—the macroscopic-scale simulations using statistical mechanics and the atomic-scale simulations using quantum mechanics."

-Ann Parker

Key Words: Accelerated Strategic Computing Initiative (ASCI), computational biology, DNA, high explosives, JEEP, material behavior, quantum molecular dynamics (QMD), semiconductor.

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AAA in the Sky for Satellites

Their numbers will continue to grow as new launch vehicles bring about more routine and lower-cost access to space. Forecasts show that during the next decade, between one and two thousand new satellites will be put in orbit. Over time, some of them inevitably will begin to fail and will need to be inspected, monitored, repaired, or removed.

Lawrence Livermore is developing a very maneuverable microsatellite that can operate as a service vehicle in space for ailing satellites. The tiny, 40-kilogram vehicle, dubbed MicroSat, will be the first truly agile, small satellite. Once deployed, it will perform close-up inspections to determine the health and operational status of other satellites in orbit (Figure 1). Because the MicroSat can get close to other satellites, it can use new types of diagnostic sensing techniques to collect data unattainable from the ground. Active vibration sensing, for example, can yield specific information on moving parts that can be used to evaluate and characterize vehicle wear and performance degradation remotely. Thermal imaging can reveal surface features invisible to the eye, including leaks and nonuniformities that may result from changes in thermal insulation or structural fatigue.

These on-orbit measurements will offer early detection of potential failures and insight into events that might limit the life of the satellite. Periodic checks could allow preventive or corrective measures and avoid unexpected system breakdowns that lead to service outages, as occurred in 1997 to a communications satellite supporting a large paging system. The Livermore MicroSat is being designed to perform autonomous docking with ailing satellites and could eventually fly missions to repair or retrieve them. A docking maneuver is shown in Figure 2.

The Livermore team of 15 engineers and technicians is led by physicist Arno Ledebuhr; engineer Joe Kordas is the deputy project leader. The MicroSat program is funded by the U.S. Air Force Research Laboratory and is a spin-off from the Clementine II Program, which consisted of an asteroid fly-by and impact experiment. That earlier project was discontinued in 1997 and redirected by the Air Force to a series of MicroSat Earth-orbit demonstrations.

The team is working toward a date in 2002 when one of its MicroSats will be flown on either the space shuttle or an expendable launch vehicle. If flown on the shuttle, the Livermore MicroSat will ride on a National Aeronautics and Space Administration *Spartan 251* "mothership carrier" spacecraft bus. The Livermore MicroSat will have to autonomously perform a series of complex tasks and conduct various close-in proximity maneuvers within a few meters of the *Spartan* carrier. It will collect stereo images and perform multiple autonomous dockings with the *Spartan*. Experiments

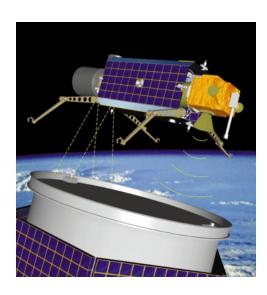


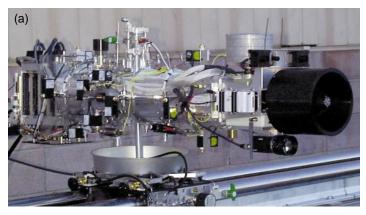
Figure 1. In this artist's rendering, a MicroSat gets a close look at a larger satellite. The goal is for the MicroSat to rendezvous with a satellite, inspect it, dock with it, service it, and verify its performance. It will look for signs of wear, including atomic oxygen and ultraviolet surface damage, micrometeoroid impacts, and debris cloud generation from leaks or other deterioration. These data can be stored on board or forwarded to ground control through an Ethernet connection.

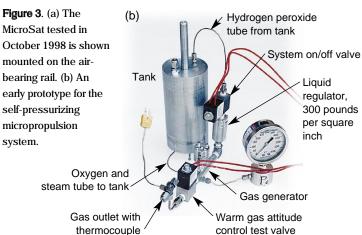
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Figure 2. Active radar or lidar, augmented by stereo imaging, will be used for precision ranging during the final docking phase. Once docked, the MicroSat will be able to repair or replace subsystems, tow or push the satellite to a different orbit, and pull "space junk" out of orbit.

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will include the transfer of data and power between the two spacecraft. The Livermore MicroSat will then maneuver itself into its original deployment canister on board the *Spartan* mothership, which will be retrieved by the space shuttle and returned to Earth. Follow-on spacecraft experiments will examine autonomous docking onto a spinning satellite, propellant transfers, and towing experiments.

Old Hardware Put to New Use

The first prototype MicroSat was constructed in 1997 with spare hardware collected during earlier program efforts. It was operated on a new dynamic air-bearing table that enabled extensive and repeated ground testing of its guidance, navigation, and control software (see S&TR, September 1998, pp. 24-26). The next prototype was based on the Clementine II asteroid-impact probe vehicle and contained the first liquid propellant propulsion system. This MicroSat design was augmented with additional support subsystems to provide stand-alone operation in orbit, including solar arrays for battery recharging, thermal management, micropower impulse radar for docking, stereo cameras for passive ranging and telepresence, and a global positioning system receiver. The third vehicle incorporated improvements in propulsion, electronics, and sensors. For future vehicles, the team wants to add grappling and robotic arms for manipulation during docking and servicing missions.

The test vehicles combine the team's unique designs, other Livermore developments, and commercial systems. To date, three prototype vehicles have been ground tested on the airbearing table, and the two most recent models have been tested outside on an air-bearing rail.

Darting about in Space

A critical aspect of the MicroSat design is its propulsion system, which must be able to move the vehicle about in orbit as well as control the satellite's attitude. There is no precedent for small, agile orbiting satellites with the large propulsion capability of the Livermore MicroSat designs. For maximum agility and range, the MicroSat must have the highest possible ratio of fuel capacity to overall mass. This goal is achieved by reducing the vehicle's dry weight and using miniaturized subsystems throughout.

Conventional spacecraft propulsion systems use highpressure-fed toxic liquid fuels, but these systems cannot be miniaturized easily. Many small spacecraft use compressed gas such as nitrogen, which works well for attitude control but not S&TR July/August 1999 Small, Agile Satellites

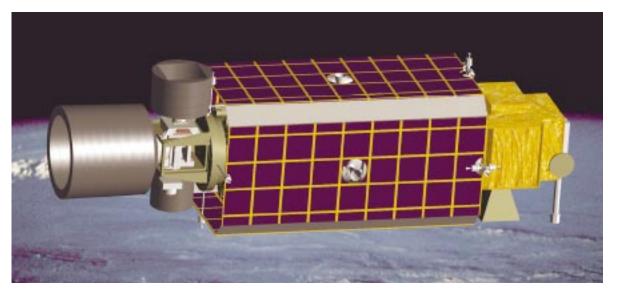


Figure 4. Artist's rendering of the MicroSat that will fly on the space shuttle.

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for maneuvering. Compressed gas tanks also tend to be heavy. "Enabling agile maneuvering on a tiny scale requires fundamental advances," notes lead propulsion engineer John Whitehead.

Liquid can be stored more efficiently (that is, in lighter weight tanks), so MicroSat's innovative propulsion system relies on the concept of making gas as needed from liquid fuel. The system supplies tiny gas jets for vehicle attitude control and small precision maneuvers and fuels liquid thrusters for large orbital maneuvers.

Most rocket fuels are toxic, but Whitehead opted for nontoxic, high-concentration hydrogen peroxide (H₂O₂) to ease experimentation and development processes and thus reduce the cost of the project. Hydrogen peroxide was the first choice because of its proven track record. The U.S. space program used it in the past, and the Russians still fly their *Soyuz* vehicles with it.

For testing purposes, the Livermore team's first prototype MicroSats used compressed nitrogen (N_2) only. The next vehicle used N_2 for attitude control but added liquid H_2O_2 thrusters for directional maneuvering. The N_2 forced the H_2O_2 out of the liquid thrusters in a pressure-fed system.

The latest version, tested in October 1998, eliminated the N_2 system altogether, saving the weight of its relatively heavy storage tanks. A patented micropump designed by Whitehead is used to self-pressurize the liquid H_2O_2 tank, with oxygen and steam derived from the propellant itself. Shown in Figure 3, the system is lighter than its predecessors, although it still requires a higher-pressure liquid tank to operate. This self-pressurized system provides a constant system pressure as

propellant is expended. It could be launched unpressurized or at low pressures, making launch safer as well.

The next step is to develop a slightly larger and more efficient pump that draws the liquid H_2O_2 out of its tank, making the satellite even more lightweight and agile. More of the system's total weight can be devoted to fuel and less to components.

Aside from the revolutionary propulsion system design, the Livermore MicroSat uses the latest generation of Power PC processors and compact PCI-format electronics. It also incorporates advanced active pixel sensors that, along with miniaturized laser ranging systems, will provide the necessary range and velocity data to allow autonomous docking by MicroSat. Figure 4 shows the team's vision for MicroSat's final design.

Ledebuhr says, "The MicroSat will move like a hummingbird darting around." Some day, near-Earth space may be dotted with these autonomous, hummingbirdlike MicroSats. They won't change flat tires, but they will help other satellites stay healthy.

–Katie Walter

Reference

"Testbeds Wring Out Technologies," *Aviation Week & Space Technology*, April 5, 1999, pp. 52–53.

Key Words: agile satellite, hydrogen peroxide propulsion, microsatellite (MicroSat).

For further information contact Arno Ledebuhr (925) 423-1184 (ledebuhr1@llnl.gov). (Continued from p. 2)

DNA analysis in the field

At Livermore's Center for Microtechnology, scientists have developed a battery-powered DNA analyzer that can quickly detect and identify microbial pathogens in biological weapons or outbreaks of infectious disease. The portable device can be operated in the field to provide critical information in a matter of minutes. Ray Mariella, director of the center, said the device "can be used in various settings, such as a hospital emergency room, where rapid analysis of samples is needed."

Called the Advanced Nucleic Acid Analyzer (ANAA), the instrument uses the polymerase chain reaction, or PCR, to produce millions of copies of an organism's identifying DNA. As the PCR progresses, synthesized complementary DNA probes, tagged with fluorescent dye and designed to attach to specific bacterial organisms, are added to the reagent. A DNA copy is measured for fluorescence to determine the presence or absence of a particular organism.

The ANAA development team is at work on a nextgeneration, handheld version of the device and aims to have a prototype later this year.

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Improving the viability of tissue welding

Researchers in Livermore's Laser Programs Directorate have developed a device that more easily and accurately measures heat resulting from tissue welding. The measurements provide feedback signals used to control a laser's output and thus maintain a preselected temperature at the tissue welding site. The device improves the viability of laser-based surgical welding, which is still in the research stage. It can also have a variety of other applications, medical and nonmedical, where control of laser temperature is critical.

The device is a two-color, mid-infrared thermometer that uses a single glass optical fiber to provide dynamic, noncontact temperature and emissivity measurements quickly and at a high spatial resolution. Peter Celliers, laser physicist, said that because of the nature of the fiber used to collect radiation,

scientists can zero in on very small points in the tissue, thus helping them obtain more accurate temperature measurements.

The work is part of a Cooperative Research and Development Agreement with Conversion Energy Enterprises of Spring Valley, New York. Conversion Energy has successfully demonstrated a laboratory prototype of the device. An upgrade is in progress, with the engineering being done jointly by Conversion Energy and Lawrence Livermore. *Contact: Peter Celliers (925) 424-4531 (celliers1@llnl.gov)*.

The last laser shots from Nova

For 15 years, the Nova laser at Lawrence Livermore had the distinction of being the world's largest laser. But with the National Ignition Facility (NIF) on the way to replacing it, Nova was retired and its components shipped off to DOE laboratories and university research centers across the country.

In late May, Nova fired its final shots in service to the nation's defense and energy projects. Although NIF is expected to be 50 times more powerful, it was Nova's work—some 14,000 experiments on its 10 separate beams—that paved the way for NIF power. Said Joe Kilkenny, deputy director of the Inertial Confinement Fusion program, "It's lasted far longer than anyone expected," adding that through Nova, "we've learned how to get more bang for the buck."

Early experiments on Nova tested the ability of the laser to convert its energy into x rays. Nova has helped researchers to better understand nuclear weapons explosions and the cores of the sun and planets. It has provided clues about radiation emitted by the intensely bright stars known as supernovae. Furthermore, the laser has created some spin-off medical technologies, aiding research to eliminate scar tissue from angioplasty surgery and to use sound waves through the blood stream to break up clots.

Now, as Nova joins its predecessor lasers—Janus, Cyclops, Argus, and Shiva—a comparable facility at the University of Rochester in New York will stand in its place until NIF is ready. *Contact: Joe Kilkenny (925) 423-4213 (kilkenny1@llnl.gov).*

Patents and Awards

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

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
M. Leslie Carman Robert T. Taylor	Method for Enhanced Longevity of In Situ Microbial Filter Used for Bioremediation U.S. Patent 5,888,395 March 30, 1999	An improved method for in situ microbial filter bioremediation based on placing an in situ microbial filter with increased operating life. A method for generating a microbial filter of sufficient catalytic density and thickness to increase replenishment interval, improve bacteria attachment and detachment characteristics, and provide endogenous stability under in situ conditions. A system for in situ water remediation.
Anthony F. Bernhardt	Electrochemical Sharpening of Field Emission Tips U.S. Patent 5,891,321 April 6, 1999	A method for sharpening field-emitter tips by electroetching/polishing. In gated field emitters, electron emission must be initiated at the lowest possible voltage. The composition of the emitter and the gate and the structure of the emitter gate are essential to low-voltage initiation. This method of sharpening the emitter tips uses the grid as a counter electrode in electroetching the emitters and can produce extremely sharp emitter tips and remove asperities and other imperfections in the emitters in relation to the specific grid hole in which the emitter resides. Emissions thus become more uniform among the emitters, and turn-on voltage is lowered.
Mark C. Hsiao Bernard T. Merritt Bernardino M. Penetrante George E. Vogtlin	Pre-converted Nitric Oxide Gas in Catalytic Reduction System U.S. Patent 5,891,409 April 6, 1999	A two-stage catalyst composed of an oxidative first stage and a reductive second stage. The first stage is intended to convert nitrogen oxide to nitrogen dioxide in the presence of oxygen. The second stage serves to convert nitrogen dioxide to environmentally benign gases that include diatomic nitrogen, carbon dioxide, and water. By preconverting nitrogen oxide to nitrogen dioxide in the first state, the catalyst enhances the efficiency of the second stage for the reduction of environmentally harmful nitrogen compounds (NO_X).
George E. Vogtlin Bernard T. Merritt Mark C. Hsiao P. Henrik Wallman Bernardino M. Penetrante	Catalytic Reduction System for Oxygen-Rich Exhaust U.S. Patent 5,893,267 April 13, 1999	Nonthermal plasma gas treatment is combined with selective catalytic reduction to enhance NO_X reduction in oxygen-rich vehicle engine exhausts.
Kenneth E. Montgomery Natalia P. Zaitseva James J. DeYoreo Russell L. Vital	Device for Isolation of Seed Crystals during Processing of Solution U.S. Patent 5,904,772 May 18, 1999	A device for isolating seed crystals during processing of solutions. The device enables a seed crystal to be introduced into the solution without exposing the solution to contaminants or to sources of drying and cooling. The device constitutes a seed protector that allows the seed to be present in the growth solution during filtration and overheating operations while at the same time preventing the seed from being dissolved by the undersaturated solution. When the solution processing has been completed and the solution cooled to near the saturation point, the seed protector is opened, exposing the seed to the solution and allowing growth to begin.

(Continued on p. 28)

Patents and Awards S&TR July/August 1999

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Michael D. Perry Jerald A. Britten Hoang T. Nguyen Bruce W. Shore	Multilayer Dielectric Diffraction Gratings U.S. Patent 5,907,436 May 25, 1999	The method for designing and fabricating dielectric grating structures with high diffraction efficiency used in reflection or transmission. By forming a multilayer structure of alternating index dielectric materials and placing a grating structure on top of the multilayer, a diffraction grating of adjustable efficiency and variable optical bandwidth can be obtained. Diffraction efficiency into the first order in reflection varying between 1 and 98 percent has been achieved by controlling the design of the multilayer and the depth, shape, and material comprising the grooves of the grating structure. Methods for fabricating these gratings without the use of ion etching techniques are described.
Harley M. Buettner William D. Daily Roger D. Aines Robin L. Newmark Abelardo L. Ramirez William H. Siegel	Electrode Wells for Powerline-Frequency Electrical Heating of Soils U.S. Patent 5,907,662 May 25, 1999	An electrode well for use in powerline-frequency heating of soils for decontamination of the soil. Heating of soils enables the removal of volatile organic compounds from soil when utilized in combination with vacuum extraction. A preferred embodiment of the electrode well utilizes a mild steel pipe as the current-carrying conductor to at least one stainless steel electrode surrounded by a conductive backfill material, preferably graphite or steel shot. A covering is also provided for electrically insulating the current-carrying pipe. One of the electrode wells is utilized with an extraction well, which is under subatmospheric pressure to withdraw the volatile material, such as gasoline and trichloroethylene (TCE), as it is heated.

Awards

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A Laboratory team that developed a system for treating cerebral aneurysms faster and less invasively has received a Federal Laboratory Consortium Award for Excellence in Technology Transfer. Team members include Abraham Lee, Duncan Maitland, Luiz Da Silva, Dean Hadley, Christopher Lee, Pat Fitch, Dan Schumann, and Jim Sommercorn.

The annual award recognizes laboratory employees who have accomplished outstanding work in the process of transferring a federal lab-developed technology to the commercial marketplace. This year, the Livermore team was one of 15 recipients nationwide.

The team's technology uses a laser-activated microgripper to release a coil inside cerebral aneurysms in less than a second. The coil seals off the aneurysm, greatly reducing the patient's risk of acute hemorraghic stroke. Duncan Maitland, group leader within the Defense and Nuclear Technologies, Engineering, and Laser Programs directorates' Medical Technology Program, said that the dramatically quick release of the coil has the potential to reduce patient health risks and lower operation costs.

Nuclear chemist **Darleane Hoffman** will receive the **Priestley Medal**, the American Chemical Society's (ACS's) highest honor, at the society's next national meeting in San Francisco in March 2000. Hoffman, chemistry professor in the graduate school of the University of California at Berkeley, helped found the Glenn T. Seaborg Institute for Transactinium Science at Lawrence Livermore and served as its first director from 1991 to 1996. The institute researches the atomic composition of synthesized elements that are heavier than uranium. Hoffman still plays an active role there as mentor, researcher, and teacher.

Only the second woman to receive the medal, Hoffman is being recognized for her work in the chemical properties of heavy elements. Among her accomplishments are the discovery of plutonium-244 in nature and the first investigations of the chemistry of element 106, seaborgium. Her many honors include the 1990 Garvan Medal, which was awarded by ACS to honor distinguished service to chemistry by women chemists, and the National Medal of Science in 1997. She was elected to the Norwegian Academy of Sciences and Letters in 1991 and the American Academy of Arts and Sciences in 1998.

On Target: Designing for Ignition

The \$1.2-billion National Ignition Facility (NIF), now under construction, will permit scientists to perform experiments for the Department of Energy's Stockpile Stewardship Program to ensure that America's nuclear arsenal remains safe and reliable. The success of NIF ignition experiments will depend upon the intricate design of 2-millimeter-diameter capsules that contain a central reservoir of deuterium-tritium (D-T) gas, a frozen D-T solid-fuel layer, and an outer ablator layer. Target designers have tested different ablator materials, including polyimide (best at high temperatures) and beryllium (best at low temperatures). Capsules will be cooled to 18 kelvins (colder than liquid nitrogen) to maintain in equilibrium the central, relatively low-density D-T gas and the high-density, 80- to 100-micrometer-thick D-T ice layer. For at least the first several years, ignition experiments will use indirect drive, in which laser light heats the inside of an open-ended gold cylinder, called a hohlraum, that encloses the ignition capsule.

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A New View of the Universe

A laser guide star and adaptive optics system developed at Lawrence Livermore is making astronomers' views of the heavens clearer than ever before. Livermore's sodium-laser guide star provides an artificial reference for viewing distant or dim celestial bodies with adaptive optics, which sharpen the blurring of images caused by our atmosphere. One system has already been installed on the University of California's Shane telescope on Mount Hamilton in California, and another is now being installed at the Keck Observatory on Mauna Kea in Hawaii.

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Scot Olivier (925) 423-6483 (olivier1@llnl.gov).

Coming Next Month

A Better Picture of Aging Materials

A report on how
Livermore scientists
are determining the
effects of aging on the
materials in stockpiled
nuclear weapons.

Also in September

- Biomedical research monitors the human radiation effects of the Chernobyl nuclear reactor accident.
- Dedication of the National Ignition Facility's target chamber marks a giant milestone in construction progress.

