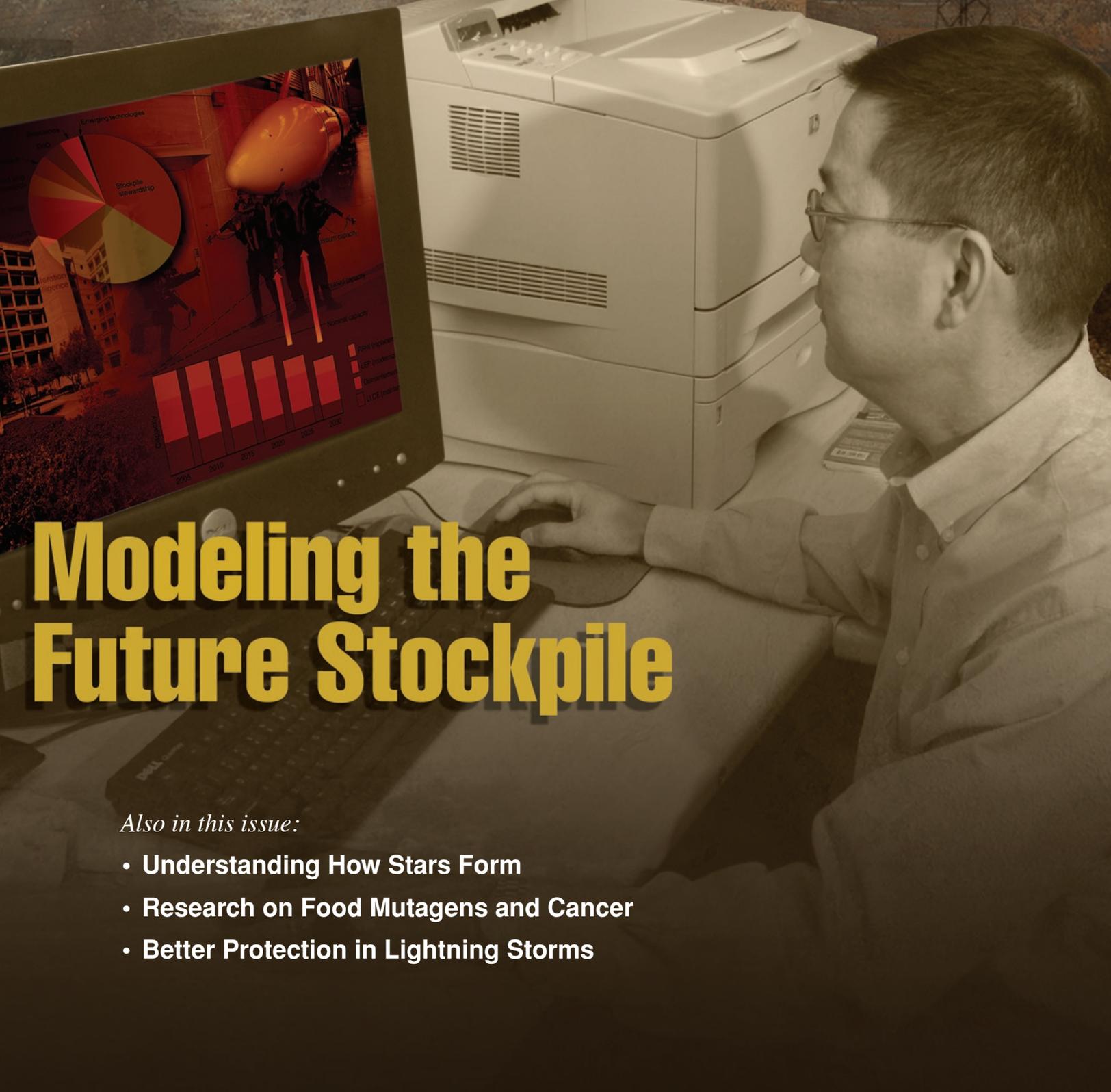


# Science & Technology

REVIEW

December 2005

National Nuclear  
Security Administration's  
Lawrence Livermore  
National Laboratory



## Modeling the Future Stockpile

*Also in this issue:*

- Understanding How Stars Form
- Research on Food Mutagens and Cancer
- Better Protection in Lightning Storms

## About the Cover

The U.S. is confronting new threats to national security in the 21st century. In this changing security environment, the National Nuclear Security Administration (NNSA) is adapting the nuclear weapons complex, or enterprise, to meet national needs for a reliable but smaller stockpile with the flexibility to respond to unanticipated threats. To help NNSA evaluate the options available, a multidisciplinary team of Livermore researchers has developed a classified computational tool based on system dynamics theory to model the entire enterprise. The article beginning on p. 4 describes the model and how it can be used to examine potential outcomes of changes. On the cover, a computational scientist works to incorporate data on the many operations of NNSA's nuclear enterprise.



Cover design: Amy Henke

## About the Review

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

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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 Technical Information 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](http://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-TR-52000-05-12  
Distribution Category UC-99  
December 2005

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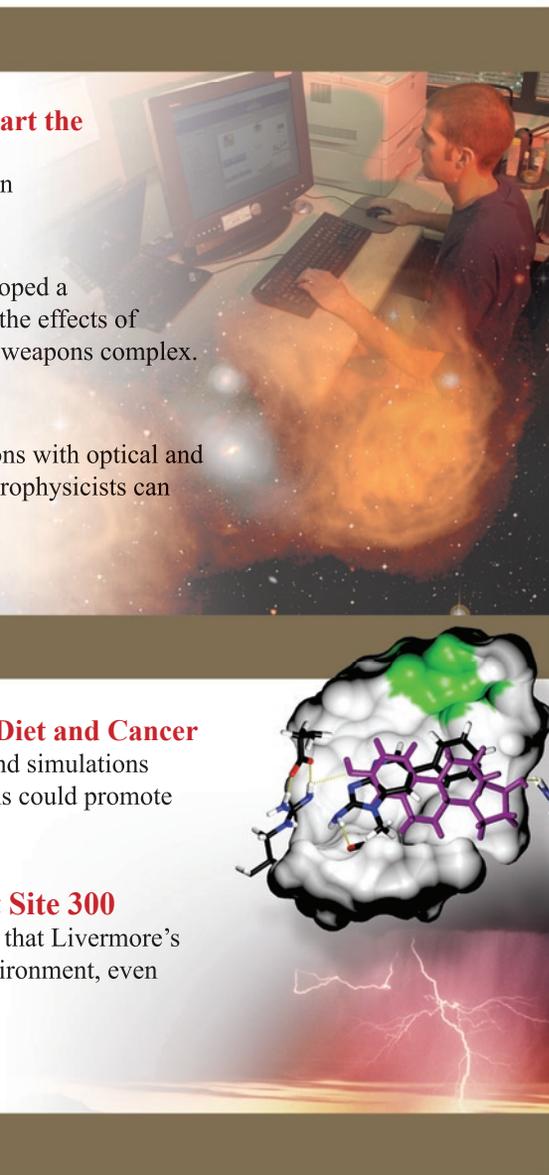
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### Scientists reveal the way nanotubes grow

In work funded by the Laboratory Directed Research and Development (LDRD) Program, Livermore scientists have clarified the growth process for nanotubes—molecules that are typically 10,000 times smaller than the diameter of a human hair. Because nanotubes are extremely strong and have good thermal conductivity, researchers want to use them in nanoscale electronic and mechanical applications. By understanding their growth structure, researchers will be better able to manipulate the use of nanotubes in technological applications.

The Livermore team performed a series of quantum molecular dynamics simulations using different initial conditions for carbon coverage on iron nanoparticles. The team chose iron as a catalyst because experimentally it has the highest rate of carbon nanotube production. In the simulations, carbon atoms bonded to the iron, forming chains that eventually interconnected to form a sheet of pentagons and hexagons.

“We were surprised that carbon and iron do not mix at the nanoscale during growth and that the tubes grew capped,” says Giulia Galli, a physicist in Livermore’s Physics and Advanced Technologies Directorate. “Our simulations clarified the growth of nanotubes on small metal nanoparticles and thus will help researchers design experiments aimed at controlled growth of nanotubes.

The team’s research appeared in the August 26, 2005, issue of *Physical Review Letters* and was featured as a highlight in the September 8 issue of *Nature Materials*.

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### A new method for making superhard materials

A research collaboration led by scientists at Lawrence Livermore found that high-pressure shock waves applied to nanocrystals may increase a material’s hardness. The research, which was funded by the LDRD Program, combined data from the first shock experiments on nanocrystalline metals with numerical simulations run on the Laboratory’s supercomputers. Results indicate that, with further development, high-pressure shock waves can be used to make superhard materials that are stronger than any materials made with current manufacturing processes.

In general, metallic materials used in everyday applications are made of small “grains” joined by grain boundaries. When the grain size is reduced to less than 100 nanometers, the material is considered nanocrystalline. Nanocrystalline materials have extraordinary properties, such as enhanced hardness. However, extremely small grains tend to slide over each other as a material deforms, which reduces the material’s hardness. “It’s like stepping into sand,” says Livermore laser physicist Bruce Remington, who participated in the research. “The material is solid, but you still sink into it.”

The team used Livermore’s Janus laser to shock samples of nanocrystalline nickel and copper. The shock waves produced by the high-intensity laser move faster than the speed of sound and generate pressures nearly 1 million times greater than atmospheric pressure. “The high pressure increased the friction among grains and decreased the sliding,” says team leader Eduardo Bringa, a materials scientist at the Laboratory. “By turning off the mechanism that softens the grains, we create a material that, being hard to begin with, is even harder during and following the shock-wave application.”

Team members caution that the research is in an early phase. If successful, it could be used to develop superhard materials for shielding military vehicles, protecting spacecraft from damage caused by interplanetary dust particles, or building safer automobile bumpers and frames. The materials also could have applications in inertial confinement fusion experiments. The team’s findings were published in the September 16, 2005, issue of *Science*.

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### Enhanced adaptive optics for Gemini Telescope

Lawrence Livermore has been selected as the lead institution to build the Extreme Adaptive Optics Coronagraphy (ExAOC) for the Gemini Telescope. Researchers from the University of California at Berkeley and Los Angeles, the Jet Propulsion Laboratory, the American Museum of Natural History, the Hertzberg Institute in Canada, and several smaller institutes will also collaborate on this project.

An enhanced adaptive optics system will allow astronomers to minimize the blurring effects of Earth’s atmosphere, so they can detect planets about 30 to 150 light years from the solar system. Adaptive optics systems use light from a relatively bright star to measure and then correct the atmospheric distortions by bouncing light off a deformable mirror. The ExAOC system will have 3,000 to 4,000 actuators to control the deformable mirror. These actuators will be made of etched silicon microelectromechanical systems instead of reflective glass, which is used on the adaptive optics system at the W. M. Keck Observatory. With the new actuators, researchers will be able to adjust the shape of the mirror by several micrometers with a precision of less than 1 nanometer and, thus, will be able to correct for atmospheric distortions at a rate 10 times greater than the Keck system. Such a high resolution will allow them to detect distant planets and learn more about how solar systems formed.

The ExAOC system is funded primarily by the National Science Foundation through the Association of Universities for Research for Astronomy. First light is predicted near the end of 2009.

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## Helping NNSA Managers Chart the Future Stockpile

**S**UCCESSIVE administrations have made clear that the future nuclear stockpile must be reliable, secure, and safe in the long term without the need for nuclear testing. The nation is committed to achieving a credible deterrent with the lowest possible number of nuclear weapons. Through the Moscow Treaty, the U.S. has already significantly reduced the number of deployed nuclear weapons.

As part of the effort to implement this vision, a number of high-level committees and task forces have taken a hard look at the nation's nuclear weapons complex, the current nuclear stockpile, and strategies of deterrence. One of the most influential reviews, the 2001 Nuclear Posture Review (NPR), called for a redefinition of the strategic triad. Created during the Cold War, the long-standing strategic triad consists of intercontinental ballistic missiles, submarine-launched ballistic missiles, and bombers. In rethinking the needs of the nation's nuclear forces in an era far removed from the Cold War, the NPR panel recommended a transition to a new triad of nonnuclear and nuclear capabilities.

One leg of the proposed triad is a responsive infrastructure, part of which would be a responsive nuclear enterprise. This element would increase the capability of the National Nuclear Security Administration (NNSA) to respond quickly to unanticipated events such as the discovery of a technical problem in stockpile warheads or the rise of a new geopolitical threat.

The current NNSA nuclear enterprise is receiving heightened scrutiny from Congress to ensure the continued reliability and safety of the nation's nuclear weapons in a cost-effective manner. However, the enterprise—three laboratories, six plants, and the Nevada Test Site—is characterized by large and aging facilities and is faced with the need to support legacy warhead designs well beyond their originally projected lifetimes. Current estimates show that operating the NNSA's Life Extension Program to maintain old warheads at the numbers and rate currently planned is likely to exceed anticipated federal funding.

Clearly, to reduce the stockpile and transition to a new strategic triad, the U.S. must transform the current nuclear enterprise to

make it more responsive. Otherwise, the nation must continue keeping many warheads in reserve to guard against surprises.

Transforming the enterprise while meeting legacy stockpile obligations is difficult without sophisticated models to aid the planning process. Within NNSA, the need for a modeling tool to test future enterprise strategies had been under discussion for some time. Our vision at Livermore was to develop a tool that would accurately represent the flow of activities within the enterprise by incorporating accurate information such as financial, production, and stockpile data. In this way, NNSA managers could see more clearly how policy decisions might affect the enterprise. They could then optimize the transition from the present infrastructure to a more responsive one while maintaining important stockpile commitments.

As described in the article beginning on p. 4, physicist Cliff Shang led a small team to build such a model. The team combined differential equations with an enormous database of information to model in extreme detail how the NNSA enterprise functions. We have been rigorously verifying and validating the new model to ensure it accurately reflects the workings of the enterprise. In this way, the task parallels our testing of new Advanced Simulation and Computing Program codes for NNSA supercomputers, which model highly nonlinear phenomena such as nuclear weapon performance. In a similar manner, the NNSA enterprise is a highly nonlinear system because of its complicated, interdependent activities.

Our hope is that this model will help not only NNSA managers but also individual NNSA sites in their efforts to meet the goal of a smaller, more responsive enterprise that can support a properly sized stockpile with reliable, safe, and secure nuclear weapons. In a time of constrained budgets, we want to provide NNSA managers with the best tools to more quantitatively inform the decision-making process as they, working with NNSA laboratories and plants, chart a path for transforming the enterprise into the future. I believe this is one of them.

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

# Modeling the Future

*A computational tool aims to help the U.S. create a responsive nuclear enterprise.*

**N**UCLEAR weapons have been a cornerstone of U.S. national security since the early 1950s. As the nation adapts to the security threats of the 21st century, the role of these weapons is changing, as is the large nuclear complex, or enterprise, that was built to research, produce, and maintain them. A series of top-level studies and reviews at the Department of Energy (DOE), its National Nuclear Security Administration (NNSA), and the Department of Defense (DoD) has called for a smaller, more agile nuclear enterprise—one that can respond quickly to a sudden change in the geopolitical environment or a discovery of an acute technical problem in the nuclear stockpile. (See the **box** on p. 9.)

NNSA Administrator Linton Brooks says his goal is to have a “responsive nuclear enterprise that is resilient to unanticipated events or emerging threats.” This need becomes particularly important as the stockpile is reduced in accordance with the Moscow Treaty, which was signed in 2001. Brooks and other analysts note that the current stockpile was developed to counter the threat posed by the Soviet Union, the nation’s principal adversary during the Cold War. Weapon scientists designed warheads to maximize the yield-to-weight ratio so a missile or bomber could carry more than one. During the Cold War, aging warheads were regularly replaced when new designs became available, but today, no new ones are being developed. The current stockpile is being maintained past its planned lifetime, and certifying the performance and reliability

of these weapons is becoming a more difficult and costly challenge.

Nuclear weapons experts are considering several options to create the modern nuclear enterprise. For example, with the support of Congress, NNSA has begun the Reliable Replacement Warhead (RRW) Program. The program’s goal is to determine whether the U.S. could replace aging warheads with ones that are more easily manufactured and cheaper to maintain, without needing to conduct nuclear experiments to validate the design changes.

RRWs would be conservative designs with large performance

margins within the design parameters validated by past nuclear data, which are important for reliability. They also would include better safety and security features. The program requires that RRW designs remain within the military requirements of the existing stockpile as well as the test-validated parameters. Production of RRWs is intended to reduce the need for a sizable secure reserve and could lead to a stockpile with substantially fewer warheads.



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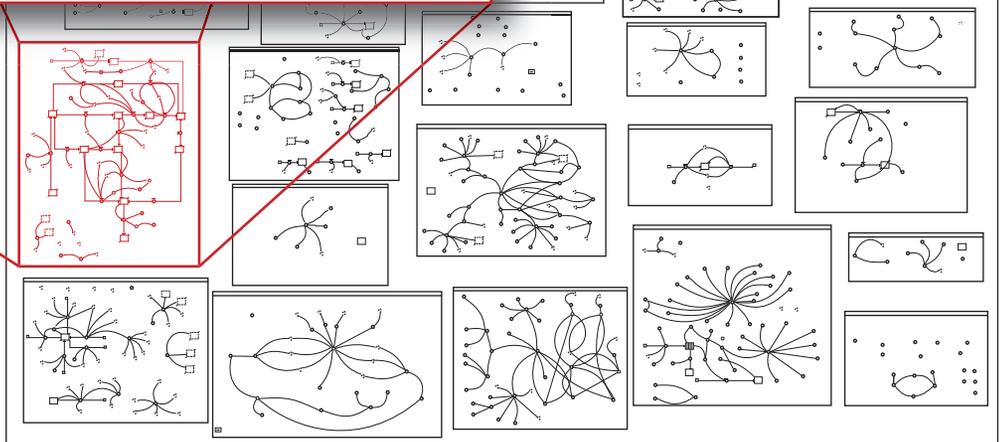
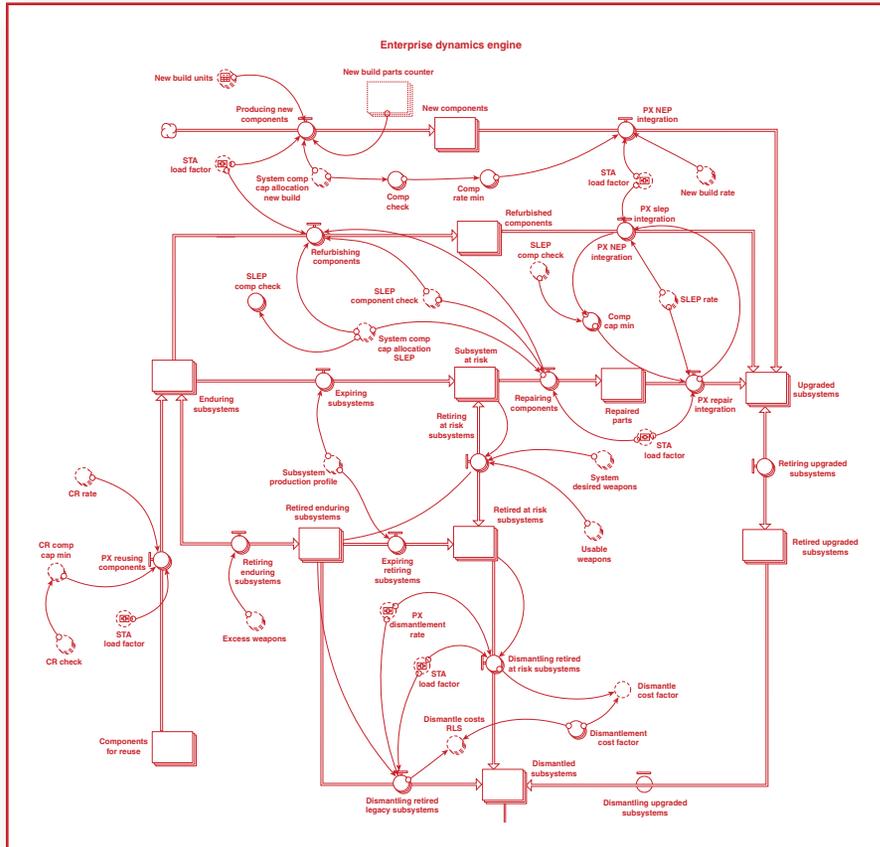
To help NNSA and individual sites evaluate such options, Cliff Shang, a physicist in Livermore's Defense and Nuclear Technologies Directorate, has developed a complex, classified tool

to model the nuclear enterprise. The code goes beyond the spreadsheets and isolated studies typically used in planning exercises. Instead, it takes a computational physics approach, using differential

equations tied to a large database to simulate proposed changes.

**Ideal for Testing Strategies**

"We're developing more quantitative tools to assist decision makers," says Shang. The Livermore model is ideal for testing strategies, finding inconsistencies, and discovering unanticipated consequences to policy options. The model couples knowledge of the stockpile with the functioning of the nuclear enterprise to capture how the enterprise really works. It can model the entire system to provide an overall view of NNSA's operations; focus on individual sites, such as a laboratory or production plant; or drill down to what Shang calls "the grubby details" of specific buildings or functionalities. The model is of interest to NNSA personnel with widely different responsibilities, including analysts who develop policies, facility



The Livermore model of the nuclear weapons complex, or enterprise, takes a computational physics approach to analyze planning options. Shown to the right is one-third of the logic diagrams that connect the differential equations describing the operations of the National Nuclear Security Administration's (NNSA's) enterprise. Above, a set of logic diagrams reveals the rich detail of warheads and components described by the equations.

managers who are concerned with building maintenance schedules, budget experts who track staffing projections, and transportation managers who are charged with delivering dismantled warhead components to the appropriate sites on schedule.

For example, the model allows users to view how fast the enterprise could respond, and in what ways, if requirements changed suddenly to address a geopolitical situation. It can also predict the effect that a severe technical problem might have on an NNSA program, and it can compare how levels of investments in the infrastructure will affect the responsiveness of the nuclear enterprise as a whole.

“Data by themselves are interesting, but they do not always show the big picture,” says Shang. “With our model, we can see realistic results to questions and hypotheses.” He notes that the model can help managers avoid making decisions that negatively affect seemingly unrelated processes. “We can change one element in a calculation and watch how it affects others. Isolated solutions may have unintended ripple effects, whether positive or negative.” One simulation showed that consolidating nuclear material in fewer buildings not only streamlined production operations but also simplified security requirements for the site. Shang is working with managers at DOE plants where nuclear material must be protected to help them plan for a more efficient yet more secure site.

In addition, the Livermore model incorporates DOE and federal policy directives. If managers run a simulation to consider the effects of building a new facility, construction outlays would increase, as expected. However, the model would also show increased spending for demolition and decontamination because DOE policy states that one square foot of old facilities must be removed for every square foot of new construction.

Designed for portability and extensibility, the model can be modified easily and the results viewed almost instantaneously on a desktop computer. Effects can be calculated out to two

decades or more. Users can also back-calculate 10 to 15 years to test the effects of strategies considered in the past.

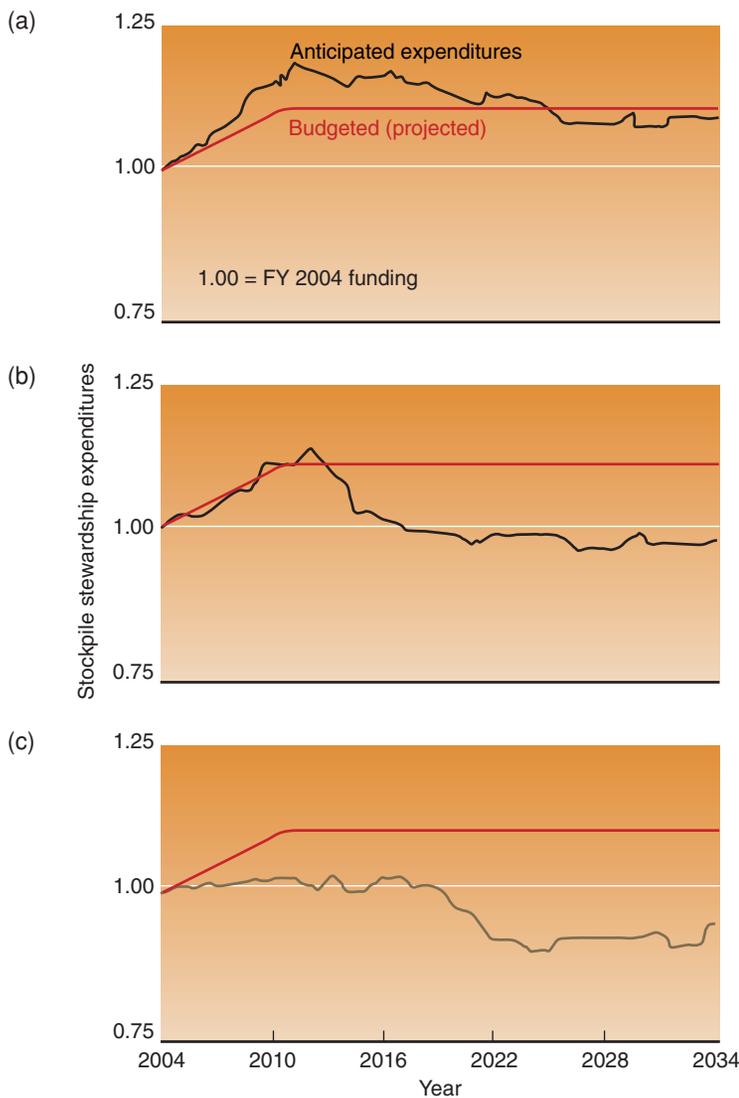
Shang notes that many businesses use complex models to determine the likely effects of strategic decisions. Similar models have been used to examine ways to improve U.S. health-care delivery and foresee how the nation would respond to an influenza pandemic.

**Work Started in 2004**

Work on the Livermore model began in April 2004. At that time, Vic Reis, former assistant secretary for DOE Defense

Programs and currently a consultant in the office of the Secretary of Energy, asked the Laboratory to help develop a method to evaluate options for transforming the nuclear enterprise. Reis met with Shang and other managers to sketch out how the nuclear weapons complex works in terms of governing equations. “I was anxious to get it started,” says Reis. “Cliff started from scratch, and we stayed in contact for six to eight months.”

Shang used system dynamics software to write a set of interlinking differential equations that describe the operations of the complex. Various Laboratory



The Livermore model shows how proposed changes to the nuclear weapons infrastructure will affect expenditures for stockpile stewardship. (a) The projected budget will not accommodate all of the proposed plans (new facilities, programs, and weapon dismantlement) in the first option. (b) The second option, which includes consolidating nuclear material storage at NNSA facilities, reduces anticipated expenditures. (c) The third option significantly reduces expenditures by implementing such programs as the Reliable Replacement Warhead Program.



Members of the model development team include (from left to right): Chris Brannan, Jeene Villanueva, Sharon Beall, Pauline Gu, Pat Sholl, and Cliff Shang, team lead.

experts contributed to the project, including a computational biologist, computer scientist, systems analyst, political scientist, budget analyst, and facility manager. The model's governing equations, similar to those called Lotka–Volterra equations, were originally developed to describe the dynamics of biological populations in which two species, such as predator and prey, interact. (Formulated independently by scientists Alfred Lotka and Vito Volterra in the 1920s, Lotka–Volterra equations are used to model ecological, social, and economic phenomena as well as chemical reactions and nucleosynthesis.)

To incorporate essential data and make the model as realistic as possible, Shang worked with all NNSA facilities and national laboratories to collect data on the stockpile, NNSA's various facilities, and their capabilities. For example, budget data include current costs and long-term projections for construction, demolition, decontamination, direct and indirect employee payrolls, and related expenses. Data on the Stockpile Stewardship Program describe refurbishment plans, production directives, and master schedules. Research, development, and testing data include details on Lawrence Livermore, Los Alamos, and Sandia national laboratories; the Nevada Test Site; and the production plants at Y-12, Pantex, Sandia, Savannah River, Kansas City, and Los Alamos. With this level of detail, users can drill down to study projects ranging from major facilities to utility upgrades at each site.

“Modeling the entire nuclear enterprise may seem like a daunting task,” says Shang “but Livermore people have extensive experience in building simulation codes and modeling complex systems.” He notes the toughest evaluators have been other Laboratory managers such as George Miller, associate director at large at Livermore and chairman of the Science and Technology Panel of the Strategic Advisory Group to U.S. Strategic Command (STRATCOM).



The Livermore model can access a large database with current information on NNSA's budget; the nation's nuclear weapons stockpile, including refurbishment plans and maintenance activities; recapitalization, demolition, and decontamination schedules; construction data, including comprehensive site plans; and program execution data, such as research and development capabilities and production capacity.

### High Marks from DoD Agencies

Shang has given presentations to managers at DOE, NNSA, and many NNSA facilities. He has also briefed managers at STRATCOM, the Defense Threat Reduction Agency (DTRA), and the office of the Secretary of Defense. The model earned high marks for thoroughness and utility, and Shang has received requests for specialized versions to help guide military agencies with their planning decisions. “What Cliff has done is remarkable,” says STRATCOM Manager Stan Gooch. “It allows senior managers

to see the impacts of policy options and budget decisions.”

STRATCOM and DTRA are collaborating with Livermore experts to develop a complementary model of the DoD enterprise. “Cliff’s model is of great interest not only to DOE but also to DoD,” says Peter Terrill, who leads the DoD Stockpile and Transformation Group. “His work has created an opportunity for a potential decision-making tool that can also incorporate the DoD nuclear infrastructure, which is a critical part of the picture that’s not well understood. As

a result, DoD is hopeful that Cliff’s work will help DOE and DoD get a holistic view of the joint nuclear enterprise, which is a critical aspect of the RRW Program.”

One of the model’s most useful applications is examining the ramifications of dismantling nuclear warheads. The U.S. currently has a large number of warheads in storage, many of them awaiting dismantlement. Although officials are working to reduce the backlog, NNSA does not have the integral capacity in facilities, budget, or personnel to accommodate warhead dismantlement

## Toward a Sustainable Stockpile

Military and policy analysts agree that the nuclear enterprise of the future should be safe and secure, affordable, and more responsive to change. The current stockpile consists of warheads developed during the Cold War, when the nation’s defense policy focused on the military might of the Soviet Union and Warsaw Pact nations. These warheads are designed to meet high performance criteria, including a high yield-to-weight ratio, but they are often difficult and costly to maintain and certify without nuclear testing.

Current plans are to maintain a stockpile of 1980s-produced warheads until about 2040. Some experts believe these plans strain the nuclear weapons production and certification infrastructure, making the nation ill-prepared to respond quickly to problems or changes in requirements. Although the plans preserve the nuclear weapons deterrent, a “ponderous and expensive enterprise [is] required to support old technology,” according to *Sustaining the Nuclear Enterprise—A New Approach*, which was written by scientists at Lawrence Livermore, Los Alamos, and Sandia national laboratories.

NNSA Administrator Linton Brooks cautions that the current stockpile was not designed for longevity. “Today, our aging nuclear weapons are being rebuilt in life extension programs that are both difficult and costly. Decisions made during the Cold War forced the use of certain hazardous materials that, in today’s health and safety culture, cause warheads to be much more costly to remanufacture. Maintaining the capability to produce these materials causes the supporting infrastructure to be larger and more complex than it might otherwise be.” He notes that small changes have been implemented over many decades, and stockpile warheads continue to evolve away from the designs originally tested underground at the Nevada Test Site. “The result is increasing uncertainty in the long-term reliability of warheads,” says Brooks.

Science-based stockpile stewardship, the nation’s program to keep the nuclear stockpile safe and reliable, has worked since its inception

10 years ago. Stockpile warheads have a documented nuclear test history, they are subjected to extensive surveillance, and issues have been addressed based on the results from nonnuclear experiments and advanced simulations. NNSA managers believe that a better long-term approach for a sustainable enterprise is to shift from a program of warhead refurbishment to one of warhead replacement.

To better evaluate this proposal, NNSA began the Reliable Replacement Warhead (RRW) Program. The goal of this program is to determine the effectiveness of replacing existing warheads with ones manufactured from materials that are more readily available and more environmentally benign than those used in current designs. Such changes would require that Cold War design constraints, which drove tight performance margins, be relaxed. These modified warheads would be much less costly to manufacture, their designs would include advanced safety technology, and their safety and reliability would be easier to certify. The proposed warheads could thus help NNSA achieve the goal of a more affordable, sustainable, and responsive nuclear enterprise.

Until the nation achieves a responsive infrastructure, it must retain a substantial number of nondeployed warheads to hedge against a technical failure of a critical warhead or delivery system or against an unforeseen threat. Establishing a responsive nuclear infrastructure, together with the RRW Program, would make possible additional stockpile reductions.

Says Brooks, “Success in realizing our vision for transformation will enable us to achieve over the long term a smaller stockpile, one that is safer and more secure, one that offers a reduced likelihood that we will ever need to test again, one that reduces NNSA and DoD ownership costs for nuclear forces, and one that enables a much more responsive nuclear infrastructure. Most importantly, this effort can go far to ensure a credible deterrent for the 21st century that will reduce the likelihood we will ever have to employ our nuclear capabilities in defense of the nation.”

while conducting its other key stockpile stewardship activities: the Life Extension Program (LEP), which refurbishes selected warheads; the Limited Life Component Exchange, which regularly replaces a few key components; and possibly, the RRW Program.

NNSA managers thus want to examine different levels of effort for the four tasks to determine how each mix would affect the complex. For example, if production begins on RRWs, the dismantlement effort would increase, and LEP activity would decrease. The model can also show how efficiencies in various RRW activities might affect the enterprise. It can then compare those projected expenditures with the life-cycle costs of selected warheads and the savings expected when expensive-to-maintain warheads are retired. The model could also delineate the effects of increased capacity if such a change is warranted.

**Incorporates Stewardship Tools**

NNSA has many existing and future stockpile stewardship capabilities and

facilities that can be used to transform the nuclear enterprise. The Livermore model helps managers determine the best use of those resources, such as the Advanced Simulation and Computing Program’s codes and supercomputers, which perform three-dimensional calculations to enhance safety and security; an improved physical properties database; and hydrodynamic, flight, and engineering tests. In addition, new facilities, such as the Dual Axis Radiographic Hydrodynamic Test Facility at Los Alamos and the National Ignition Facility at Livermore, are beginning to make important contributions. The model shows production delays if key facilities are not in use or must operate at reduced capacity. At the same time, it can indicate enhanced confidence in the stockpile as new resources become available and can show how stockpile stewardship tools help guard against technological surprise.

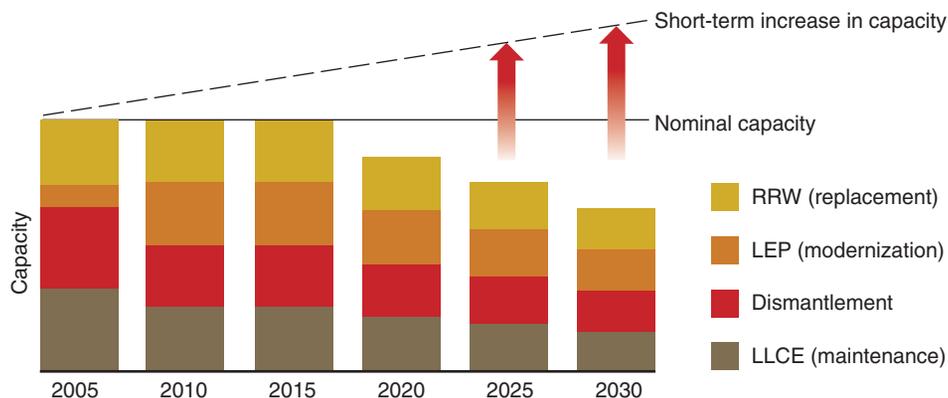
Nuclear weapons experts are working on a more complete model that combines both DoD and NNSA assets, data, and plans. The DoD components will include data on delivery systems, such as intercontinental

ballistic missiles, bombers, and submarines, as well as DoD operations, maintenance schedules, and planned acquisitions. “If the President says that because of a changing geopolitical situation, we must revise the nuclear weapons policy, our requirements for both warheads and delivery systems might change,” says Shang. “A combined DOE–DoD model will help decision makers determine how the two departments together can meet new or evolving policy directives.”

Reis successfully used system dynamics models to help explain the Fiscal Year 2006 Energy Bill as it advanced through Congressional committees. He is developing an even more comprehensive view of the nuclear enterprise that includes the weapons complex and the nuclear power industry. This model will examine the interrelationships between civilian and defense applications of nuclear energy and issues such as climate change and nonproliferation.

The Livermore model will continually be refined, expanded, and tailored to meet new user needs. Livermore physicists believe their modeling expertise, honed on physical systems as large as supernovae and as small as subatomic particles, can help managers plan for a more efficient and responsive nuclear enterprise, one based on a sustainable stockpile.

—Arnie Heller



Representative data show different model scenarios for stockpile stewardship activities, such as the Life Extension Program (LEP), which refurbishes selected warheads; the Limited Life Component Exchange (LLCE), which regularly replaces a few key components; warhead dismantlement; and the proposed Reliable Replacement Warhead (RRW) Program. The model can also project the effects from increasing capacity to respond to an unanticipated threat or a technical problem.

**Key Words:** Life Extension Program (LEP), Limited Life Component Exchange (LLCE), nuclear enterprise model, Reliable Replacement Warhead (RRW) Program, stockpile stewardship.

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# A Peculiar Burst of Stars

*Livermore astrophysicists find evidence that radio jets emitted from black holes give rise to new stars.*

**L**OOKING up to the vast expanse of the sky on a clear night, stargazers see a showy sparkle of planets, stars, and galaxies. And for every celestial body they can see, countless more escape view.

Advanced technologies allow today's astronomers to visualize heavenly bodies that past astronomers—from Hipparchus and Aristarchus to Galileo and Kepler—could not have imagined. However, even with the most powerful optical telescopes, they do not get the whole picture.

What they cannot see in this astral show are details of galaxies, supernovas, distant quasars, and other objects that emit electromagnetic radiation at wavelengths outside the region of visible

light. Many celestial objects emit radio waves—electromagnetic radiation with a wavelength much greater than that of visible light. (See the **box** on p. 13.) Scientists have found that by capturing the emitted signals with radio telescopes and studying the sky with optical telescopes, they can piece together a more complete picture of the astrophysical phenomena at work in the universe. (See the **box** on p. 15.)

Astrophysicists Wil van Breugel and Steve Croft at Livermore's branch of the University of California's Institute for Geophysics and Planetary Physics are using this radio astronomy technique to examine black holes and the gas jets

that emanate from them. Their research indicates that these radio jets may trigger the formation of new stars.

### Finding the Invisible

Van Breugel and his team are studying a starburst system called Minkowski's Object near the NGC 541 radio galaxy. This arc of perhaps 10 million stars, which spans 32,000 light years, may have originated in the warm, "clumpy" gas at the edge of the galaxy's radio jet. The idea that radio jets induce star formation is relatively new. Several decades ago, when astronomers discovered the first radio jet associated with a galaxy, they believed the

pairing was caused by a chance contact with an older galaxy. "Researchers had a lot of theories about what was going on but no evidence to support them," says van Breugel. Today, with optical charge-coupled devices and a new generation of powerful radio telescopes, scientists can acquire more detailed data, and this new evidence is helping to shape their conclusions.

In the late 1990s, van Breugel and his team developed an efficient method using radio sources to pinpoint extremely distant galaxies. In 2000, as part of a Laboratory Directed Research and Development (LDRD) project, they used this technique

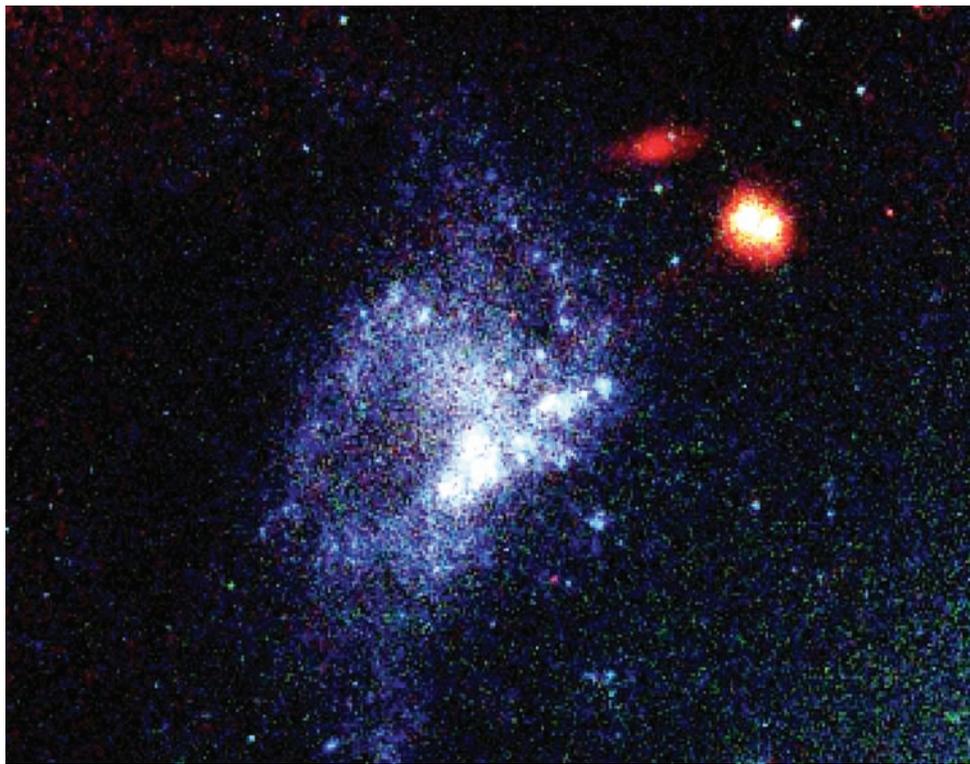
to find radio galaxies in the early universe. In the process, they discovered the most distant radio galaxy known to date—powered by an active black hole or quasar 12.4 billion light years away. With this method, researchers can investigate how galaxies form and determine the role played by supermassive black holes.

To examine the NGC 541 radio galaxy, van Breugel and Croft combined data from the Very Large Array radio telescope near Socorro, New Mexico; the Hubble Space Telescope (HST); and one of the twin telescopes operated by the W. M. Keck Observatory and located at the summit of Hawaii's dormant Mauna Kea volcano. NGC 541 is relatively close to Earth, at just 216 million light years away. Van Breugel and Croft wanted to determine if the peculiar burst of stars they had observed was a rejuvenated older galaxy or a completely newborn colony of stars.

Images and spectra of Minkowski's Object taken by HST and the Keck telescopes in both the infrared and optical regions indicate that the system contains young stars—a mere 10 million years old. Because of this finding and similar discoveries of jet-galaxy pairings, the collocation of Minkowski's Object and the radio jet no longer seems to be a chance happening. Researchers now believe that black holes and the radio jets that shoot out of them are likely triggering star formation.

### A Star Is Born

This star formation process, in which radio jets cause interstellar gas clouds to collapse and form new stars, is relatively rare today. But the phenomenon may have been more common and significant in creating galaxies in the early universe. Much more hydrogen gas would have been available then because relatively few stars and galaxies had consumed it earlier

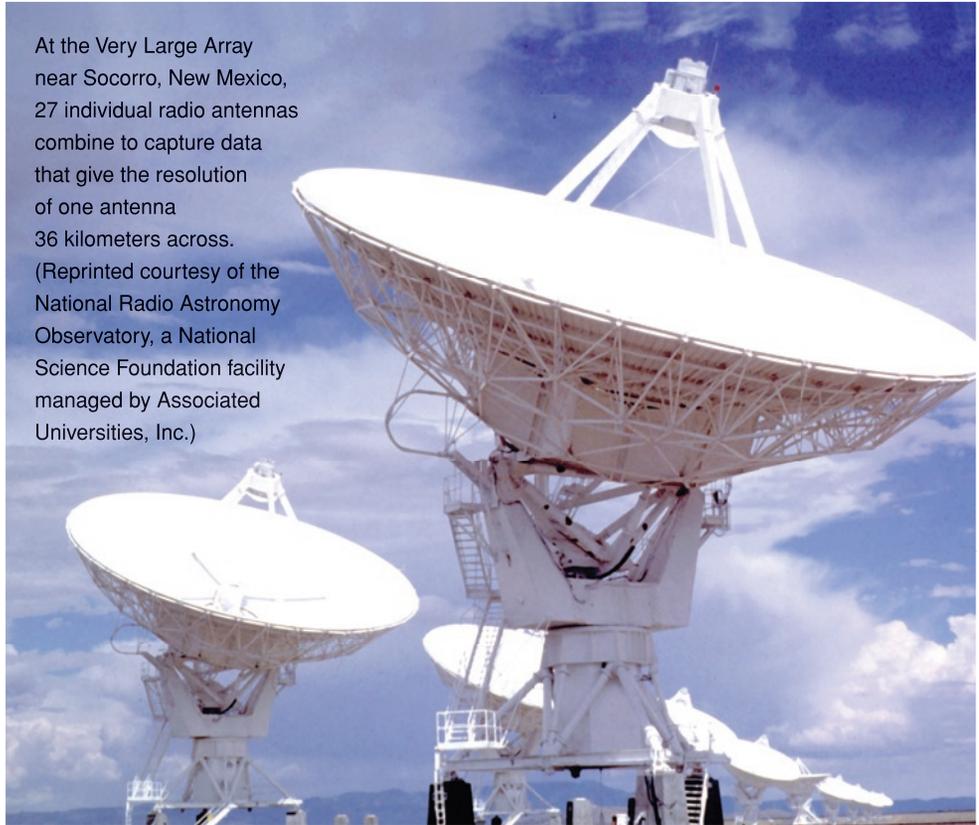


This false-color image of Minkowski's Object is a composite of three images—two taken in visible light by the Hubble Space Telescope (the blue and green channels) and one taken in infrared light by a telescope at the W. M. Keck Observatory (the red channel). The blue colors of the young stars in Minkowski's Object contrast with the older double star nearby and a faint background galaxy (red).

during their formation. Black holes were also more active. “This certainly isn’t the dominant way stars are formed,” says Croft, “but the conditions we observe around Minkowski’s Object do not appear to be exceptional.”

Normally, stars form from the collapse of cold, molecular gas clouds. When warm, dense gas is abundant in the interstellar medium—the region between stars—the violent matter and energy of the radio jets could collide with the gas, compressing the clouds and causing them to cool faster than usual. This cooling, in turn, hastens the process of star formation. Van Breugel’s observations of NGC 541 agree with this hypothesis. The team’s research shows that when a radio jet collides with warm, dense hydrogen near the parent galaxy, the medium begins to cool and forms a large neutral hydrogen cloud from which stars are subsequently born. Radio waves emitted by this cloud provide key data, but optical instruments cannot detect such long wavelengths.

At the Very Large Array near Socorro, New Mexico, 27 individual radio antennas combine to capture data that give the resolution of one antenna 36 kilometers across. (Reprinted courtesy of the National Radio Astronomy Observatory, a National Science Foundation facility managed by Associated Universities, Inc.)



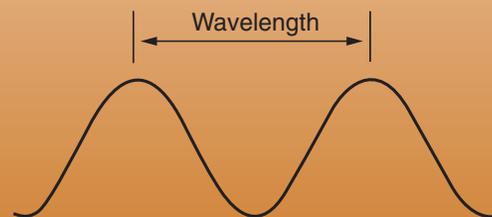
## The Electromagnetic Spectrum: From Radio Waves to Gamma Rays

Radio waves, visible light, x rays, and all the other parts of the electromagnetic spectrum are fundamentally the same thing. They are all types of electromagnetic waves, differing from each other only in wavelength. Wavelength is the distance between one wave crest and the next. The longest wavelengths are radio waves, which can be the size of buildings. The shortest—gamma rays—are smaller than the nucleus of an atom.

Electromagnetic waves also can be described by their energy and frequency, and these characteristics are related to the others in a precise mathematical way. Thus, when describing the spectrum, scientists may refer to the energy of an x ray or the wavelength of a microwave or the frequency of a radio wave.

Electromagnetic radiation also consists of photons. These massless particles travel in a wavelike pattern and move at the speed of light. Each photon contains a certain amount, or bundle, of

energy. The only difference between the various types of electromagnetic radiation is the energy of the photons, with radio waves at the low-energy end of the spectrum and gamma rays at the high-energy end.



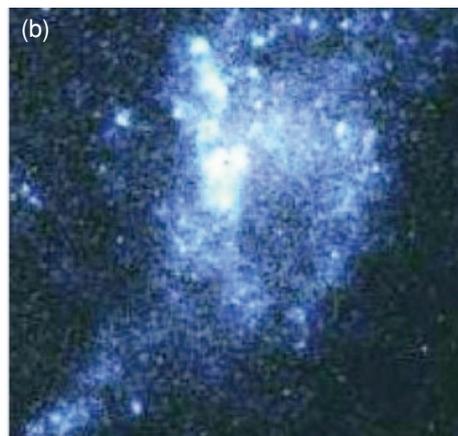
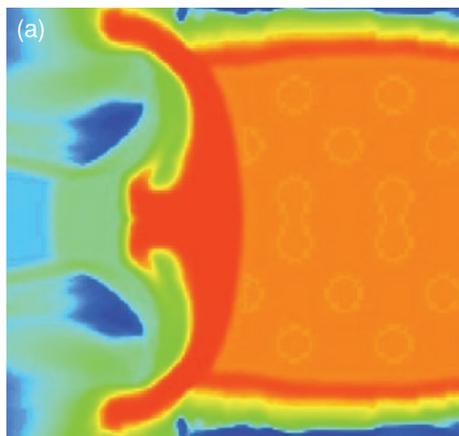
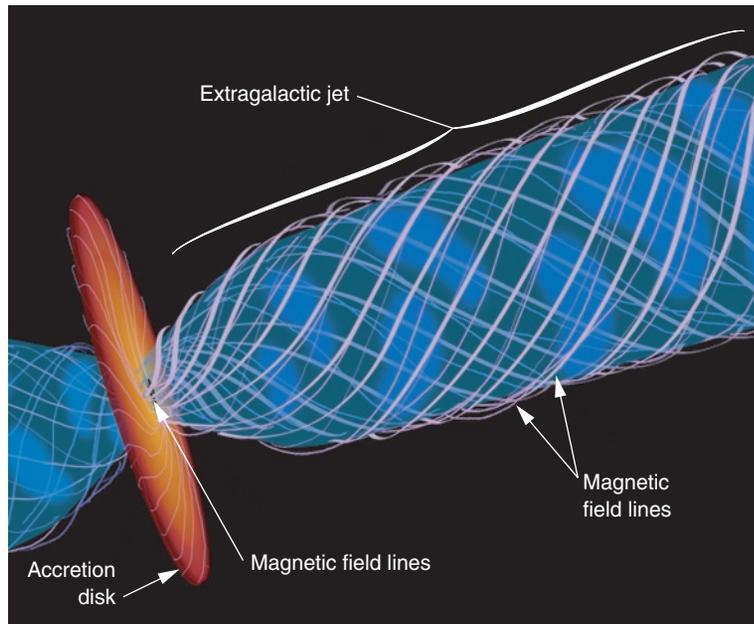
The distance between two adjacent wave crests of an electromagnetic wave is its wavelength.

### Black Holes: Give and Take

For van Breugel, the discovery that black holes can give as well as receive is poetic justice. “Twenty years ago, we would have thought this idea was

a fantasy,” says van Breugel, whose fascination with black holes goes back to the 1980s. “The fact that these big, bad black holes can actually give birth to new stars is exciting.”

Accretion disks rotating around black holes can be hundreds of light years across. The disk has a cold outer region and an ultrahot inner region and fuels black holes by feeding matter into them. Magnetic fields help collimate powerful radio jets that expel material from the accretion disk at high speeds.



A comparison of (a) an intermediate density distribution plot from numerical simulations with (b) a similarly scaled observation of Minkowski's Object shows clear similarities between the distribution of the postshock gas within the simulated cloud (red) and the regions of active star formation within Minkowski's Object.

Recent evidence shows that black holes are likely common objects at the centers of galaxies. A black hole is an object with so much mass concentrated in a relatively small area that its escape velocity—the velocity necessary for a nearby object to escape the hole's gravitational pull—is greater than the velocity of light. Thus, scientists reason, nothing near a black hole can escape its gravitational pull—not even light. Research suggests that black holes inhabiting the centers of powerful radio galaxies have billions of times the mass of the Sun and would fit within a space the size of the solar system.

Astrophysicists do not agree on the mechanisms involved when violent radio jets shoot out from the vicinity of a black hole. One leading theory involves the interaction of the magnetic fields generated by the accretion disks that rotate around supermassive black holes. An accretion disk is a giant ring of gas and dust and can be hundreds of light years across. The disk has a cold outer region and an ultrahot inner region that lies a few billion miles from the black hole. The accretion disk fuels the black hole by feeding matter into it. Through a process not fully understood, some gas in the disk is drawn out by magnetic fields, which creates the radio jets.

### Radio Astronomy at Work

“According to our astronomical observations,” says van Breugel, “energetic feedback by jets from active black holes can significantly affect the interstellar medium in galaxies in ways that had not been previously considered.” Most theories of galaxy evolution assume that this black-hole feedback will slow down or shut off star formation. Van Breugel and Croft found that active black holes might occasionally have a positive effect that enhances star formation.

To better understand this effect, van Breugel also investigated the effects of high-energy particles on interstellar dust grains that control the efficiency of the star-formation process. Working with Livermore colleagues from the Chemistry and Materials Science and Physics and

Advanced Technologies directorates, he began laboratory experiments irradiating interstellar dust analogs with high-energy particles.

Van Breugel notes that Livermore provides an excellent environment for the study of active black holes and their

role in forming galaxies. “Gaining an understanding of the relationship between the radio jets and star formation requires complex, multidimensional numerical simulations,” says van Breugel. He credits the computer modeling done with Livermore astrophysicist Peter Anninos’s

## Give Me Land, Lots of Land: A Radio Astronomy Primer

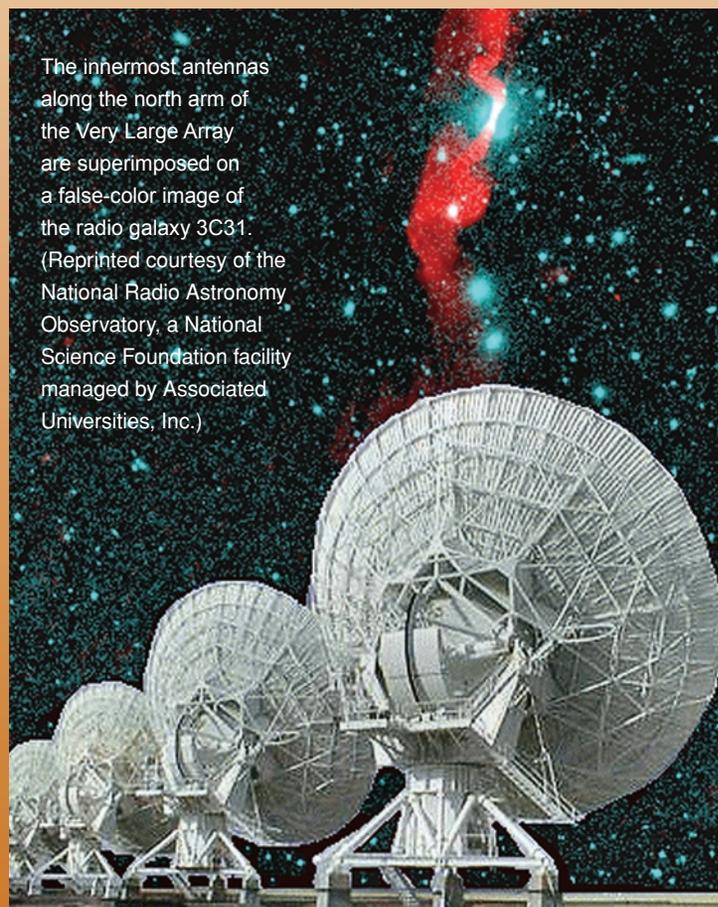
Radio waves penetrate much of the gas and dust in space and pass through the terrestrial atmosphere with little distortion. Radio astronomers can therefore obtain a much clearer picture of stars and galaxies than is possible by means of optical observation, as long as they emit at radio wavelengths.

Radio telescopes work in much the same way as optical telescopes. Just as optical telescopes capture the visible light emitted from celestial objects, radio telescopes capture the electromagnetic radiation in the radio wavelength region. Radio telescopes comprise a large radio antenna and a sensitive radio receiver. The most common radio telescopes, such as those that make up the Very Large Array (VLA) near Socorro, New Mexico, look similar in design to a satellite television dish. Because cosmic radio sources are so weak, the parabolic dish that captures the incoming radiation must be very large and the radio receiver, or radiometer, must be highly sensitive. Signal-processing techniques are used to detect astronomical radio signals that can be as much as a million times weaker than the noise generated in the receiver.

Because radio waves are so long, the best possible telescope to capture them would be, perhaps, many kilometers in diameter. The physical constraints of designing and constructing such an instrument are obvious. By using a technique called interferometry, astronomers can capture the same results by grouping many instruments at some distance from one another and having them work together as if they were one instrument. The VLA is just such a telescope system. Its 27 individual radio antennas capture data that can be combined electronically so that the array effectively functions as one giant antenna. Although each antenna is only 25 meters in diameter, the combined data from the antennas gives the resolution of an antenna that is 36 kilometers across.

The world’s largest and most powerful radio telescope to date is the Very Long Baseline Array (VLBA), a system of ten radio telescope antennas that are controlled remotely from the Array Operations Center in Socorro, New Mexico. The VLBA spans more than 5,000 miles with stations from Mauna Kea on the Big Island of

Hawaii to St. Croix in the U.S. Virgin Islands. Each station has a dish antenna 25 meters in diameter, as well as a control building housing a computer, tape recorders, and other equipment for collecting the radio signals captured by the antenna. The VLBA provides the sharpest vision of any telescope—optical or radio—on Earth or in space.



The innermost antennas along the north arm of the Very Large Array are superimposed on a false-color image of the radio galaxy 3C31. (Reprinted courtesy of the National Radio Astronomy Observatory, a National Science Foundation facility managed by Associated Universities, Inc.)

COSMOS code for much of the direction the work on jet-induced star formation has taken. (See *S&TR*, March 2003, pp. 4–11.)

COSMOS, a massively parallel radiation-hydrodynamics code developed at the Laboratory, is easily adaptable to probe astrophysical problems. The code has been used to simulate such events as the development of accretion disks in black holes and the evolution of the universe. A key simulation for van Breugel and Croft's research was to predict the chemistry of an environment after radio jets collide with the interstellar medium.

COSMOS incorporates 27 chemical reactions, including both collisional and radiative processes for atomic hydrogen and helium gases as well as molecular hydrogen chains. With it, scientists can simulate the dynamics of the cooling of the gas cloud, a critical step in star formation. "If warm gas cools and produces neutral

hydrogen that is dense enough, we should get star formation," says Croft. "The simulations showed that the presence of neutral hydrogen was, indeed, likely in the surrounding environment of Minkowski's Object, which was confirmed by our observations."

Both Croft and van Breugel point out that much more work is needed in the search to determine how the universe began. "It's not the end of the story," says van Breugel. "We have many complicated questions, and we'll need both observational data and simulations to find the answers."

For instance, van Breugel wants to use the COSMOS code to help determine the age of Minkowski's Object and the properties of the jets, which are relatively brief outbursts in the life of galaxies. "The only way to understand these things is to look at what's out there and figure out how jets interact with the interstellar medium," he says.

By combining computer simulations with both optical and radio astronomical techniques, van Breugel is certain that today's astrophysicists will find a few more answers and, certainly, many more questions for the next generation of scientists to pursue.

—*Maurina S. Sherman*

**Key Words:** accretion disks, black holes, COSMOS code, early universe, electromagnetic spectrum, gas clouds, Minkowski's Object, molecular hydrogen, nearby galaxies, NGC 541, neutral hydrogen, radio astronomy, radio emission, radio interferometry, radio jets, radio telescope, star formation, Very Large Array (VLA).

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# Exploring the Link between Diet and Cancer

**T**HE link between the human diet and cancer presents an intriguing puzzle for scientists. Research indicates that different foods and how they are prepared can increase a person's risk for cancer. Cooked muscle meats such as beef, pork, and fowl are one such food. They contain a class of tumor-causing mutagens called heterocyclic amines that target specific organs. For example, 2-amino-1-methyl-6-phenylimidazo[4,5-*b*]pyridine (PhIP), the most abundant mutagen produced in cooked foods, may cause tumors in the breast, prostate, and colon of laboratory animals. Scientists have yet to explain the connection, but a Livermore team funded by the National Cancer Institute is finding new evidence to solve this puzzle.

Led by biomedical scientist Kristen Kulp, the team is combining breast cell-based assays with computational modeling and nuclear magnetic resonance (NMR) to better understand the cell-growth process. This work is part of the Laboratory's ongoing research on diet and cancer, which is funded by the National Institutes of Health and the Department of Defense's Breast Cancer Research Program. Results from the team's experiments and simulations indicate that PhIP competes with the estrogen hormone estradiol, thereby disrupting the hormone's regulatory role in cell growth.

Livermore's studies of food mutagens are a spin-off from early efforts to understand the human health hazards of coal gasification and oil-shale retorting. Curiously, the chemical processes that occur when oil shale is heated are similar to those occurring when food is cooked, and both processes produce mutagenic arylamines. In the 1970s, the National Institute of Environmental Health, learning of the oil-shale project, asked the Laboratory to use its expertise to study food mutagens.

## An Attempt to Displace Estrogen

Heterocyclic amines form when amino acids, creatine (a chemical found in muscles), and sugar react at high cooking temperatures. Researchers have identified 17 heterocyclic amines that may pose a cancer risk in humans. Kulp's team is studying three of them—PhIP, 2-amino-3,8-dimethylimidazo[4,5-*f*]quinoxaline (MeIQx), and 2-amino-1,6-dimethylfuro[3,2-*e*]imidazo[4,5-*b*]pyridine (IFP)—as well as a PhIP metabolite called N<sup>2</sup>-hydroxy-PhIP.

PhIP is similar in structure to the hormone estradiol, which stimulates cell growth in the breast and other parts of the body

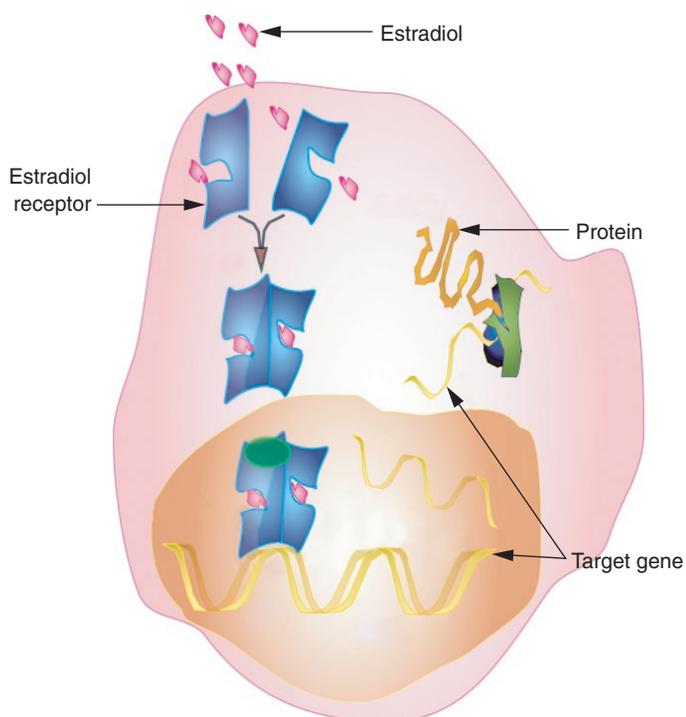
by binding to estrogen-receptor proteins. Estrogen receptors also modulate gene expression in the developing fetus and in adolescents as secondary sexual characteristics develop. Estrogen receptors belong to a class of proteins called nuclear receptors, all of which contain a ligand-binding domain. When estradiol binds to this domain in an estrogen receptor, it activates the receptor.

Two phases in the metabolic pathway of PhIP mimic that of estradiol. During the first phase, PhIP oxidizes into a hydroxylated intermediate, N<sup>2</sup>-hydroxy-PhIP. In the second phase, metabolizing enzymes convert N<sup>2</sup>-hydroxy-PhIP to a more biologically reactive form, generating esters that can bind DNA and cellular proteins. "The body converts heterocyclic amines into a water-soluble form that can be excreted," says Kulp. "The reactive compounds formed in this process can attach to DNA and cause mutations that are believed to lead to cancer. In addition to the cell damage caused through this pathway, we've also discovered that PhIP binds directly to the estrogen receptor and may play a role in regulating cell growth."

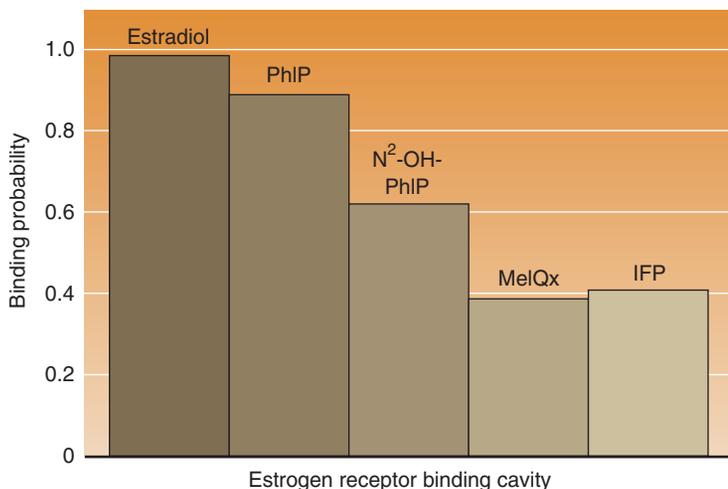
The team's results could explain the tumor specificity in certain organs. Direct binding to the estrogen receptor's ligand-binding domain may promote cancer. "When PhIP activates the estrogen receptor and related cell-growth pathways, it may enhance the damage by accelerating the rate at which mutated cells duplicate," says Kulp.

## Simulating the Positions of Molecules

To study potential binding interactions between heterocyclic amines and the estrogen receptor, Kulp's team generated models



The hormone estradiol stimulates cell growth in the breast and other parts of the body by binding to an estrogen-receptor protein. Estrogen receptors also modulate gene expression in the developing fetus and in adolescents during puberty.



Computational analysis shows the probability that three heterocyclic amines and one metabolite will compete with estradiol at the estrogen-receptor binding cavity. PhIP = 2-amino-1-methyl-6-phenylimidazo[4,5-*b*]pyridine; MelQx = 2-amino-3,8-dimethylimidazo[4,5-*f*]quinoxaline; and IFP = 2-amino-1,6-dimethylfuro[3,2-*e*]imidazo[4,5-*b*]pyridine. N<sup>2</sup>-hydroxy-PhIP is a PhIP metabolite.

on the Laboratory's Multiprogrammatic Capability Resource supercomputer, which can process 11 trillion operations per second. With high-resolution simulations, researchers can observe, in hours or days, the numerous positions the heterocyclic amines may assume relative to the estrogen receptor. By contrast, experiments would take months or even years to produce the same data.

For the modeling studies, the team obtained a structure for the estrogen receptor from the Protein Data Bank, an international repository for protein structures. Team members set up a control model by calculating the position coordinates of estradiol in the estrogen receptor's ligand-binding domain. They then used an algorithm to specify the number of docking, or binding, steps they wanted to observe and compared positions for PhIP, N<sup>2</sup>-hydroxy-PhIP, IFP, and MelQx with those for the control model.

The team's calculations showed that PhIP attaches directly to the estrogen receptor's ligand-binding domain. However, the probability of it doing so is less than that for estradiol. In addition, N<sup>2</sup>-hydroxy-PhIP is oriented in the same docking position to the estrogen receptor as PhIP, but N<sup>2</sup>-hydroxy-PhIP does not compete with estradiol for binding. Computational biologist Brian Bennion explains, "To compete with estradiol in the estrogen-receptor binding cavity, a heterocyclic amine or its metabolite must have the same orientation and arrangement of atoms. The hydroxy atoms in N<sup>2</sup>-hydroxy-PhIP are not arranged in a way that would make it as easy as it is for PhIP to bind at the estrogen-receptor site. The other heterocyclic amines we examined, MelQx and IFP, have three fused heterocyclic rings in their molecular structure, which limits interactions even more."

### Tuning into a Molecule's Frequency

Experiments with NMR spectroscopy—one of the experimental methods used to determine protein structure for the Protein Data Bank—confirmed the simulation results that PhIP binds to the estrogen-receptor protein. With NMR, a molecule's nuclei will resonate to a unique radio frequency, providing physical, chemical, electronic, and structural information about the molecule. Livermore researchers have developed methods that use NMR in competition assays to study whether molecules compete for the same binding location on a protein.

Determining whether PhIP competes with estradiol for the estrogen receptor's ligand-binding domain was particularly challenging. "Estrogen receptors are sensitive proteins," says physical chemist Monique Cosman, who leads the Biomolecular NMR Group at Livermore. "For example, if we shake them or try to concentrate them, they will aggregate and form a precipitate, making it impossible to collect data." Another challenge is that some proteins are only active in a high-salt environment, but PhIP and estradiol are only soluble in a 100-percent organic solvent, such as dimethyl sulfoxide (DMSO). The two environments are compatible only at less than 5-percent DMSO.

To ensure that precipitate did not form, the team used low concentrations of estrogen receptor, PhIP, and estradiol and extended the run times for the NMR experiments. “A typical NMR experiment uses a sample concentration that is 100 to 1,000 times greater than we used,” says Cosman. “To adjust for the low concentrations, we ran the experiments for four days to increase the number of scans collected. Then we averaged them over time to increase the signal-to-noise ratio. With this approach, we detected, for the first time, that PhIP and estradiol do in fact compete for binding in the same site on the estrogen receptor.”

When examined with NMR, small molecules such as PhIP exhibit a weak, positive signal called the nuclear Overhauser effect (NOE). The much larger estrogen-receptor protein exhibits a strong, negative NOE signal. If a small molecule binds to a protein, the characteristics of the NOE for the protein will be transferred to the small molecule.

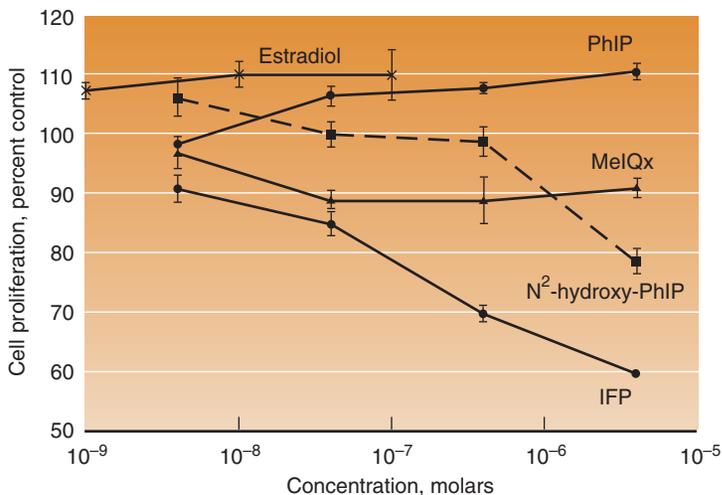
Adding PhIP to the sample solution changed the NOE signal for PhIP from positive to negative, indicating that PhIP was bound to the estrogen-receptor protein. When estradiol was added, the signals reverted to weakly positive. This change indicated that estradiol competitively displaced PhIP and that both ligands were binding to the same site on the protein. The NMR data thus confirmed the computational results that PhIP binds to the same site on the estrogen-receptor protein but not as strongly as estradiol.

### Increased Growth of Cancer Cells

The Livermore team also examined whether heterocyclic amines influence cell proliferation. Using *in vitro* assays, researchers compared cells treated with a heterocyclic amine to untreated cells. This study indicated that treatment with only PhIP increases cell proliferation in human breast-cancer cells up to 40 percent and almost doubles estrogen-receptor activity compared with the activity in untreated cells. Results from the cell assays are consistent with those from the computer simulations, which predicted that the probability of PhIP binding to the estrogen receptor is almost as high as that of estrogen. In contrast, the cellular assays demonstrated that N<sup>2</sup>-hydroxy-PhIP, MeIQx, and IFP inhibit estrogen-receptor activation, also consistent with the team’s simulations.

One explanation of these results is that the binding mechanism for MeIQx and IFP differs from that for PhIP and N<sup>2</sup>-hydroxy-PhIP. MeIQx and IFP may even bind in other regions of the estrogen-receptor protein that somehow prevent activation.

Kulp notes that the concentrations of PhIP examined by her team are orders of magnitude higher than what a single cell might be exposed to after a meal of cooked meat. However, prolonged exposure to PhIP over a lifetime may add to the total estrogenic burden on the body. In addition, the biological consequence of exposure to heterocyclic amines may differ when they are



Assays of breast-cancer cells show that adding PhIP increases cell proliferation, as does the estrogen hormone estradiol, which regulates gene growth. In contrast, adding MeIQx, IFP, and N<sup>2</sup>-hydroxy-PhIP do not increase proliferation.

combined with other foods. Previous Livermore studies showed that the cooking method also affects the formation of the different heterocyclic amines. (See *S&TR*, July 1995, pp. 6–25; September 1995, pp. 6–23; April 2001, pp. 4–11.)

The Livermore researchers are evaluating the possible benefits of soy and green tea to determine if exposure to such foods will inhibit the activation. They also want to expand their NMR research to examine other heterocyclic amines and hope to conduct additional studies on PhIP. “We have good evidence now that PhIP can bind to the same site as estradiol,” says Cosman. “Next, we’re planning studies to directly map its orientation at the binding site.”

By demonstrating through experiments and simulations that PhIP can activate estrogen receptors and stimulate breast-cancer cell proliferation, the Livermore team is helping to determine how dietary constituents may affect the growth of hormone-sensitive cancers. More importantly, better understanding of these mechanisms may lead researchers to develop potent therapeutics for treating breast cancer.

—Gabriele Rennie

**Key Words:** 2-amino-1,6-dimethylfuro[3,2-*e*]imidazo[4,5-*b*]pyridine (IFP), 2-amino-3,8-dimethylimidazo[4,5-*f*]quinoxaline (MeIQx), 2-amino-1-methyl-6-phenylimidazo[4,5-*b*]pyridine (PhIP), estradiol, estrogen-receptor protein, food mutagen, heterocyclic amine.

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# When Lightning Strikes at Site 300

**L**OCATED 29 kilometers east of Livermore, the Laboratory's Site 300 houses experimental facilities for explosives testing and research. One safety issue affecting operations is the frequent thunderstorms that occur in the Altamont Hills. The staff at Site 300 tracks weather systems in the area, and safety procedures include different levels of lightning alerts, up to and including halting work on explosives and evacuating personnel. Each alert day could reduce the efficiency of the site's operations. To better protect employees and facilities, a team of electrical engineers has developed a certified protection system that eliminates the need for costly work stoppages and building evacuations.

## Flash Facts

Lightning is random, unpredictable, and dangerous. It occurs when rapidly rising air in a thunderstorm interacts with rapidly falling air to create widely separated positive and negative charges within a cloud. The electrical current in a flash averages about 25,000 amperes and can go up to 400,000 amperes. Voltages can be hundreds of millions of volts, and the air ionized by a flash can reach nearly 28,000°C, more than four times the temperature on the surface of the Sun.

In the most common type of cloud-to-ground lightning, negative charges emerge from the bottom of a cloud and create ionized channels, called stepped leaders. The leaders' strong electric field induces streamers of positively charged ions to develop at the tips of grounded pointed objects, such as lightning rods, trees, and blades of grass. The streamers flow upward and join the negatively charged leaders, creating a pathway to the ground. A pulse of current, called a return stroke, travels through the streamer object and up the ionized channel to the charge center within the cloud. Additional negative discharges, called dart leaders, often move down this ionized path, thus forming subsequent return strokes.

## The Explosive Connection

According to the National Lightning Safety Institute, some 2,000 ongoing thunderstorms around the world cause about 100 cloud-to-ground strikes each second. Site 300 averages 50 alert days per year based on data from the last 3 years, and each alert may reduce the efficiency of operations. No strikes to Site 300 facilities have been verified, but lightning has struck nearby power poles and lines and the open ground.



Personnel and facility safety is always the top priority in operational planning at Site 300. In analyzing the work procedures during thunderstorm alerts, Cal Dibble, a project manager in Livermore's Plant Engineering Department, believed the operations could be improved. He proposed to investigate structural improvements at the site and worked with a team of Livermore engineers to develop and certify a lightning protection system.

"In the past, we depended on lightning rods attached to buildings," says Livermore engineer Mike Ong, who researches electrical safety. When used on a wooden structure, lightning rods will guide a current along the path of least resistance—down the metal pole or wire and into the ground. However, lightning rods are not as effective with typical explosives facilities, which have rebar in the walls and ceiling.

Work involving explosives is of particular concern during lightning storms. The safety limit for currents flowing through some detonators is less than 1 ampere, but peak lightning currents may hit tens of thousands of amperes. Therefore, a critical part of the lightning protection system is to separate explosive components from the current-conducting objects and possible arcs from objects in a room.

To do that, the Livermore engineers want each room, or cell, to act like a Faraday cage and shield the components inside the room from lightning strikes outside. In an ideal world of frictionless surfaces and massless springs, the Faraday cage would be a solid metal shell of perfectly conducting metal. If the outside of this ideal cage were struck by lightning, currents and electric fields would be conducted down the outside surface of the shell to the ground, never reaching the shell's interior surface. In the real world, buildings or rooms can only approximate a Faraday cage, and measurable fields and currents will leak inside the structure. Faraday cages prevent internal arcs by minimizing the electric fields within a cage.

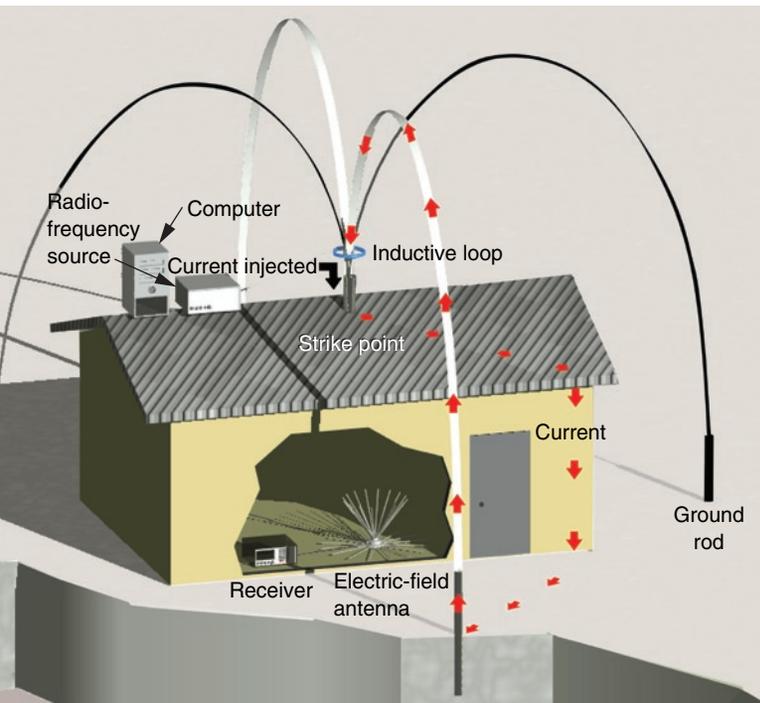
"A car's metal frame approximates a Faraday cage," says Ong, "so being inside a car can be a fairly safe place during a lightning

storm, as long as the person inside stays away from the ‘shell’ of the car. At Site 300, we want to design rooms so most of the electric fields from a lightning strike will remain outside the building and not penetrate enough to create an arc of current that can reach an explosive.”

### Re-creating a Bolt from the Blue

To determine each facility’s Faraday-cage effectiveness, Livermore engineer Todd Clancy worked with Dibble and others to measure the conducting capability of each wall in a room. Most buildings at Site 300 are made of concrete reinforced with metal rebar, which provides a pathway for a lightning current to travel to the ground. Moisture absorbed by the concrete also acts as a conductor, drawing current down the wall into ground. The reinforced concrete thus creates a Faraday-cage effect for those buildings.

However, any metal that penetrates a structure’s wall, such as a water pipe or phone line, provides an alternate pathway for the currents and fields to enter a building. To retain the integrity of the Faraday cage, electricians bonded these metallic structures to the building’s rebar, so that all of the conducting material is interconnected.



For the Site 300 experiments, wires connected grounded rods to likely strike points at the top of the building being tested. Milliampères of current were inductively injected through the strike point and driven through the facility’s ceilings and walls to the ground. The current then traveled through the ground rods and back through the wires.

Clancy then conducted experiments to determine the potential currents and electric fields that a lightning strike might generate inside each cell. For these experiments, wires connected likely strike points at the top of a building to metallic rods driven into the ground around the facility. Milliampères of current with a frequency range similar to that of lightning were injected inductively through the strike point. A broadband antenna measured the fields at various points along the wall and in the center of the cell. A probe was used to measure the currents injected at likely strike points.

The current was driven through the facility’s ceilings and walls to the ground, and then it traveled through the ground rods and back through the wires. “The voltages produced were generally highest at the ceiling and the top of walls and lowest at the foot of the wall and on the floor,” says Clancy.

Team member Charles Brown ran the experimental data through signal-processing calculations to extrapolate the measured currents to lightning-strike proportions. “First, we used experimental data to compute a wall’s impedance, which relates the wall’s floor-to-ceiling voltage to the injected current,” says Brown. “Then using signal-processing techniques, we extrapolated the wall’s response to that of a current of lightning-strike proportions and computed the necessary standoff distance.”

Even when the standoff distance is doubled to increase the safety margin, it is about 15 centimeters from the wall. Standoff lines are then painted on the floors of each room, and all explosives components must be located inside the painted lines before a building can be certified for lightning protection. “This requirement mitigates the danger of an electrical arc hitting the explosive,” Brown says. “Our team is very conservative in determining standoff distances.”

### Certification and Staying Safe

According to Clancy, the team has certified most of the appropriate facilities at Site 300, and personnel are being trained. With this certified protection system, the facilities do not have to shut down under threatening conditions, which will save the Laboratory close to \$250,000 a year.

Now, when the thunder rolls, employees at Site 300 can continue their jobs, knowing that they and the explosives inside the buildings are safe from any bolts from the blue.

—Ann Parker

**Key Words:** explosives, Faraday cage, hazard management, lightning, signal processing, Site 300, workplace safety.

**For further information contact Charles G. Brown (925) 423-4435 (brown207@llnl.gov).**

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

## Patents

### **Method and System for Optical Figuring by Imagewise Heating of a Solvent**

**Michael C. Rushford**

U.S. Patent 6,936,182 B2

August 30, 2005

This system provides a method for imagewise etching the surface of a substrate, such as thin glass, in a parallel process. When the substrate surface is placed in contact with an etching solution, the etch rate increases with increasing temperature. Local thermal gradients are then generated individually in different regions of the solution's boundary layer to imagewise etch the substrate surface in a parallel process. In one configuration, a local heating gradient is produced at selected locations chosen from an indexed array of addresses. A computer processor can then activate each address independently and specify the etching rate for each region. An interferometer can also be included to monitor the system's progress in real time over the entire surface area and deterministically control the computer processor.

### **Tapered Laser Rods as a Means of Minimizing the Path Length of Trapped Barrel Mode Rays**

**Raymond J. Beach, Eric C. Honea, Stephen A. Payne, Ian Mercer, Michael D. Perry**

U.S. Patent 6,937,636 B1

August 30, 2005

The maximum trapped path length of a barrel mode can be dramatically reduced by tapering the diameter of a flanged barrel laser rod over its length. This design limits the ability of the trapped spontaneous emission to negatively affect laser performance through amplified spontaneous emission. Laser rods with polished barrels and flanged end caps are being used in diode-array end-pumped laser systems to confine diode-array pump light. In these systems, the pump light can be introduced into one or both ends of the laser rod and ducted down the length of the rod via the total internal reflections that occur when the light strikes the rod's barrel. However, such rods are susceptible to barrel mode paths that can trap spontaneous emission over long path lengths. If this trapped spontaneous emission is then amplified through stimulated emission, the stored energy available to the desired lasing mode can be effectively depleted, which will affect the laser's performance. The trapped spontaneous emission can be reduced by introducing a taper onto the laser rod.

### **Creating Ensembles of Decision Trees through Sampling**

**Chandrika Kamath, Erick Cantu-Paz**

U.S. Patent 6,938,049 B2

August 30, 2005

This system for decision-tree ensembles includes modules to read and sort data, evaluate a potential data split according to some criterion using a random sample of the data, split the data, and combine multiple decision trees in ensembles. The decision-tree method is based on statistical sampling techniques and includes the steps for each module.

### **Carbon Nanotube Array Based Sensor**

**Christopher L. Lee, Aleksandr Noy, Stephan P. Swierkowski, Karl A. Fisher, Bruce W. Woods**

U.S. Patent 6,946,851 B2

September 20, 2005

This sensor system has an electrode with an array of carbon nanotubes and a second electrode, both of which are positioned with an air gap between them. A measuring device senses changes in electrical capacitance between the first electrode, which has the carbon nanotube array, and second electrode.

### **High Stroke Pixel for a Deformable Mirror**

**Robin R. Miles, Alexandros P. Papavasiliou**

U.S. Patent 6,947,188 B2

September 20, 2005

This mirror pixel can be fabricated using standard microelectromechanical systems-based methods for a deformable mirror. The pixel is electrostatically actuated and is capable of the high deflections needed for spaced-based mirror applications. In one configuration, the mirror has three layers: a top mirror layer, a middle layer consisting of flexures, and a comb-drive layer. The flexures of the middle layer are attached to the mirror and comb-drive layers, and the comb drives are attached to a frame via spring flexures. Several mirror pixels can be used to construct a large mirror assembly. The actuator for the mirror pixel may be configured as a crenellated beam with one end secure or as a scissor jack. The mirror pixels may be used in various applications requiring high-stroke adaptive optics.

### **Cylindrical Microlens with an Internally Reflecting Surface and a Method of Fabrication**

**Raymond J. Beach, Barry L. Freitas**

U.S. Patent 6,948,341 B2

September 27, 2005

This high-numerical-aperture cylindrical microlens, which includes an internally reflective surface, will deviate light from its original propagation direction. The fast microlens can be used in optically conditioning laser diodes, laser diode arrays, and laser diode bars.

### **Biomedical Nuclear and X-Ray Imager Using High-Energy Grazing Incidence Mirrors**

**Klaus-Peter Ziock, William W. Craig, Bruce Hasegawa,**

**Michael J. Pivovarov**

U.S. Patent 6,949,748 B2

September 27, 2005

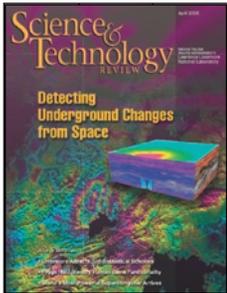
This approach for imaging radiation sources located in a subject is being considered for various medical applications. The approach uses grazing-incidence optics to form images of radiopharmaceuticals administered to a subject. These are true-focusing optics; that is, they project a real and inverted image of the radiation source onto a detector possessing spatial and energy resolution.

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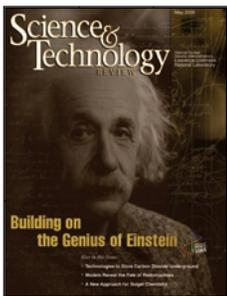
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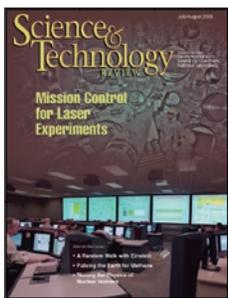
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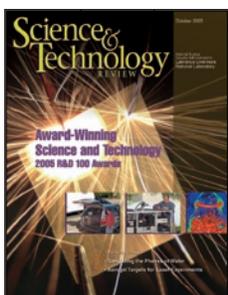
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### Modeling the Future

A Lawrence Livermore team has developed a complex classified tool to help the National Nuclear Security Administration (NNSA) and individual NNSA sites evaluate options for transforming the nuclear weapons complex, or enterprise. The code takes a computational physics approach to simulate proposed changes to the enterprise. Differential equations connect to a large database with detailed information on weapons in the stockpile and the many facilities that design, build, and maintain them. NNSA managers can use the model to test strategies, find inconsistencies, and discover unanticipated consequences to policy options. The model can provide an overall view of NNSA operations, or it can focus on individual sites. A complementary model is being developed for the Department of Defense.

**Contact:**  
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### A Peculiar Burst of Stars

Astrophysicists in the Livermore branch of the University of California's Institute for Geophysics and Planetary Physics are combining computer simulations with optical and radio astronomical techniques to better understand how stars form. In this project, the team used data from the Very Large Array radio telescope in New Mexico, the Hubble Space Telescope, and telescopes at the W. M. Keck Observatory in Hawaii. COSMOS, a computer code developed to simulate high-energy physical processes for Livermore nuclear physics research, provided simulations of the astrophysical events. The team's research focused on a starburst system called Minkowski's Object near the NGC 541 radio galaxy, which is 216 million light years from Earth. Research results indicate that the radio jets emanating from black holes may trigger the formation of new stars.

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# The Mystery of Crystal Formation



Livermore scientists are closer to understanding how nature grows crystals.

#### *Also in January/February*

- *Simulating materials at the nanoscale helps scientists design nanodevices.*
- *Real-time measurements of plutonium as it is created in a nuclear reactor are now possible with an antineutrino detector.*
- *Livermore engineers push the limits to fabricate and measure superprecise laser targets.*

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