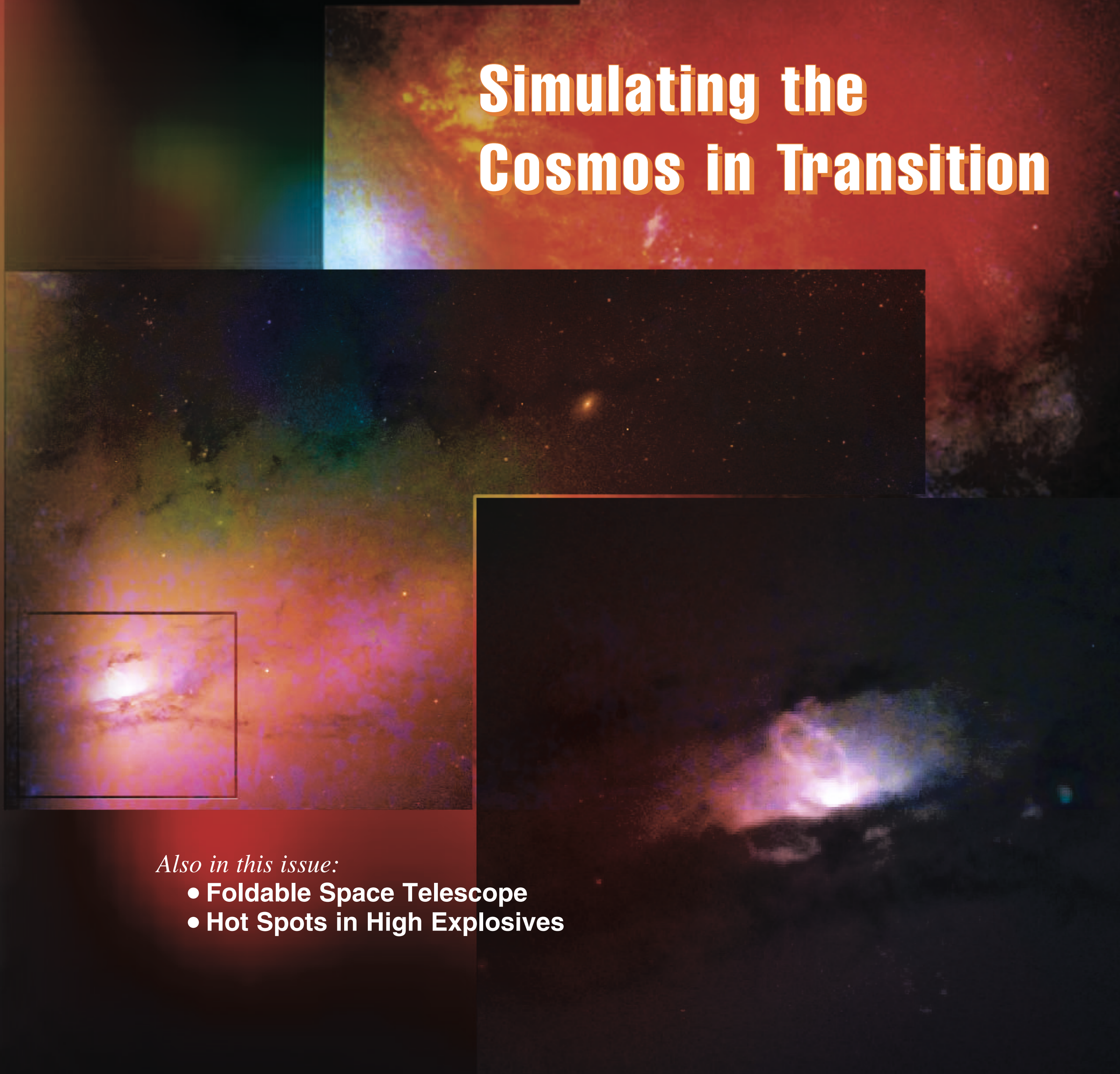
March 2003

Science & Technology REVIEW

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

Simulating the Cosmos in Transition



Also in this issue:

- Foldable Space Telescope
- Hot Spots in High Explosives

About the Cover

On the cover are several telescope images of black holes and surrounding matter. Black holes suck in anything that comes within their gravitational field and let nothing escape. They are fascinating but not wholly understood. At Lawrence Livermore, an astrophysical code called COSMOS is being used to model the complex interactions of rotating black holes with nearby gas. The model is difficult to create, but COSMOS is up to the challenge. Its capability to simulate a variety of astrophysical events in one, two, and three dimensions is described in the article beginning on p. 4.

Cover design: Lew Reed

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on 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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National Nuclear Security Administration

Prepared by **LLNL** under contract No. W-7405-Eng-48

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S&TR, a Director's Office publication, is produced by the Innovative Business and Information Services Department under the direction of the Office of Policy, Planning, and Special Studies.

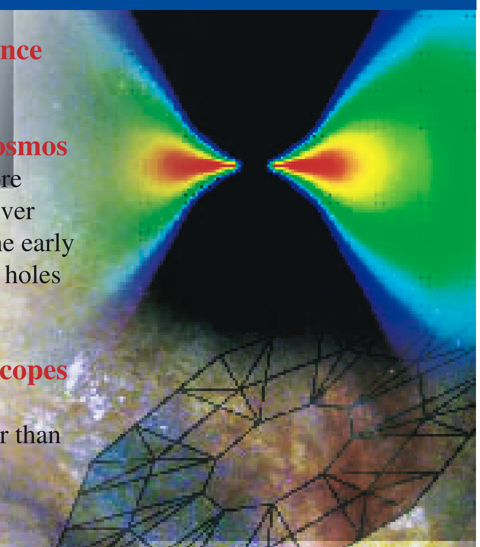
S&TR is available on the Web at www.llnl.gov/str/.

Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-52000-03-3
Distribution Category UC-99
March 2003

Features



Research Highlight

Departments

Delving further into climate change

Researchers at Livermore have completed several studies to better understand climate change.

Evaluating energy technologies. Late in 2002, Livermore researchers Ken Caldeira and L. John Perkins collaborated with a team of international researchers to evaluate a series of advanced energy technologies that do not emit carbon dioxide or that limit its release to the atmosphere. The candidate technologies include terrestrial, solar, and wind energy; solar-powered satellites; biomass; nuclear fission; nuclear fusion; fission-fusion hybrids; and fossil fuels from which carbon has been removed.

The researchers concluded that current technologies are not helpful to stabilizing the climate. Says Martin I. Hoffert of New York University, lead author of the study report, ". . . scientific innovation can only reverse this trend if we adopt an aggressive, global strategy for developing alternative fuel sources that can produce up to three times the amount of power we use today. Currently, these technologies simply don't exist—either operationally or as pilot projects."

Assessing geoengineering schemes. Using models that simulate the interaction between global climate and land ecosystems, Livermore researchers have shown that compensating for the carbon dioxide greenhouse effect by decreasing—geoengineering—the amount of sunlight reaching the planet could create a more vigorous ecosystem.

Bala Govindsasamy, Starley Thompson, Philip Duffy, Ken Caldeira, and University of Wisconsin collaborator Christine Delire published a report in the November 26, 2002, online edition of *Geophysical Research Letters*. They modeled the effect of various schemes to reduce sunlight reaching Earth's surface and determined that the reduction would have little effect on the terrestrial biosphere. "In fact," says Caldeira, "turning down the Sun a bit reduces evaporation and therefore gives plants more water for photosynthesis so that they may actually grow better in a geoengineered world than they do today." However, researchers strongly caution against adopting geoengineering interventions because of the risks of system failure and unpredictable responses from Earth's climate system.

Measuring tropopause height. Climate researchers have discovered another sign of human effects on global climate. They have observed that the height of the tropopause—the transition zone between the troposphere and the stratosphere—has increased, and those increases agree with projections made by climate models of greenhouse warming. The warming affects atmospheric temperature, which in turn affects tropopause height.

The observations and modeling undercut claims that no warming has occurred during the last two decades because satellite temperature measurements of the troposphere have shown little or no warming. According to Livermore researcher Benjamin Santer, "Our best understanding is that this increase [in tropopause height] is due to two factors: warming of the troposphere, which is caused by increasing greenhouse gases, and cooling of the stratosphere, which is mainly caused by depletion of stratospheric ozone. Tropopause height changes give us independent evidence of the reality of recent warming of the troposphere."

In addition to Santer, Livermore scientists James Boyle, Krishna Achutarao, Charles Doutriaux, and Karl Taylor teamed with researchers from the National Center for Atmospheric Research, National Aeronautics and Space Administration's Goddard Institute for Space Studies, Max Planck Institute for Meteorology, and Institut für Physik der Atmosphäre in Germany to report their findings in the online *Journal of Geophysical Research–Atmosphere*.

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Looking for small objects beyond Neptune

At the winter meeting of the American Astronomical Society in early January, a collaboration of astronomers, including several from Lawrence Livermore, presented their work to search for small, cometlike bodies in the outer solar system with four half-meter telescopes.

In normal practice, astronomers detect comet bodies by looking for the light reflected by them. But the astronomers on the Taiwanese–American Occultation Survey (TAOS) Project will instead be searching for those rare moments when one of the objects passes between telescopes and a nearby background star. During one of these brief moments, scientists will be able to study objects that are much too faint to be seen in reflected sunlight, even with the largest telescopes.

TAOS is probing the Kuiper Belt, known only through two objects (Pluto and its moon Charon) until a flood of its bodies was discovered in the 1990s. Much about the region remains unknown, but all theories about it predict that there are many more small objects than large ones. TAOS scientists believe that their technique will allow them to detect objects as small as 3 kilometers in diameter. It is believed that there are billions of objects this small in the outer solar system. "The TAOS survey will provide data on remnants of our early solar system and early planet formation," says Livermore astronomer Kem Cook. "It will provide us insight into how the solar system evolved. We'll be looking at the smallest objects that anyone has seen."

The collaboration is made up of scientists from the Institute of Astronomy and Astrophysics in Taiwan, University of Pennsylvania, National Central University in Taiwan, Yonsei University in South Korea, and National Aeronautics and Space Administration as well as Livermore.

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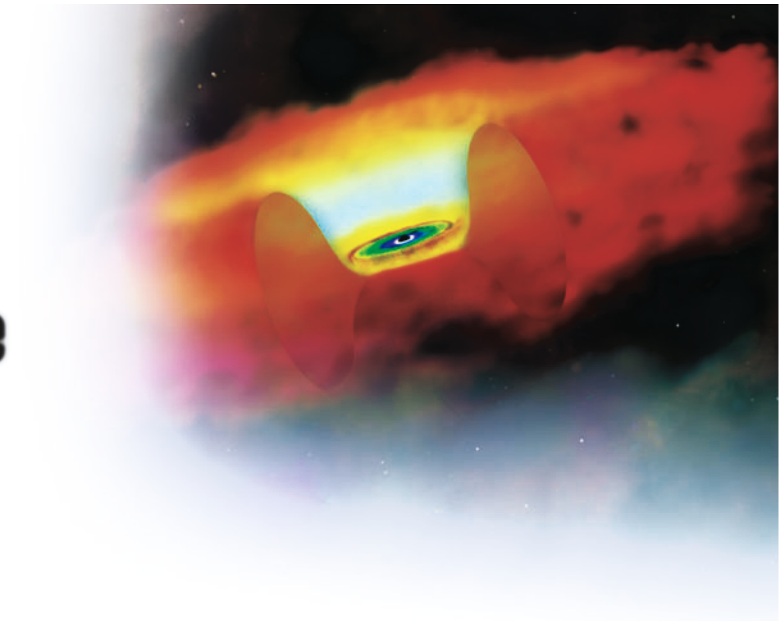
Basic Science Is Creative Science



MOST great scientific discoveries have resulted from a willingness to suspend judgment and a refusal to be boxed in by conventional wisdom. Astronomer Edwin Hubble discovered in the 1920s that the universe is expanding. As unlikely as this seemed then, later measurements have shown that Hubble was right. Einstein's special and general theories of relativity represented a truly revolutionary way of understanding the universe when they were proposed almost 100 years ago. Yet discoveries since then—black holes and their furious gravitational power are but one example—have proven Einstein right.

At Livermore, we encourage our scientists to think creatively—outside the box—in finding solutions to challenges they encounter. While most news about Lawrence Livermore centers on the applied science we do—maintenance of the nation's nuclear stockpile or the development of ever more powerful lasers—none of those advances would be possible without experiments, theory, and simulations that delve into science at its most basic. Basic and applied science are synergistic pursuits, with advances in either feeding back in often unexpected ways. For example, the development of the laser is a true applied science breakthrough that has opened up many avenues for exploring basic science from equations of state to the fusion process that powers stars. Basic research tests the creativity of scientists, keeping them intellectually agile, and may produce unexpected results that lead down new paths.

The COSMOS code, described in the article beginning on p. 4, is an excellent example of the basic science that our scientists pursue. This new simulation tool leverages not only their abilities and creativity but also the unique resources available at this Laboratory. Having trained as an astrophysicist (I worked on neutron star formation in supernova collapse), I take particular interest in Livermore's research in astrophysics. Early on, I discovered that astrophysics is superb training for a career at Livermore. Because stars and weapons operate in similar ways, new discoveries in one area are bound to spill over and benefit the other. Some of our nation's greatest astrophysicists, such as James Wilson and Stirling Colgate, move continuously between weapons and astrophysics in their careers.

With COSMOS, scientists can simulate a variety of astrophysical events in two and three dimensions, from early cosmology to the creation of stars. COSMOS incorporates more complex physics than almost any other similar code. It is the first astrophysical code that considers the process of cooling, a critical factor in the congealing of stellar gas and dust that creates stars. Its flexibility and power leave it with few peers. The astrophysics community is excited about COSMOS, which will surely find many users outside the Laboratory.

COSMOS is the brainchild of a Livermore astrophysicist who not only had a great idea but also an awareness of all that the Laboratory has to offer. COSMOS simulations would not be possible without Livermore's massively parallel terascale computers to manipulate enormous quantities of data representing complex physics in multiple dimensions.

People become scientists because they want to understand the workings of the universe around them. Exciting basic scientific pursuits such as COSMOS act as magnets, drawing the best and brightest young scientists to Livermore and enhancing our reputation in the greater scientific community. The success of our national security missions depends on the quality of our science and technology and, perhaps more fundamentally, upon the quality of our scientists. It is only with their passion for science—and the creativity that passion breeds—that we can succeed.

■ Bruce Goodwin is associate director for Defense and Nuclear Technologies.

A New Code Simulates the Cosmos

A Livermore astrophysicist's code can model almost anything from a small black hole to the entire universe.

By day, Livermore astrophysicist Peter Anninos works on stockpile stewardship projects. Many astrophysicists at Lawrence Livermore work primarily in the weapons program to safeguard the reliability of the nuclear stockpile because the two fields have so much in common: the fusion process that powers stars is the same one that unleashes the deadly energy of a thermonuclear weapon. "Astrophysics is about as close to Weapons 101 as you can get in college," he says.

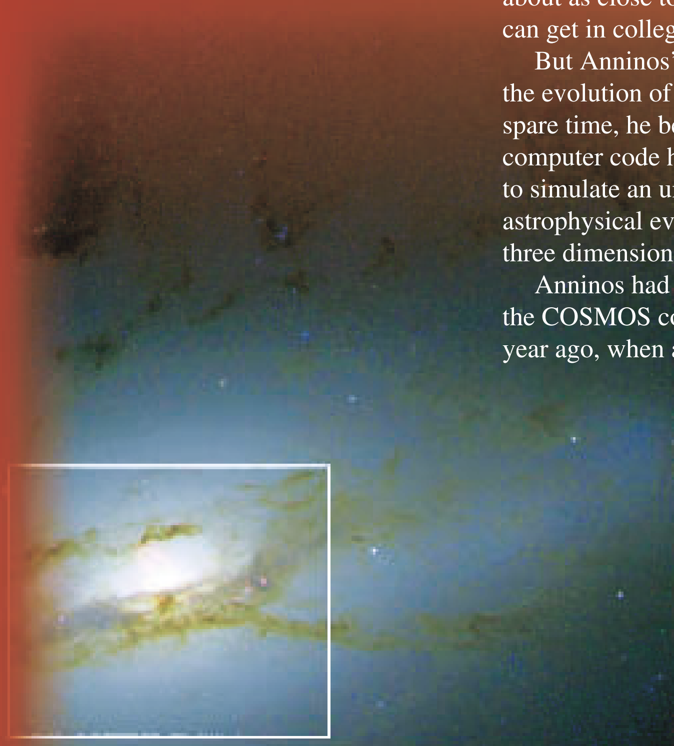
But Anninos's first love is cosmology, the evolution of the universe. In his spare time, he began to develop a new computer code he called COSMOS to simulate an unprecedented variety of astrophysical events in one, two, or three dimensions.

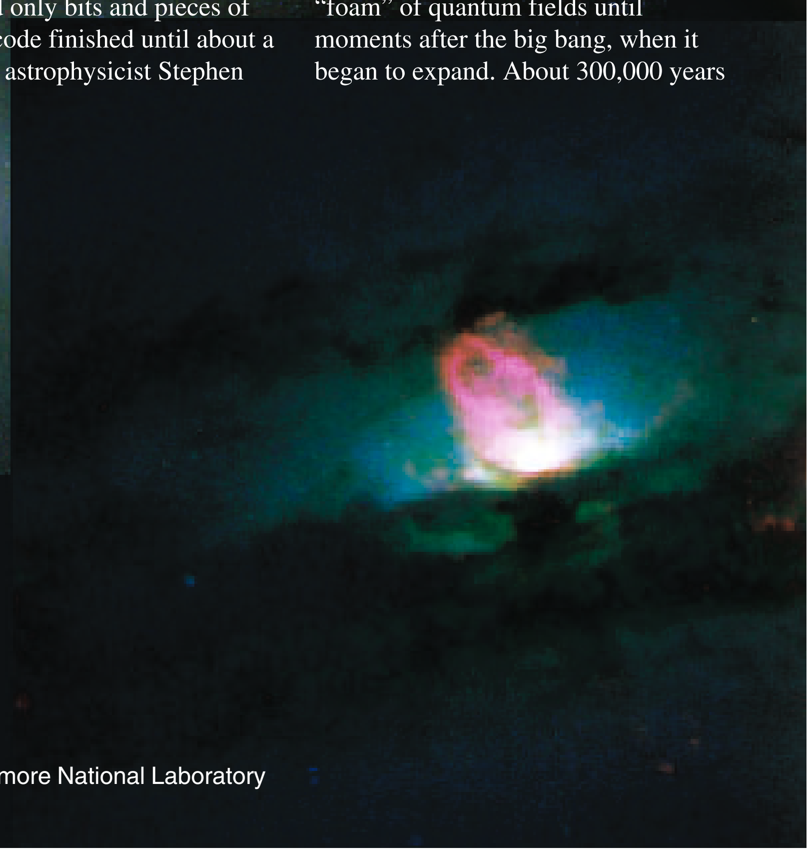
Anninos had only bits and pieces of the COSMOS code finished until about a year ago, when astrophysicist Stephen Murray instigated the hiring of Chris Fragile as a postdoctoral fellow to perform astrophysics research full time. Fragile, who transformed a fascination with black holes into a career in astrophysics, has fleshed out the code with Anninos and performs most computer runs.

Now virtually complete, COSMOS can model almost anything from a small black hole to the entire universe. (See the box on p. 7.) It has already been applied to an ambitious array of astrophysical problems: the evolution of the very early universe, accretion of matter by black holes, star formation, and the evolution of dwarf galaxies.

The Universe in Transition

The young universe was a hot, dense "foam" of quantum fields until moments after the big bang, when it began to expand. About 300,000 years





later, hydrogen atoms first appeared when temperatures had cooled enough for electrons and nuclei to join. Hundreds of millions of years later, matter began to come together to form stars and galaxies. (See the box on p. 8.)

Anninos recently used COSMOS to model one of the phase transitions that took place just after expansion began, when the universe was about a hundred-thousandth of a second old. During this transition, the most fundamental forms of matter—quarks and gluons—joined to become protons and neutrons. Because particles that contain three quarks, including protons and neutrons, are known collectively as hadrons, this event is known as the quark–hadron phase transition. While a few other researchers have examined early cosmology in one spatial dimension, Livermore's simulations of the quark–hadron transition are the first in multiple dimensions.

In the universe of today, matter is spread haphazardly in clumps with vast areas of some unknown substance—perhaps dark matter—in between. Astrophysicists surmise that the manner in which the early phase transitions took place may be the cause of this unevenness. These phase transitions may also have given rise to a population of primordial black holes and may have set the foundation for the production of galactic and extragalactic magnetic fields.

"If the quark–hadron phase transition were turbulent," says Anninos, "the universe would be more homogeneous today. We wanted to find out how stable—or unstable—the transition boundaries were to flow perturbations and shock collisions. We also wanted to determine whether destabilizing mechanisms play a role in how hadrons evolve and mix."

It is possible that bubbles and droplets of varying phases may have coexisted for a time, resulting in an uneven production and distribution of hadrons. The simulation shown in the figure below illustrates how these bubbles may have behaved as a wall of hadronic material collides with an isolated bubble of hadrons. The background is initially composed of supercooled quark material. But the expanding hadronic regions quickly convert quarks into hadrons immediately behind a detonation or shock front. However, as shocks pass through the cooled hadron regions, they reheat the hadrons. Reheating may either decompose the hadrons back into their quark constituents or simply impart a spectrum of thermal fluctuations to the hadrons. The simulations provide clear evidence of the formation of quark "nuggets" that may still survive today in the form of dark matter.

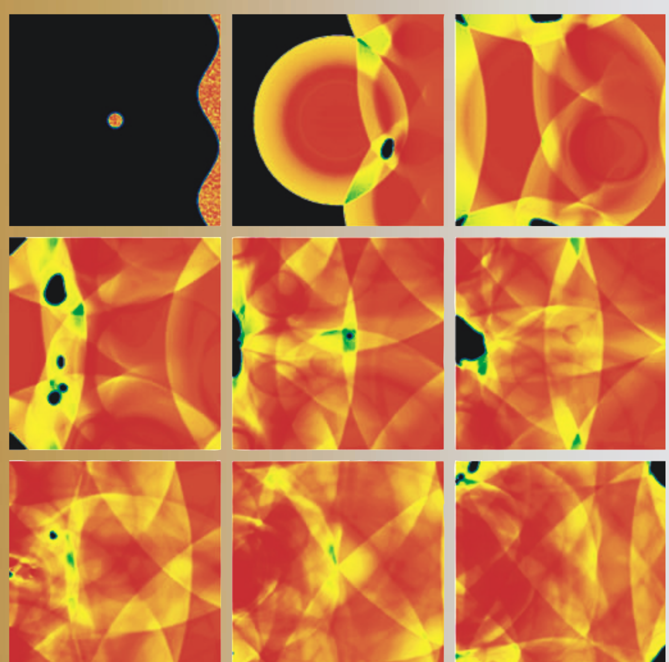
Although the team's simulations to date show complex behavior, there is no evidence of hydrodynamic turbulence during this transition period, at least for the cases they investigated.

The Tug of Black Holes

Black holes tugged at Chris Fragile's imagination when he was younger. Black holes also tug madly at anything that comes within their gravitational field, sucking in dust, gas, and even stars. According to the general theory of relativity, black holes drag space–time around them in a spiraling whirlwind.

Although a black hole itself is not visible, hot matter that orbits around it is. The gases closest to the black hole are very hot and emit x rays. Further away from the black hole, cooler material emits visible radiation.

Black holes are suspected to exist in the center of all galaxies. In October



In this simulation, a wall of cold hadronic material collides with an isolated bubble of hadrons. Although the background is initially composed of supercooled quarks, the expanding hadronic regions quickly convert quarks into hadrons immediately behind the detonation or shock front. There is also clear evidence of the formation of quark "nuggets" (the dark spots) that potentially may have survived to the present as dark matter.

2002, scientists reported having found strong evidence for a dense black hole more than two million times as massive as our Sun in the center of the Milky Way Galaxy. After tracking the paths of several stars in the vicinity of the presumed black hole for 10 years, they discovered at least one star in an orbit that may send it to its death in the black hole in about 15 years. Another indicator of the presence of a black hole is the speed with which things move. In our galaxy, most objects move at about 100 kilometers per second. Near black holes, however, they may move as fast as 9,000 kilometers per second.

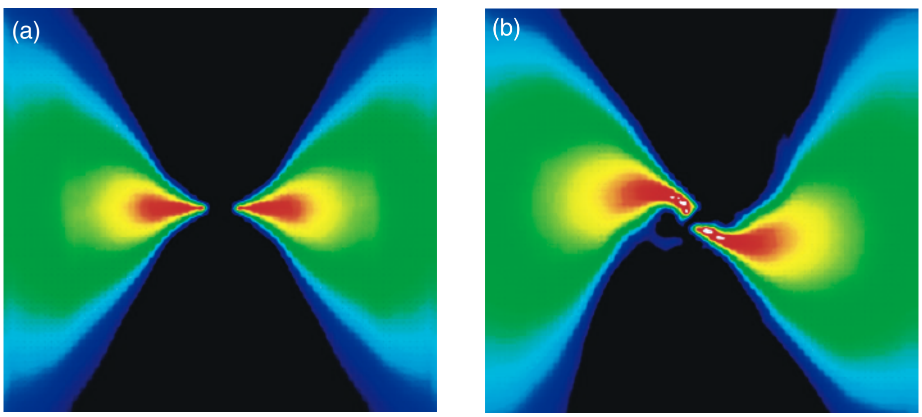
Fragile is modeling single rotating black holes with a disk or torus of gas being sucked into them, a process known as accretion. The topmost figure below shows a model of an accreting gas torus around a black hole. In one version, a black hole has its spin axis aligned with the angular momentum axis of the torus. Although they are spinning in opposite directions (180 degrees from each other), the black hole accretes the most material from the torus in this position.

In another version, the spin axis is tilted 30 degrees relative to the angular momentum axis of the same accreting gas torus. No one has modeled such a tilted black hole torus before, although they are expected to exist in nature.

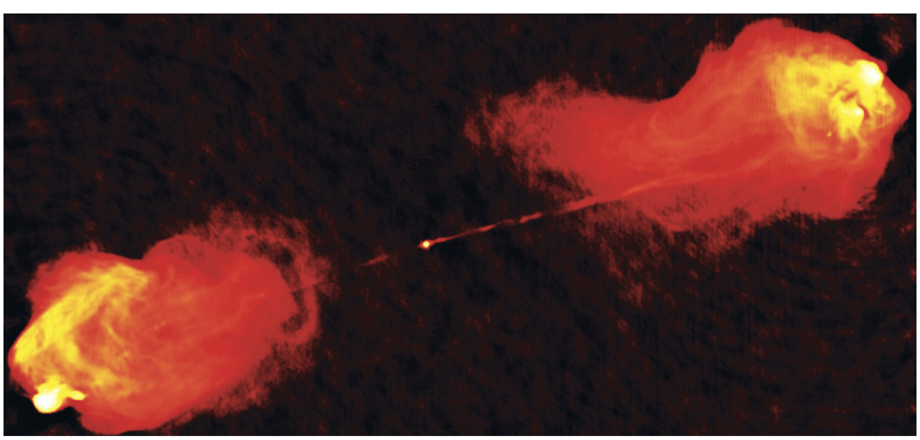
The tilt angle produces important differences in the geometry of the accretion pattern, particularly close to the black hole. Here, spiraling space–time produces what is known as frame dragging, a general relativistic effect, which causes the shape of the torus to warp. Frame dragging also affects how much of the gas can eventually be captured by the black hole, which in turn will affect how bright the system's x rays are.

For constructing the model, COSMOS currently uses a three-dimensional Cartesian mesh, which has a uniform grid of zones that describe discrete elements of the model. "To have enough zones to get far out in the torus, we end up with just a few around the black hole," Fragile says. "That means the resolution around the black hole isn't as good as we would like."

One solution is to add zones at the black hole without adding them further out in the torus, creating a nonuniform grid. The other is to create a spherical grid, which would resemble a globe with the black hole at the center. But modeling in this way is difficult, especially near the boundaries of the black hole where gravity is strongest. The challenges never stop.



(a) Simulation of the spin axis of a black hole aligned with the angular momentum axis of the torus. (b) The black hole spin axis is tilted 30 degrees relative to the angular momentum axis of the same accreting gas torus. No one had modeled a tilted black hole torus such as this before. The tilt produces major differences in how the black hole accretes matter.



A radio telescope reveals this image of high-energy radio jets coming from a massive black hole.

Cosmic Fireworks

Black holes don't just pull cosmic junk in. They also spit it out. For decades, astronomers have observed massive rotating black holes in the centers of some huge elliptical galaxies that spew high-energy jets, as shown in the figure at left. These narrow streams of high-velocity particles emit radiation in the form of radio waves, but their exact nature and how they interact with their surroundings remain a mystery.

In 1985, before he came to Livermore, astronomer Wil Van Breugel led a team studying whether a radio jet emanating from elliptical galaxy NGC 541 was interacting with a cooler cloud of gas and causing the formation of stars. Such an event is known as a jet-induced starburst. His team used radio and optical imaging as well as optical spectroscopy to compare emissions from NGC 541 with emissions from a confirmed prototypical starburst galaxy.

"The idea of a jet triggering a starburst in a cloud made news," says Van Breugel. "But many scientists didn't believe it at the time. It seemed too much like science fiction."

At the time, many thought the gas might be part of a preexisting galaxy that happened to be nearby. Furthermore, it was unclear if it was even possible for a jet to trigger the collapse of a gas cloud.

More recently, much more sensitive observations by Van Breugel and others using the Hubble Space Telescope and the Keck Observatory on Mauna Kea, Hawaii, indicate that jet-induced star formations do indeed occur and may even have been a common phenomenon in the early universe when galaxies were forming. In young galaxies, much of the gas has yet to form into stars. Jets may help this process by pushing gas clouds to higher densities, forming stars a bit sooner than they would if only gravitational forces acted. In powerful jets, star formation is probably initiated by shocks that move sideways, along the edge of the jets.

"Understanding this process of jet-induced star formation requires numerical simulations with complex, multidimensional computer codes such as COSMOS," says Van Breugel. A COSMOS simulation of jet–cloud

Inside COSMOS

Given Peter Anninos's interest in cosmology, COSMOS is an appropriate name for the code he developed. When Anninos first began work on it, he was hoping to simulate such isolated phenomena as black holes and neutron stars in three dimensions. These all require modeling nonlinear interactions between different sources of matter and highly relativistic gravitational fields.

COSMOS is unusual in being easily adaptable to either relativistic or Newtonian astrophysical phenomena. The exceedingly strong gravitational fields in effect immediately after the big bang, during the initial inflation of the universe, and near black holes are governed by the laws of relativity. In contrast, classical Newtonian physics governs cosmological and astrophysical events that occur in the presence of much weaker gravitational fields. Examples include the creation of stars and galaxies during which gravity behaves in a fashion more familiar to us.

The general and special theories of relativity provide a unified description of space and time as a single continuous fabric called space–time. The general theory also describes gravity through the notion of "curved" space–time and governs the motion of all objects in the presence of this curvature. For instance, general relativity predicts that when a large enough mass is concentrated in a small enough volume, that mass distorts the space around it so much that a part of space wraps itself up and leaves the rest of normal space behind. This is a black hole. Anything that falls into the black hole—including light—can never get out.

Codes that can simulate relativistic flows in the presence of ultrastrong gravitational fields have been around for some time, but each has been "tuned" to a particular purpose, such as modeling black hole dynamics, cosmological gravitational waves, or binary neutron stars. COSMOS, in contrast, is designed for generic applications so that with only minor modifications, it can simulate a variety of events.

Astrophysics models are very computationally intensive. COSMOS could have only been developed at an institution such as Lawrence Livermore with its massively parallel terascale computers. To date, the code has run successfully on several different Livermore computers.

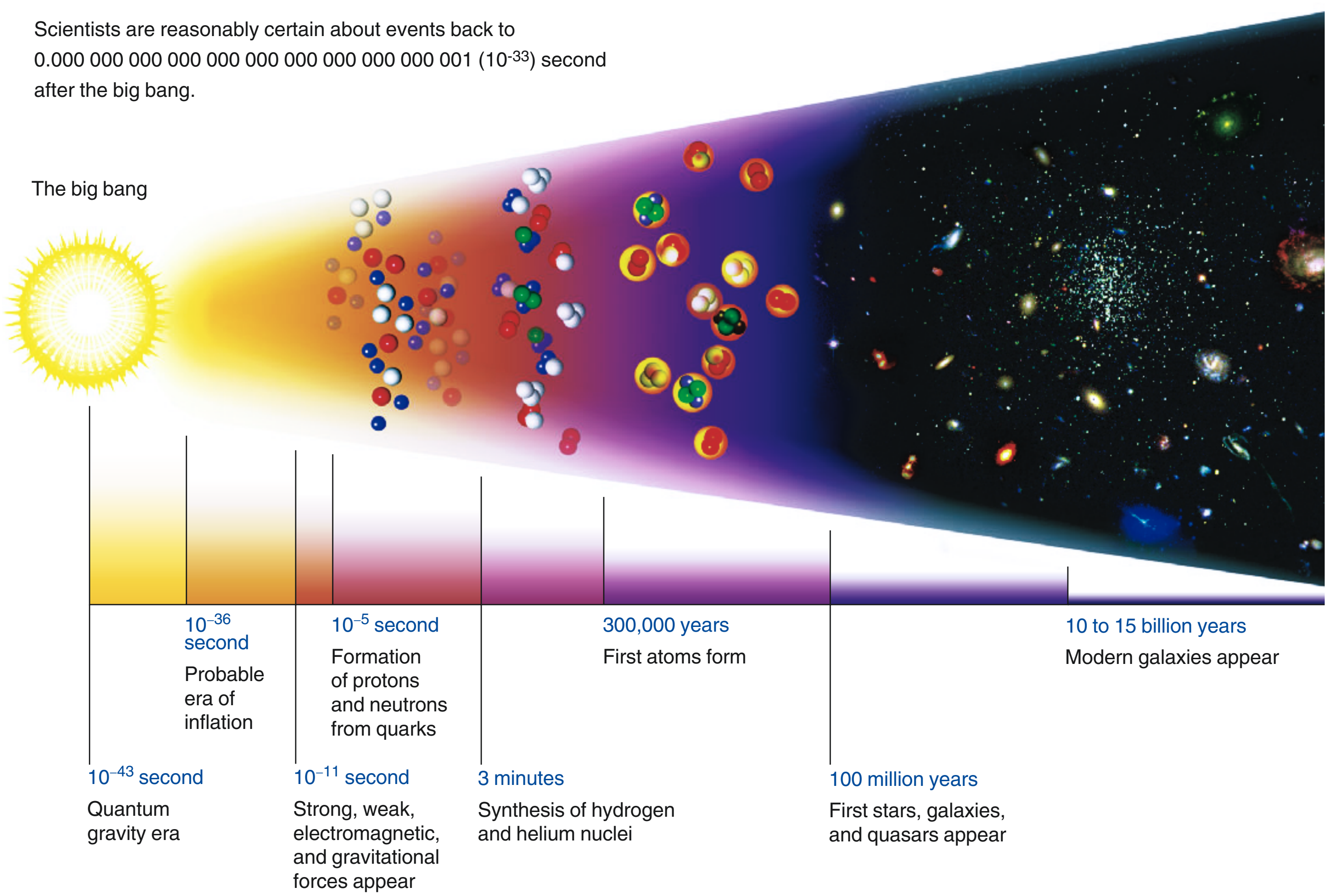
"Most astrophysical problems are inherently multidimensional," notes Anninos, so he designed COSMOS to run in up to three dimensions. It currently uses a uniform mesh, composed of quadrilateral-shaped zones in two dimensions and hexagonal-shaped zones in three. Although all calculations that have been run to date use Cartesian coordinate systems, the code can be adapted to curvilinear meshes as well.

How the Universe Started

The Standard Model of cosmology says that the big bang happened about 15 billion years ago. In the first moments after that cataclysmic event, the universe was still a single hot, dense entity in which all the forces we know today—the strong, electromagnetic, weak, and gravitational—were unified. In the first hundred-billionths of a second after the big bang, the four forces came into being, one by one, in a series of rapidly occurring phase transitions.

The most elementary particles—quarks and gluons—briefly floated freely. But during the final phase transition of the early universe, at about a hundred-thousandth of a second after the big bang, they became bound together to form the protons and neutrons that make up ordinary matter today. Three minutes after the big bang, protons and neutrons first formed nuclei of hydrogen and helium in a process known as nucleosynthesis. The universe was 300,000 years old before electrons and nuclei joined to form any atoms heavier than a simple proton–neutron hydrogen atom. All heavier elements—nitrogen, oxygen, iron, copper, and so on—were created much later in stars, which began to develop when the universe was 100 million to about 1 billion years old.

At the time of electron–nuclei combination, the radiation temperature of the universe was about 3,000 kelvins. The universe has expanded and cooled since then such that its radiation temperature today is just 3 kelvins. This temperature corresponds to that of the microwave radiation that rains down upon us today from all directions, radiation that has been traveling through the universe since it decoupled from matter. This radiation is just one of many clues that have allowed scientists to solve the puzzle of how the universe got started.



interactions, using temperature, density, and velocity data estimated from observed systems such as NGC 541, is shown in the leftmost figure below. Livermore's simulations are the first ever to incorporate cooling, a critical component of the process of star formation.

Van Breugel wants to use COSMOS to help answer a number of questions: What is the range of jet and shock velocities that allows the clouds to collapse rather than heat up and disperse? What are the required densities and temperatures of the gas in the star-forming clouds? What is the chemical composition of the clouds, that is, how important is the cooling efficiency of the gas? These answers will provide valuable insight into the nature of the jets themselves and the physical conditions in galaxies as they form.

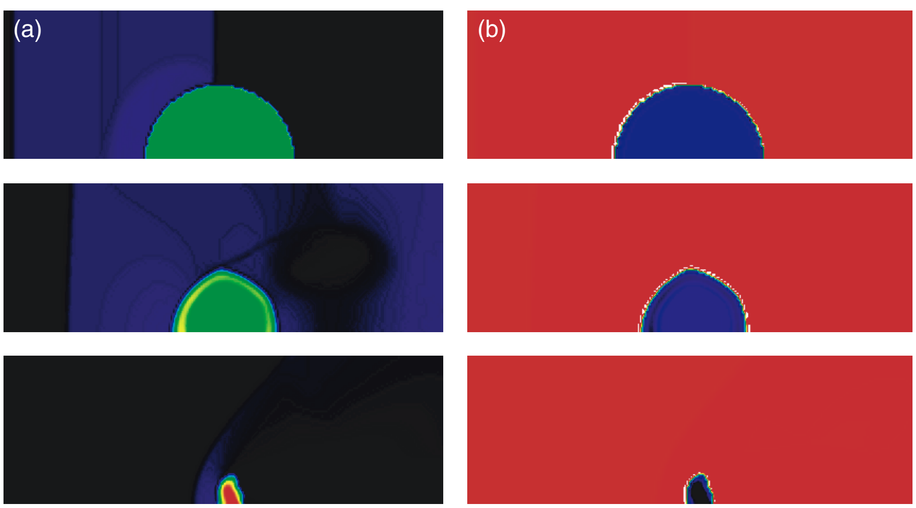
These new calculations may also help to determine whether feedback from active jets, emanating from the vicinity of black holes, helps or hinders the growth of galaxies. A few years ago, scientists discovered that the masses of black holes and their parent galaxies are closely related, making the feedback mechanism an important issue in astrophysics today.

Galactic Building Blocks

Astrophysicist Stephen Murray, like Anninos, is primarily a weapons physicist. But, together with colleagues at the University of California at Santa Cruz, he obtained funding from the National Aeronautics and Space Administration to study dwarf spheroidal galaxies, which orbit much more massive galaxies.

"Dwarf galaxies were most likely the first galaxies to form in the early universe," Murray says. "They are likely the building blocks of larger galaxies. So the number of dwarf galaxies we observe today are probably the remnants of a much larger initial population, most of which went to form our own galaxy. These survivors make excellent laboratories for studying how stars form in the early universe and may tell us something about the early evolution of more massive galaxies."

Because dwarf spheroidal galaxies are the smallest type of dwarf galaxy, one might expect them to be simple laboratories for studying star formation. But astronomers find that they exhibit a variety of histories. Some show evidence of only a single burst of star formation while others show signs of having had multiple bursts. Yet others appear to have had more or less continuous star formation over their lifetimes. Some contain differing amounts of heavy elements, while others show little variation from star to star. Understanding the reasons for such variety requires looking at the many factors that affect dwarf spheroidal galaxies. Murray and Fragile have used COSMOS to simulate two phenomena



For star formation to occur, a cloud of gas must first cool enough for hydrogen molecules to begin to form. As the cloud cools, it will also become denser. This simulation shows some of the early steps in the cooling and condensing process caused by the interaction of a radio jet with a cloud of gas. The jet is not visible because it is larger than the cloud and covers the whole grid. (a) Over a span of 1.4 million years, the cloud of gas increases in density by a factor of 1,000. (b) At the same time, the temperature of the cloud of gas cools from 5,000 kelvins to less than 800 kelvins.

Dwarf spheroidal galaxies are not very photogenic. Here, the Pegasus dwarf spheroidal galaxy is hiding among brighter stars. (Keck Observatory image, courtesy of P. Guhathakurta, University of California at Santa Cruz.)

in these galaxies that relate to their evolution: enrichment and tidal stripping.

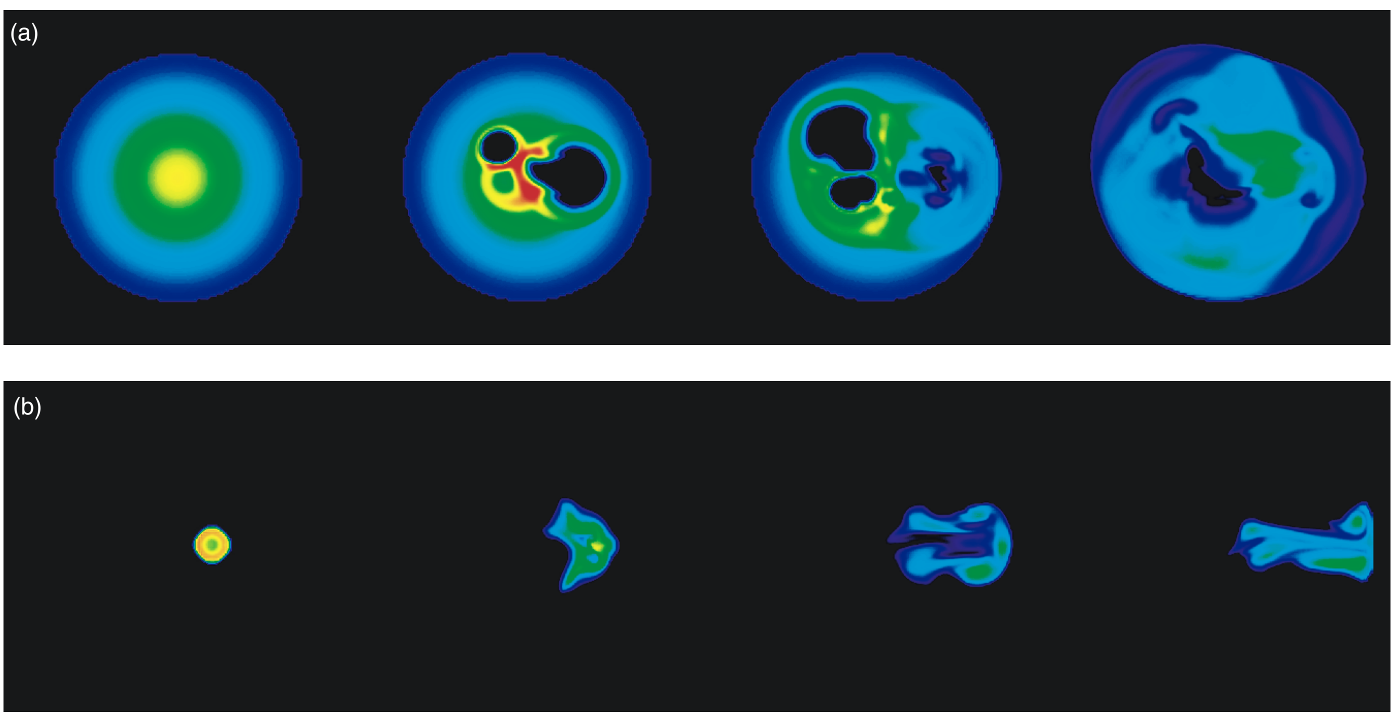
Enrichment is the process by which elements heavier than helium are created and dispersed into the universe. Most such elements are formed by nuclear fusion within the cores of stars much more massive than the Sun. When these stars die, they explode as supernovas, dispersing the elements they have created into space. The heavy elements are then mixed into the galactic gas from which a subsequent generation of stars may form. Only through countless stellar deaths over the millennia have there come to be elements heavier than helium in amounts comparable to those seen in the Sun.

Murray and Fragile examined the ability of dwarf spheroidal galaxies to retain gas expelled by supernovas. Simulations with COSMOS examined the effects of multiple supernova explosions at random locations throughout the cores of dwarf galaxies. A three-dimensional code was essential because no assumptions could be made about the symmetry of the system.

The simulations showed for the first time how supernova gases can "chimney" their way out of the galaxy without mixing with galactic material. This effect may explain why some dwarf spheroidal galaxies have less heavy-element enrichment than would be expected from their history of star formation. The material ejected from supernovas in dwarf galaxies would almost certainly be captured by massive galaxies that form after the dwarfs. Such preenrichment may help to explain why astronomers studying our own Milky Way Galaxy find very few stars lacking in heavy elements.

Factors external to the dwarf galaxy may also explain their evolution. Tidal stripping is a process whereby massive galaxies strip material from their smaller neighbors. This transfer of mass to the larger galaxy is a galactic-scale version of black hole accretion. "Big galaxies make bad neighbors," says Murray with a smile.

His team modeled a dwarf galaxy under the influence of a larger nearby galaxy. If its gas is ionized and heated, either by external or internal sources, then the gas may be rapidly lost from the system, preventing the formation of subsequent generations of stars. The result, in the presence of a massive galaxy, is to limit the ability of the dwarf system to form multiple



(a) Plots reveal the density of gas along slices through the center of an initially undisturbed dwarf galaxy. Following a fairly rapid burst of several supernovas near the center of the galaxy, substantial disturbance of the gas is visible. (b) The concentration of enriched material from the first supernova "chimneys" its way out of the galaxy. This chimneying effect is a new discovery in dwarf spheroidal galaxies and may explain why some such galaxies have less heavy-element enrichment than might be expected.

generations of stars or, in extreme cases, to form any stars at all.

An Expanding COSMOS

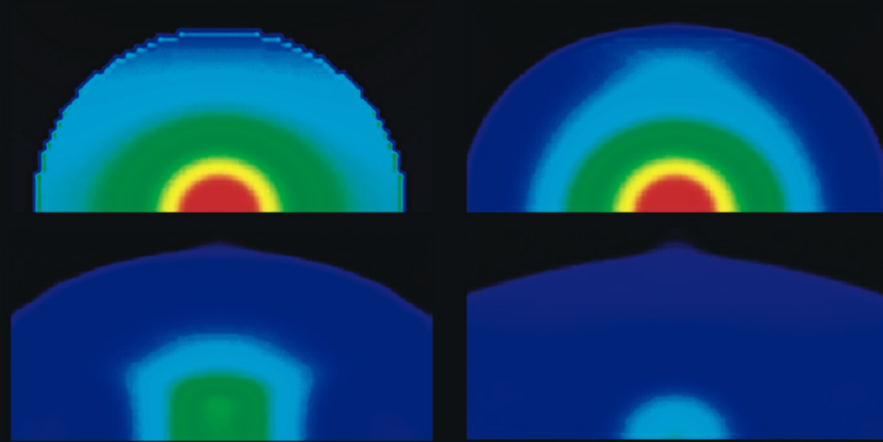
As observational data continually improve, astrophysics codes must be able to keep up and include as many physical processes as possible.

"The code is mostly done," says Anninos. "Now we're concentrating on actually using it. But in the next year or two, we'll be adding more physics to it."

He and Fragile plan to add photon transport and neutron diffusion to the code, and they will modify the existing system of equations for radiation chemohydrodynamics to include magnetic fields. To improve the code's accuracy and efficiency for problems requiring varying degrees of spatial resolution—such as the black hole torus simulations—they will add some form of adaptive grid technology to the code.

"COSMOS is just beginning to give us the 'why' and 'how' of astronomers' observations," says Anninos. As the code's capabilities are expanded, it will bring observations into ever clearer view.

—Katie Walter



Over the course of 190 million years, a nearby massive galaxy steals material from a dwarf spheroidal galaxy in a process known as tidal stripping.

Key Words: astrophysics, black hole accretion, COSMOS code, dwarf galaxies, early cosmology, radio jetcloud interactions, star formation.

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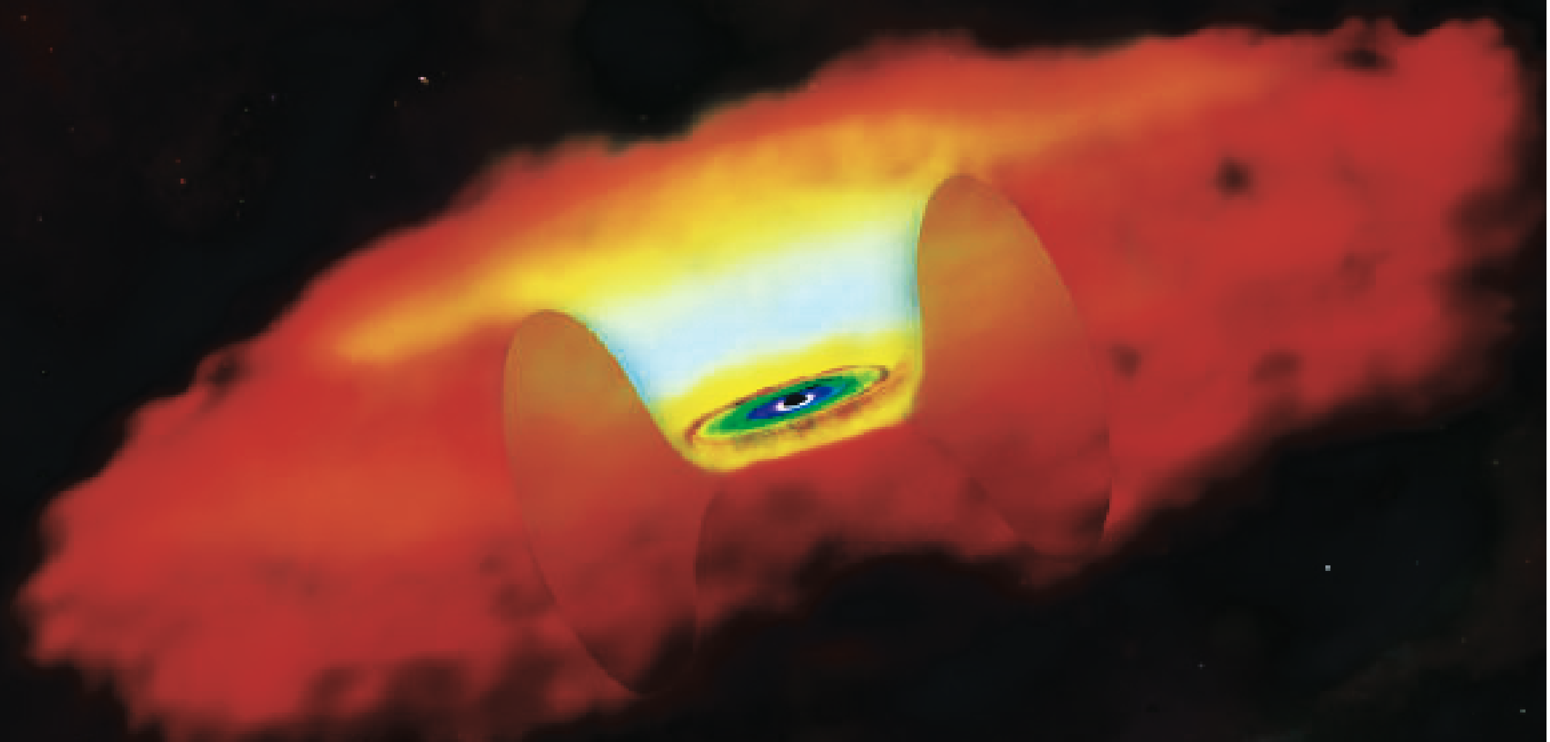


A Giant Leap for Space Telescopes

Eyeglass is a lightweight, flexible, and foldable space optic.

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

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

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

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

Neatly Packaged, Easily Fielded

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

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

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

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

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

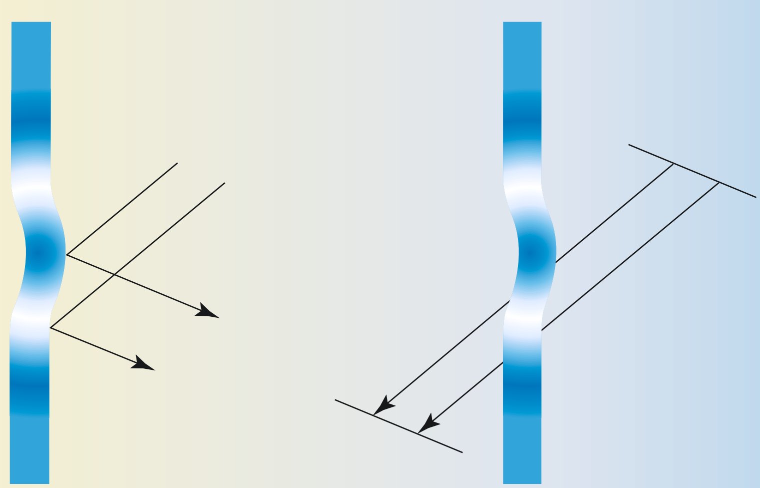
No Motors Required

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

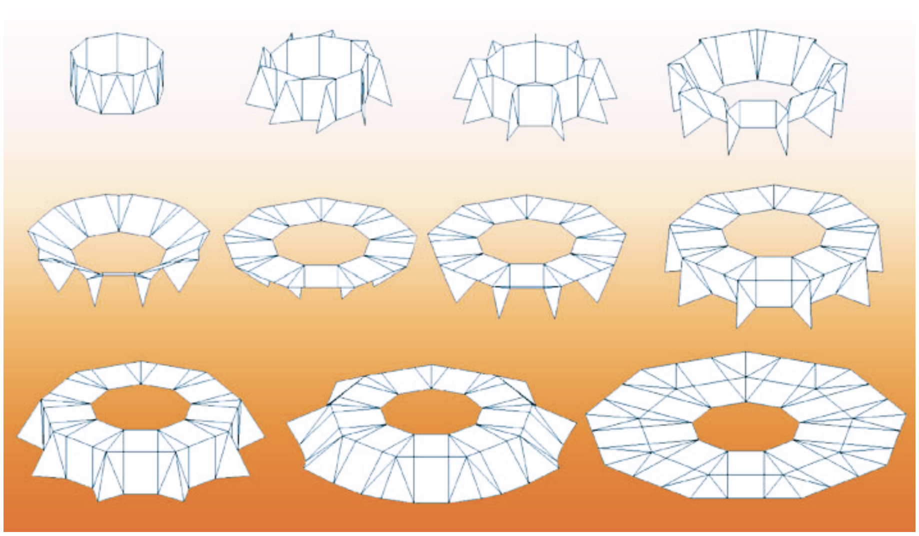
Furthermore, transmissive diffractive lenses are themselves more lightweight. Compared to traditional lenses, the amount of optical material that is required to focus light with a diffractive lens is quite small. For example, Hubble's 2.5-meter mirror weighs 800 kilograms. A 25-meter mirror made more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

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

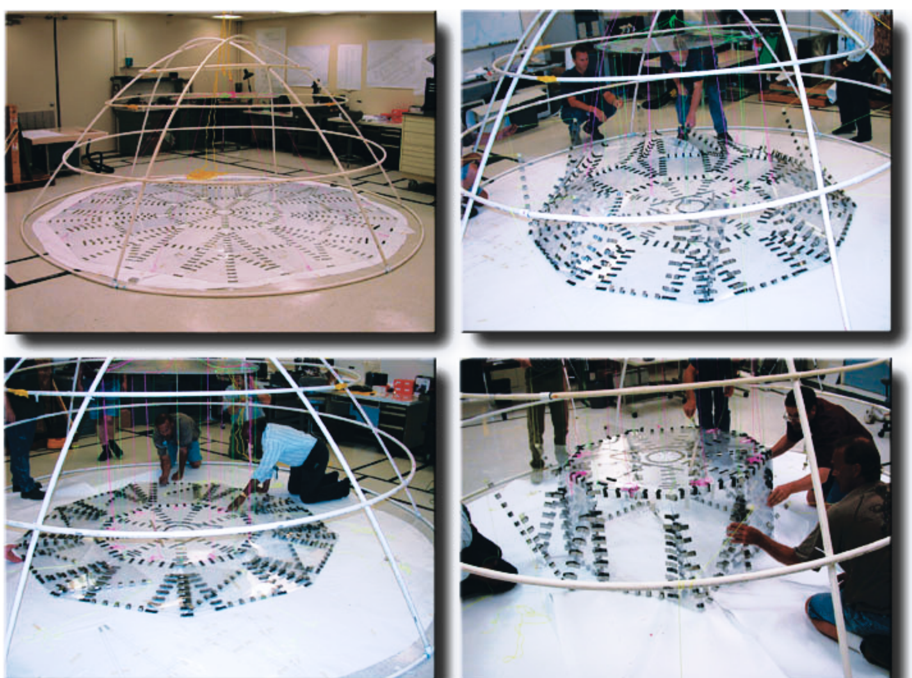
"It's difficult to fold something that is curved, like a mirror. It's much easier to fold something that is flat, like a diffractive lens, especially one that is made of many flat segments," says Hyde. He cites concerns about whether a lens made of many fragile glass segments can survive the severe



In contrast to common mirror lenses, transmissive diffractive optics are relatively insensitive to surface imperfections such as bumps and ripples. Because mirrors reflect light, surface ripples double the magnitude of the bump. Light passing through a ripple on the surface of a thin glass or plastic diffractive optic experiences the same path as light passing next to the ripple, thereby minimizing any distortion.



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



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

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

A Color-Corrected Telescope

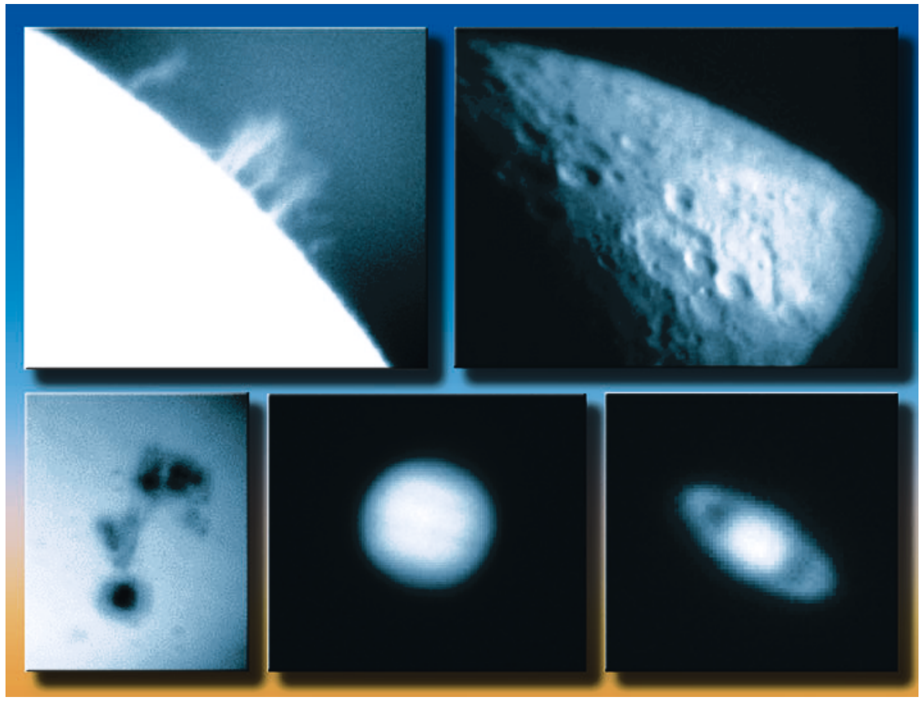
The team has been building and testing increasingly advanced diffractive lenses with materials that are considered suitable for space missions. They started by defining the requirements for a space mission, selecting and characterizing the best materials to make a diffractive lens, and developing fabrication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

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

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

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

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



In 1999, the team developed a color-corrective optic and incorporated it into the first large diffractive telescope. This telescope, which measured 20 centimeters in diameter and 20 meters long, successfully imaged the lunar surface, sunspots, solar flares, Jupiter, and Saturn.

First Segmented Lens

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

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

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

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

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

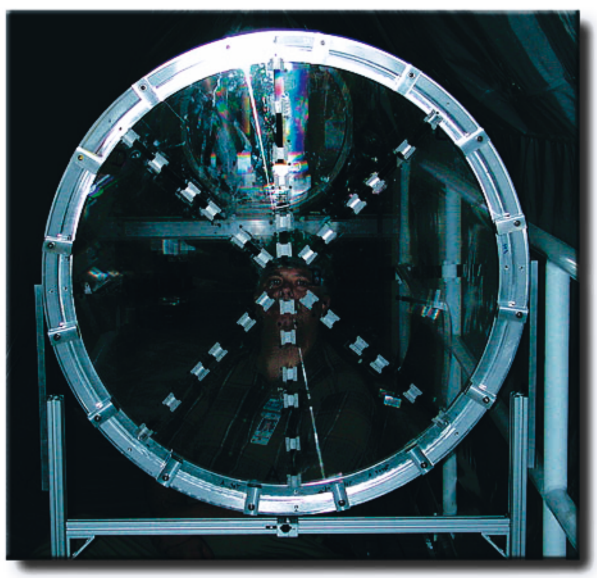
Panels Polished and Etched

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

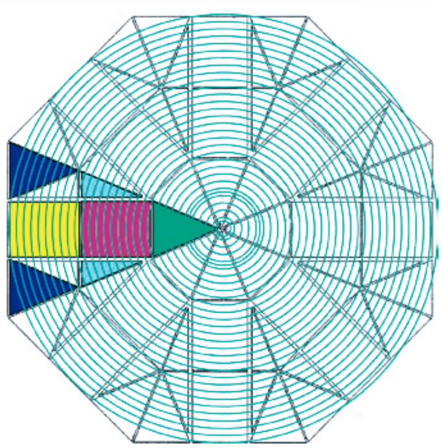
The glass sheets contained several micrometer-deep ripples; they needed to be smoothed to a flatness within about 0.1 micrometer to obtain the required optical quality. Because traditional grind-and-polish techniques are expensive and become increasingly risky for thinner and thinner sheets of glass,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

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

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



In 2001, the team built its first segmented lens. The lens measured 75 centimeters in diameter and was assembled from six foldable panels precisely aligned and joined to each other.



The final 5-meter lens is composed of 72 segments: 16 rectangles measuring 654 by 790 millimeters, 32 right triangles measuring 327 by 790 millimeters, and 24 isosceles triangles measuring 654 by 790 millimeters. The panels are divided into eight "petals" consisting of three isoceles triangles, four right triangles, and two rectangles. Each petal covers 45 degrees, or one-eighth of 360 degrees. One of the petals is highlighted. The circular lines suggest some of the 19,105 circular etched grooves that focus the light.

Assembling the Panels

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

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

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

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

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

Upon delivery at its testing location, the horizontal lens was lifted by a crane to a vertical position and then secured. The lens was illuminated at night with 532-nanometer laser light, producing 1- to 2-centimeter-diameter image spots. Although the optical test was successful, Hyde calls it a rudimentary test because, as expected, air currents and the lack of the panels' complete flatness caused some distortion of the focused spot. An ideal testing environment, Hyde says, would be an underground tunnel at the Department of Energy's Nevada Test Site. Nevertheless, the test at Livermore was considered appropriate for this first-generation lens.

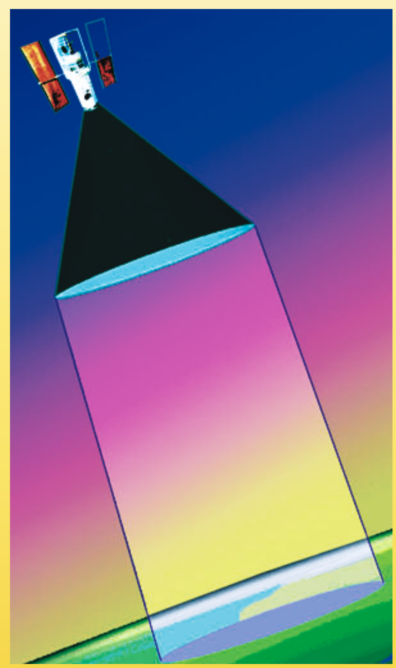
Magnifying Glass and Eyepiece at Work in Space

In high Earth orbit, the Livermore-conceived Eyeglass diffractive telescope would consist of two spacecraft: a 25-meter-aperture Magnifying Glass and a 1-meter-aperture Eyepiece. Two vehicles are required because of the Eyeglass telescope's large aperture and optical slowness. That aperture and optical combination confers large manufacturing tolerances but also dictates a focal length of about 1 kilometer. Such a length is impractical for a single spacecraft, so the Eyeglass telescope would be split into two separate but cooperating vehicles.

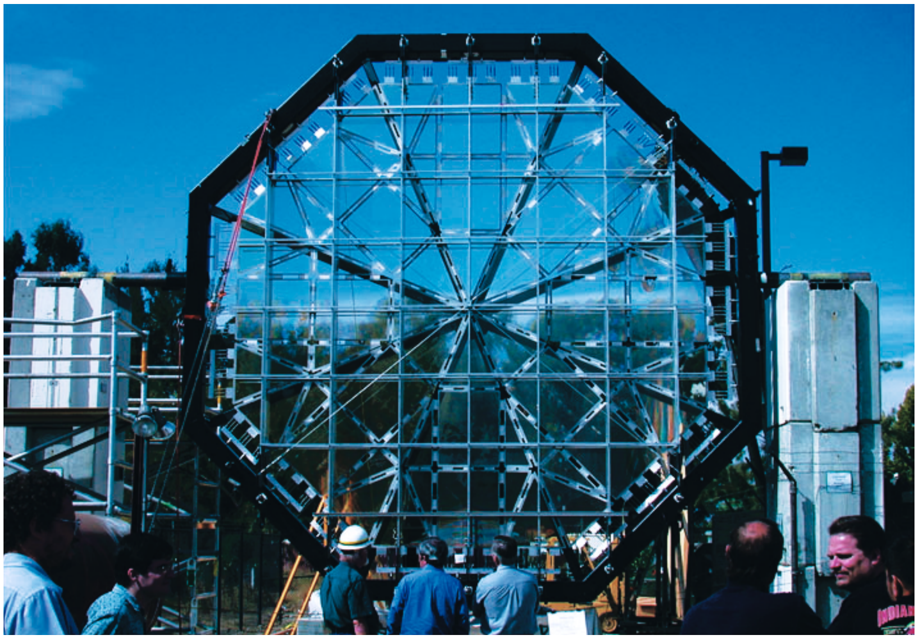
Under this arrangement, the Magnifying Glass vehicle holds the large-aperture diffractive lens and, with the aid of a gyrowheel, swivels the lens to point toward desired targets. The Magnifying Glass gathers and focuses light to a spot about 1 kilometer away, where the light is collected by the mobile Eyepiece. The compact Eyepiece also performs the color correction necessary to obtain accurate images in visible light of all wavelengths. "The two separate vehicles must remain properly aligned so that they function together as a high-precision, steerable telescope," says Livermore physicist Rod Hyde, creator of the Eyeglass concept.

Hyde says that after being deployed in space, the giant lens would be kept flat by being held in tension by rotating the lens along its axis at about 10 revolutions per minute. However, spinning would make it harder to swivel the Magnifying Glass so it could image another target. Hyde solves this problem by placing a counter-rotating gyrowheel inside the center of the lens. Although the gyrowheel would replace the centermost glass panels, these make up only a small portion of the lens and are not essential.

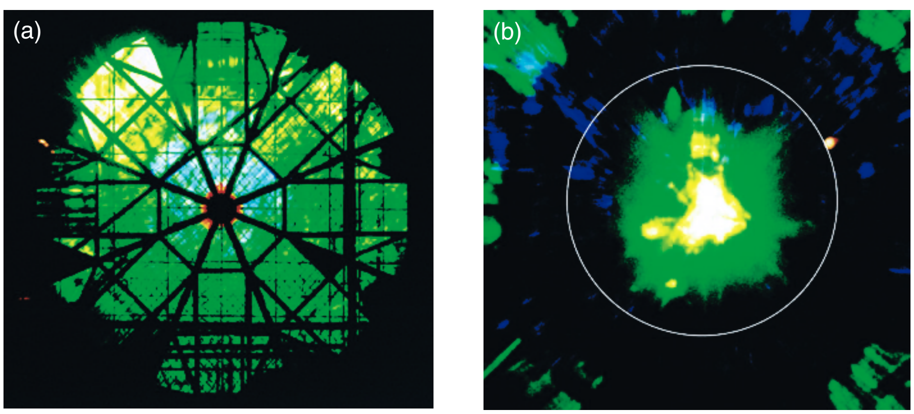
While in space, the thin glass panels must withstand exposure to meteoroids and vacuum, sunlight, and radiation. Fortunately, glass holds up well to the extreme conditions of space. Hyde calculates that based on data recorded by existing satellites, a 10-year exposure in space would result in damaging one ten-thousandth of the Eyeglass lens surface. Impact from meteoroids would likely create either craters or holes located about every 2.5 centimeters and many accompanying cracks. Fortunately, the cracks would not grow because the lens would be under low tension. Also, the lack of water vapor in space makes glass much more resistant to spreading cracks.



The Eyeglass diffractive telescope would consist of two spacecraft: a 25-meter-aperture Magnifying Glass and a 1-meter-aperture Eyepiece.



The completed lens, mounted in a steel and aluminum frame and ready for optical testing.



(a) The lens during optical testing. Some of the panels are obstructed by the supporting frame. (b) The 1- to 2-centimeter focal spot produced by the lens when illuminated with 532-nanometer laser light.

On the Map

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

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

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

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

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

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

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

—Arnie Heller

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

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For more information about diffractive optics:

www.llnl.gov/nif/lst/diffractive-optics/newtecheye.htm

Checking Out the Hot Spots

WHEN a high-explosive material detonates, several events happen virtually instantaneously. A shock wave slams into the material, compresses it with pressures up to 400,000 times that of Earth's atmosphere, and causes it to release chemical energy, which heats it to over 3,500°C. The heat releases power approaching 10 billion watts per square centimeter to sustain the shock wave, which travels as fast as 10 kilometers a second. All of these reactions occur within less than a millionth of a second.

High explosives are an essential component of a nuclear weapon because they initiate the nuclear reaction. The study of high explosives has been an integral part of nuclear weapons research for Livermore scientists since 1952, when the Laboratory began operations. However, it has been a challenge for the scientists to find avenues for observing exactly what happens during high-explosive detonations, given the speed and extreme conditions in which they happen.

The National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program, which began in 1994, placed emphasis on another aspect of high-explosive research. Because the program's mission is to ensure the safety of the nation's nuclear stockpile without underground testing, Livermore weapon scientists focused their research on how high-explosive material may change in an aging stockpiled nuclear weapon.

A crucial part of high-explosive research is the study of voids, or defects, in high-explosive material. Normally, a defect is seen as something that makes a material less than perfect. But voids in high explosives are an important part of the ignition process, because they enable the material to explode. Voids are small pockets—usually between 1 to 20 micrometers in size—either filled with air or, in some cases, a byproduct gas of the surrounding crystalline high-explosive grains or polymer binder. During the detonation process, the shock wave deforms and compresses the material, which then engulfs the area occupied by the voids. What remains are hot spots—small isolated regions of high explosive at a much higher temperature than the surrounding material. These hot spots are where ignition of the high explosive begins.

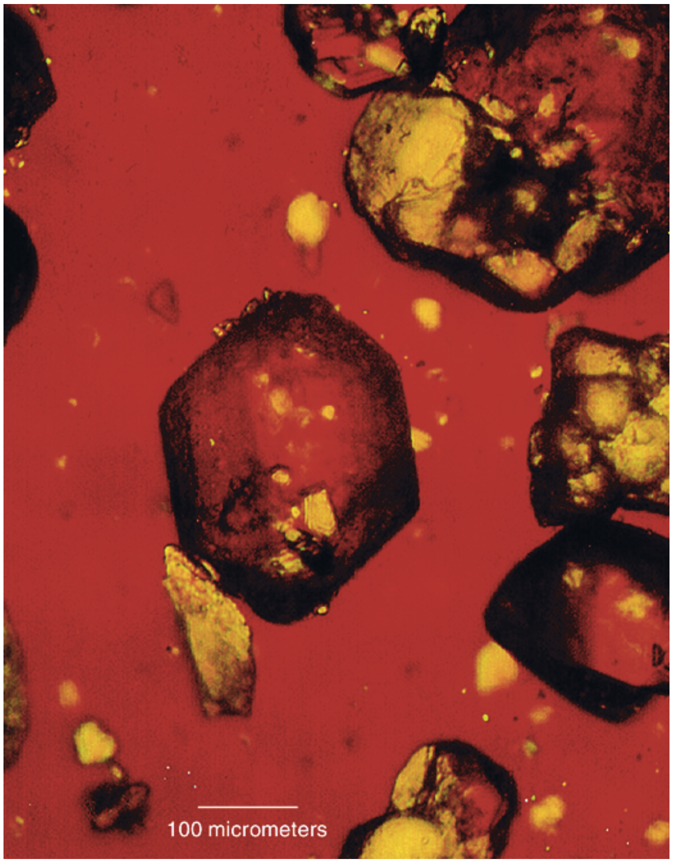
A Long History

The research involving voids is a study of balance. Material with too few voids will result in too few hot spots, making ignition difficult. In addition, if hot spots are too small, they will cool prematurely, preventing ignition. But high explosives with too many voids can be too sensitive and explode from mishandling.

Investigating the role of hot spots in explosives has never been easy. Historically, scientists relied on rules of thumb in materials science, laboratory testing of explosives, and accident analysis to determine the dynamics of explosive materials. All of these methods are time- and labor-intensive.

In early experiments, scientists crushed a piece of explosive material on a glass plate and identified small spots of light seen from underneath as hot spots. Eventually, their research capabilities expanded, and they began using simple computational models. The early models were limited, however, because they treated the explosive as a homogeneous material. High explosives are anything but. They are composed of various constituents and can include one or more crystalline components, plastic binders, and voids.

The chemistry that occurs in a detonation can also be complex. For example, 300 different reactions can occur when the high-explosive material tetranitro tetraazacyclooctane (HMX) detonates. Depending on the circumstances of combustion, each reaction can involve different pathways. Models developed at Livermore in the 1970s were based on this realization but needed considerable experimental calibration.

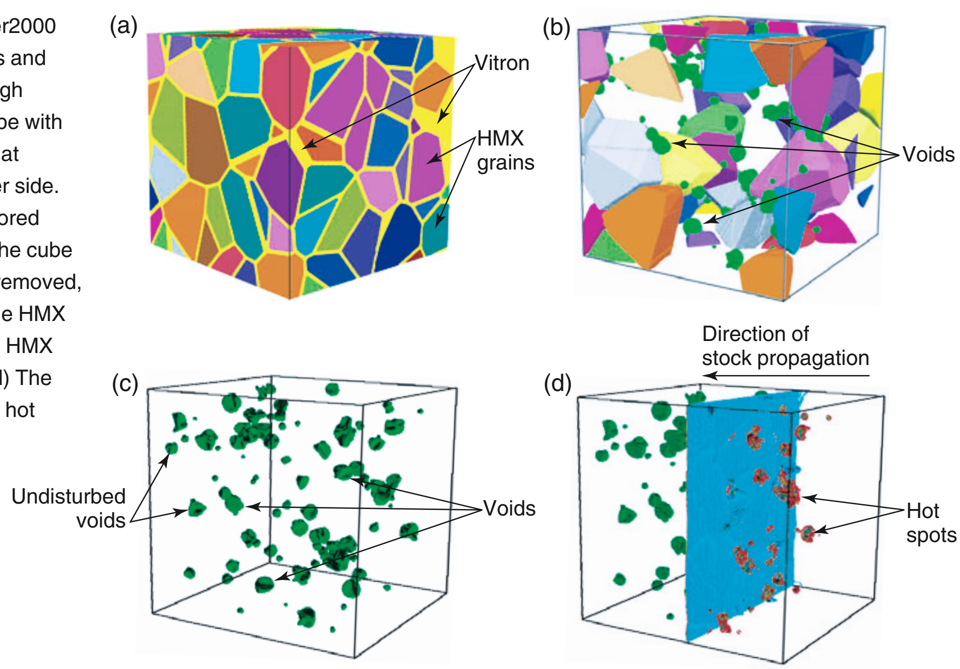


Defects, or voids, are a necessary component in a high explosive because they cause the material to ignite. This photomicrograph shows defects in a 150-micrometer HMX crystal.

With the development of supercomputers, scientists have the capability to simulate high-explosive detonation and, in particular, observe hot spots in action. "The importance of hot spots in explosive materials has been known since the 1940s," says computational physicist Jack Reaugh. "Until recently, however, observing hot spots in detail has been extremely difficult." For several years now, Reaugh has been studying hot spots and voids using hydrodynamic computational codes, which describe material flow under extreme pressures. (See *S&TR*, June 1999, pp. 12–18.) In his first simulation in 1999, Reaugh designed a cube with 36 HMX particles, each 0.05 millimeter in size. He then simulated the detonation of the cube on a computer workstation using ALE3D, a three-dimensional computational code developed at Livermore.

In the fall of 2001, Reaugh, with the help of physicist Stew Keeton, took advantage of Livermore's new TeraCluster2000 (TC2K) supercomputer and ran a new simulation, again with ALE3D and using 128 of the TC2K's processors for 500 computing hours. This time, the cube contained a more complex combination of simulated HMX. The cube measured 100 micrometers per side—about the diameter of a human hair—and contained about 100 grains of HMX represented by various geometric shapes, along with a light-colored fluorocarbon polymer binder between the grains. Voids were inserted into the cube so that they made up 1 percent of its volume. The simulation generated a shock wave that swept across the cube. It hit the material at 120,000 times Earth's atmospheric pressure at sea level. The compression collapsed the voids and transformed them into isolated hot spots with temperatures of over 900 kelvins—100 to 200 kelvins higher than the surrounding material.

This simulation, performed on the TeraCluster2000 supercomputer, tracked the evolution of voids and resulting hot spots during detonation of the high explosive HMX. (a) The simulation uses a cube with approximately 100 grains of high explosive that measures approximately 100 micrometers per side. The shaded grains are HMX and the light-colored veins are a polymer binder called Viton. (b) The cube with the binder and some of the HMX grains removed, so that the voids, located between some of the HMX grains, are visible. (c) The cube with all of the HMX and binder removed, showing all the voids. (d) The shock wave moves through the cube, leaving hot spots where the voids used to be.



Refining the Model

"The sequence of events revealed in the TC2K simulation showed how important supercomputer capabilities are to this field of study," Reaugh says. As in most new work, the first attempt gave Reaugh some ideas on how to improve the model for the next simulation. "A big portion of this project is just designing the model," he continues, "and each pass improves it." He could see, for example, that the simulated HMX crystals were too big and that he needed to change the chemical reaction rates and transport properties.

Through an effort funded under the joint Department of Defense–Department of Energy Munitions Technology Development Program, Reaugh collaborated with Livermore scientists whose experimental work gauged Reaugh's results. Part of Reaugh's work focuses on how flames propagate between hot spots and how propagation speed affects the response of the explosive to high-pressure shocks. For the TC2K simulation, Reaugh estimated the distance between the hot spots based on his calculations of flame speed at high pressure. Meanwhile, chemist Joe Zaug and his colleagues used the high pressures of a diamond anvil cell for HMX experiments in which they measured propagation speeds at over 300,000 atmospheres. The experiments showed the flame speed to be up to 100 times faster than Reaugh initially calculated for the simulation. "This meant that the hot spots could have been 100 times farther apart than I originally thought," Reaugh says.

At the same time, theoretical chemist Riad Manaa performed quantum molecular dynamics calculations—that is, calculations of the interactions between atoms and electrons—to determine the rate of chemical decomposition of HMX at high temperature and pressure. "When we compared results, Manaa's calculations showed the decomposition to be happening much faster than we thought. In fact, his rates are almost fast enough to account for the difference between our estimate of the flame speed and Zaug's measurements," notes Reaugh.

The differences pointed out that additional capabilities were needed in the computational code. "We were able to see things that needed to be improved with ALE3D so that it could deal gracefully with some very stressing calculations that we're planning for the future."

Building on these observations, Reaugh's group ran a new simulation in September 2002. The simulation was performed on Livermore's most powerful supercomputer, ASCI White, part of NNSA's Advanced Simulation and Computing (ASCI) Program. The new model cube was designed for optimum use of ASCI White and incorporated lessons learned from the previous simulation. Again, HMX was used. The variety of grain sizes was increased dramatically. Voids amounting to 2 percent of the volume were inserted into the explosive grains. The new cube measured approximately 300 micrometers per side and contained 93,000 grains, quite a jump from the 100 grains used in the previous simulation. Just generating the initial cube assembly took 400 processors about 4 computing hours. By reducing the level of detail but retaining the distribution of voids, engineer Tom Reitter and Reaugh, with the help of computer support associate Estella McGuire, were able to simulate the propagation of a shock wave through a brick consisting of four cubes stacked end to end. That simulation took less than 100 hours and showed the shock wave speeding up as reactions behind the shock front built up pressure. "This simulation never could have been done without the computational power that we have now," Reaugh says.

Improvements to the simulation were tested in September 2002. The simulation used a new cube that consisted of approximately 93,000 grains of different shapes and sizes. Voids shaped like spheres were inserted into the grains. This simulation also incorporated improvements to the equations of state for explosive products and the chemical reaction kinetics models.

Details of a Larger Picture

With the powerful supercomputers and codes now available, scientists can simulate high-explosive detonations in sufficient detail to observe detonation behavior under a multitude of parameters. "Whereas before, we had to rely on piecemeal data from tests," notes Reaugh, "now, the details of ASCI simulations help us to interpret what went on in the experiment."

Because the simulations will also help scientists understand how high explosives respond during manufacturing, shipping, and storage, they will not only benefit the Stockpile Stewardship Program but also help the high-explosives industry.

The study of explosive materials is at once becoming more comprehensive and more focused.

—Laurie Powers

Key Words: ALE3D, Advanced Simulation and Computing (ASCI) Program, chemical kinetics, high explosives, high-pressure activities, hot spots, HMX, hydrodynamics codes, TeraCluster2000 (TC2K), voids.

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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

Illumination Box and Camera System
Jeffrey S. Haas, Fredrick R. Kelly, John F. Bushman, Michael H. Wiefel, Wayne A. Jensen, Gregory L. Klunder
U.S. Patent 6,454,939 B1
September 24, 2002
A hand-portable, field-deployable thin-layer chromatography (TLC) unit and a hand-portable, battery-operated unit for development, illumination, and data acquisition of TLC plates. Both contain many miniaturized features that permit a large number of samples to be processed efficiently. The TLC unit includes a solvent tank, a holder for TLC plates, and a variety of tool chambers for storing TLC plates, solvent, and pipettes. After processing in the TLC unit, a TLC plate is positioned in a collapsible illumination box, where the box and a charge-coupled-device (CCD) camera are optically aligned for optimal pixel resolution of the CCD images of the TLC plate. The TLC system includes an improved chamber for chemical development of TLC plates that prevents solvent overflow.

Glow Discharge Detector
Jackson C. Koo, Conrad M. Yu
U.S. Patent 6,457,347 B1
October 1, 2002
A highly sensitive electronic ion cell with a constant wave glow discharge detector used for measuring trace elements in helium carrier gas. The detector, which is controlled through a biased resistor, can detect the change of electron density caused by impurities in helium carrier gas by many orders of magnitude greater than that caused by direct ionization or electron capture. The glow discharge detector uses a floating pseudoelectrode to form a probe in or near plasma. By using this probe, the detector can directly measure the large variation of electron density due to trace amounts of impurities.

Optical Fiber Head for Providing Lateral Viewing
Matthew J. Everett, Billy W. Colston, Dale L. James, Steve Brown, Luiz Da Silva
U.S. Patent 6,466,713 B2
October 15, 2002
The head of an optical fiber comprising the sensing probe of an optical heterodyne sensing device includes a planar surface that intersects the perpendicular-to-axial centerline of the fiber at a given polishing angle. The planar surface is coated with a reflective material so that light traveling axially through the fiber is reflected transverse to the fiber's axial centerline and is emitted laterally through the side of the fiber. Alternatively, the planar surface can be left uncoated. The given polishing angle must be no greater than 39 degrees or must be at least 51 degrees. The emitted light is reflected from adjacent biological tissue, collected by the head, and then processed to provide real-time images of the tissue. The method for forming the planar surface includes shearing the end of the optical fiber and applying the reflective material before removing the buffer that circumscribes the cladding and the core.

Actinide Removal from Spent Salts
Peter C. Hsu, Erica H. von Holtz, David L. Hipple, Leslie J. Summers, Martyn G. Adamson
U.S. 6,471,922 B1
October 29, 2002
A method for removing actinide contaminants (uranium and thorium) from the spent salt of a molten salt oxidation reactor. Spent salt is removed from the reactor and analyzed to determine the contaminants present and the carbonate concentration. The salt is dissolved in water; then one or more reagents are added to precipitate the water, and one or more reagents are added to precipitate the thorium as thorium oxide and/or the uranium as either uranium oxide or as a diuranate salt. The precipitated materials are filtered, dried, and packaged for disposal as radioactive waste. About 90 percent of the thorium and/or uranium present is removed by filtration. After filtration, salt solutions having a carbonate concentration greater than 20 percent require further cleanup using an ion exchange column, which yields salt solutions that contain less than 0.1 part per million of thorium or uranium.

System and Method for Ultrasonic Tomography
Waleed Sami Haddad
U.S. Patent 6,475,150 B2
November 5, 2002
A system and method for doing both transmission mode and reflection mode three-dimensional ultrasonic imaging. The multimode imaging capability may be used to provide enhanced detectability of cancerous tumors within a human breast. Similar imaging systems are applicable to other medical problems as well as to a variety of nonmedical problems in nondestructive evaluation.

Chemical Sensor System
Christopher B. Darrow, Joe H. Satcher, Jr., Stephen M. Lane, Abraham P. Lee, Amy W. Wang
U.S. Patent 6,480,730 B2
November 12, 2002
An implantable chemical sensor system for medical applications that permits selective recognition of an analyte using an expandable biocompatible sensor, such as a polymer, that undergoes a dimensional change in the presence of the analyte. The expandable polymer is incorporated into an electronic circuit component that changes its properties (for example, frequency) when the polymer changes dimension. As the circuit changes its characteristics, an external interrogator transmits a signal transdermally to the transducer, and the concentration of the analyte is determined from the measured changes in the circuit. This invention may be used for minimally invasive monitoring of blood glucose levels in diabetic patients.

Optically Generated Ultrasound for Enhanced Drug Delivery

Steven R. Visuri, Heather L. Campbell, Luiz Da Silva
U.S. Patent 6,484,052 B1
November 19, 2002
High-frequency acoustic waves, analogous to ultrasound, can enhance the delivery of therapeutic compounds into cells. The compounds delivered may be chemotherapeutic drugs, antibiotics, photodynamic drugs, or gene therapies. The therapeutic compounds are administered systemically or, preferably, locally to the targeted site. Local delivery can be accomplished through a needle, cannula, or a variety of vascular catheters, depending on the location of routes of access. To enhance the systemic or local delivery of the therapeutic compounds, high-frequency acoustic waves are generated locally near the target site and preferably near the site of compound administration. The acoustic waves are produced via laser radiation interaction with an absorbing media and can be produced via thermoelastic expansion, thermodynamic vaporization, material ablation, or plasma formation. Acoustic waves temporarily permeate the membranes of local cells, increasing the diffusion of the therapeutic compound into the cells, allowing for decreased total body dosages and side effects, and enabling new therapies.

Mitigation of Substrate Defects in Reflective Reticles Using Sequential Coating and Annealing

Paul B. Mirkarimi
U.S. Patent 6,489,066 B2
December 3, 2002
A buffer layer to minimize the size of defects on a reticle substrate before a reflective coating is deposited on the substrate. The buffer layer is formed either by a multilayer deposited on the substrate or by a plurality of sequentially deposited and annealed coatings deposited on the substrate, which may comprise multilayer and single layer coatings. The multilayer deposited and annealed buffer layer coatings may be of the same material as or different material than the reflective coating thereafter deposited on the buffer layer.

Process for Fabricating a Charge Coupled Device

Alan D. Conder, Bruce K. F. Young
U.S. Patent 6,489,179 B2
December 3, 2002
A monolithic three-dimensional charged-coupled device (3D-CCD) that uses the entire bulk of the semiconductor for charge generation, storage, and transfer. The 3D-CCD provides a vast improvement of current CCD architectures that use only the surface of the semiconductor substrate. The 3D-CCD is capable of developing a strong electric field throughout the depth of the semiconductor by using deep (buried) parallel (bulk) electrodes in the substrate material. Using backside illumination, the 3D-CCD architecture enables a single device to image photon energies from the visible to the ultraviolet and soft x ray and out to higher energy x rays of 30 kiloelectronvolts and beyond. The buried or bulk electrodes are electrically connected to the surface electrodes, and an electric field parallel to the surface is established with the pixel in which the bulk electrodes are located. This electric field attracts charge to the bulk electrodes independent of depth and confines it within the pixel in which it is generated. Charge diffusion is greatly reduced by the electric field, which is strong because of the proximity of the bulk electrodes.

Delivery System for Molten Salt Oxidation of Solid Waste

William A. Brummond, Dwight V. Squire, Jeffrey A. Robinson, Palmer A. House
U.S. Patent 6,489,532 B1
December 3, 2002
A delivery system for safely injecting solid waste particles, including mixed wastes, into a molten salt bath for destruction by the process of molten salt oxidation. The delivery system includes a feeder system and an injector that allow the solid waste stream to be accurately metered, evenly dispersed in the oxidant gas, and maintained at a temperature below incineration temperature while entering the molten salt reactor.

Borehole Induction Coil Transmitter

Gale Holladay, Michael J. Wilt
U.S. Patent 6,489,772 B1
December 3, 2002
A borehole induction coil transmitter that is a part of a cross-borehole electromagnetic field system used for underground imaging applications. The transmitter consists of four major parts: (1) a wound ferrite or mu-metal core, (2) an array of tuning capacitors, (3) a current driver circuit board, and (4) a flux monitor. The core is wound with several hundred turns of wire and connected in series with the capacitor array to produce a tuned coil. This tuned coil uses internal circuitry to generate sinusoidal signals that are transmitted through the earth to a receiver coil in another borehole. The transmitter can operate at frequencies from 1 to 200 kilohertz and supplies sufficient power to permit the field system to operate in boreholes separated by up to 4 meters.

Method and Apparatus for Dynamic Focusing of Ultrasound Energy

James V. Candy
U.S. Patent 6,490,469 B2
December 3, 2002
Method and system for noninvasively detecting, separating, and destroying multiple masses (tumors, cysts) through a plurality of iterations from tissue (for example, breast tissue). The method and system may open new frontiers in noninvasive treatment of masses in biomedicine, along with the expanding technology of acoustic surgery.

Awards

On November 26, 2002, **Edward Teller** received the **Secretary's Gold Award**, the Department of Energy's highest honorary award, for his outstanding contributions to science and the security of the nation. Energy Secretary Spencer Abraham presented the award during a visit to the Laboratory. In doing so, Abraham said, "Dr. Teller is one of the giant figures of the 20th century, whose contributions to winning both World War II and the Cold War are immeasurable. But I believe that Edward Teller should also be regarded as one of the most important figures of the 21st century. Dr. Teller did not just help make the world safe from tyranny and aggression. He helped usher in the era of supercomputing that drives so much of our current science. His unwavering support for scientific education has inspired countless young men and women to pursue lives in the sciences."

Physicist **Steve Allen** has been selected as a **Distinguished Lecturer** by the **American Physical Society's Division of Plasma Physics**. He is one of six lecturers chosen from around the nation who will travel to U.S. colleges and universities during 2002–2003 to share their expertise with a broad audience. Allen will be discussing his work in plasma physics, specifically, "Improving Tokamak Confined with 'Plasma Surgery' and 'Plasma Floating.'" Allen, who works in the Physics and Advanced Technologies Directorate, is the program leader for Livermore's collaboration on the DIII-D tokamak, an effort between Lawrence Livermore and General Atomics in San Diego.

Don Correll, director of the Laboratory's Science and Technology Education Program, and this year's chair of the lecturer selection committee, said that having Laboratory scientists selected "gives the Laboratory an opportunity to be recognized for its high-caliber work in plasma physics."

Mimi Alford has received the **Aegis Award** for producing "A Journey Through Time . . . The History of Engineering at LLNL." The Aegis is a national award that is intended to recognize excellence in video and film production among nonbroadcast organizations, such as corporations, government, and universities. Alford's video is a 20-minute history of the Engineering Directorate and includes hundreds of clips and archival film such as rare footage of John F. Kennedy at the University of California at Berkeley meeting with Director Emeritus Edward Teller and several other former Laboratory directors. Alford had been collecting footage from employees for nearly 20 years. The video was one of several produced for the Laboratory's 50th anniversary celebration.

A New Code Simulates the Cosmos

A new Livermore astrophysics code called COSMOS can model almost anything from a small black hole to the entire universe. It is unusual in being easily adaptable to either relativistic or Newtonian astrophysical phenomena. COSMOS incorporates several ways to simulate hydrodynamic as well as radiative cooling, chemistry, self-gravity, relativistic scalar fields, and several other physics packages to accurately address a wide range of problems. COSMOS has already been applied to an ambitious array of astrophysical problems: a phase transition during the early moments of the young universe, accretion of matter by black holes, star formation caused by the interaction of gas clouds and jets emanating from massive black holes, and the evolution of dwarf spheroidal galaxies. In the near future, several new features will be added to the code, including adaptive grid technology to allow varying degrees of spatial resolution.

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A Giant Leap for Space Telescopes

A Livermore team is developing a radically new technology to solve the difficulties inherent in building and fielding a high-quality space telescope far larger than ever deployed. The concept, called Eyeglass, uses diffractive optics (also called Fresnel lenses) instead of mirrors or conventional glass lenses. Because it is lightweight, flexible, and able to be segmented and folded, an Eyeglass diffractive telescope could be neatly packaged in a space launch vehicle. It would also be easy to field in space because as a thin, flat membrane, it would not need large, heavy backings, trusses, or motors to maintain its shape, as do telescopes using mirrors. The team has been building increasingly advanced diffractive lenses with materials that are considered suitable for space missions. The largest lens measures 5 meters in diameter and is composed of 72 folding panels of thin glass. The lens is the largest optical quality lens in the world. It is twice as big as, yet 10 times lighter than, the primary mirror for the Hubble Space Telescope.

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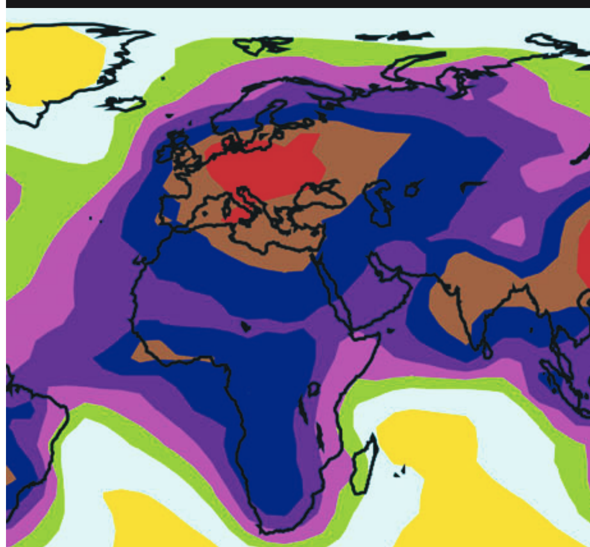
U.S. Government Printing Office: 2003/583-060-70034

Coming Next Month

Aerosols and the Climate Change Puzzle



Computer simulations are revealing the effects of human-caused atmospheric aerosols on global climate.

Also in April

- ***Examining neutrino transformation over time and distance helps scientists to better understand the physical forces guiding the universe.***
- ***A common input/output library for massively parallel computing is now in wide use.***
- ***A new three-dimensional fluid dynamics simulation code is used to explain a perplexing secondary instability in the mixing of two fluids with different densities.***

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