June 1999

Science & Technology REVIEW

U.S. Department of Energy's
Lawrence Livermore
National Laboratory

Catching the Drift of Atmospheric Hazards

Also in this issue:

- Modeling Detonation Details
- Collaboration Ignites Laser Advances
- Predicting Material Performances through Multiscale Models

About the Cover

Lawrence Livermore's Atmospheric Response Advisory Capability (ARAC) was founded in the 1970s to predict the atmospheric dispersion of radioactivity from nuclear incidents. Today, its ability to simulate the transport and fate of a variety of atmospheric releases makes it a valuable resource for emergency planning and response. One such hazardous release—a dense cloud of oil-laden smoke from a recent tire fire in Tracy, California—is pictured on the cover. Our report on ARAC accomplishments and on how its codes model atmospheric releases begins on p. 4.

Photograph by: Enrique Gutierrez, *Tracy Press*

About the Review

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

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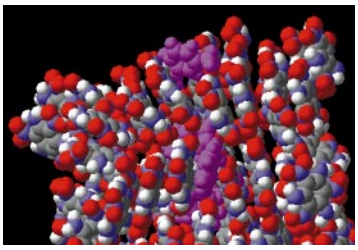

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Photograph by: Enrique Gutierrez, *Tracy Press*

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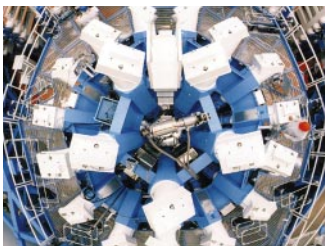

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Fission and antimatter created by Lab laser

Lawrence Livermore researchers recently reported to the centennial meeting of the American Physical Society in Atlanta, Georgia, that they had used the world's most intense and powerful laser, the Petawatt, to generate a hot, short-lived fireball of energy that produced antimatter and stimulated nuclear fission in a millimeter-thick target.

Physicist Tom Cowan teamed with colleagues from the Laser Programs Directorate, National Aeronautics and Space Administration's Marshall Space Flight Center, the University of Alabama, Harvard University, and the GSI laboratory in Germany to produce the surprising results.

Cowan described the research as opening the door to the world of "photonuclear physics," in which science that once was the province of huge particle accelerators can now be approached through "a new, high-energy regime of laser–matter interactions."

The research team believes that it may be possible in the future to create ultrabright and detailed stroboscopic images of nuclear and atomic structures—and possibly even of proteins—by using powerful x rays and gamma rays created by bouncing extremely short laser pulses off oncoming streams of electrons.

Contact: Thomas Cowan (925) 422-9678 (cowan3@llnl.gov).

Using radar for the right spin

A recently tested Laboratory radar technology aims to speed up rotor-blade balance adjustment and dramatically reduce maintenance costs for U.S. Marine and Navy V-22 Osprey helicopters.

The radar device, which uses microwave impulse radar technology, was successfully tested on mock V-22 Osprey rotor blades at Bell Helicopter's Ground Test Article Facility in Arlington, Texas, in early April.

"We were able to successfully demonstrate that this system meets the U.S. Navy's requirements," said electrical engineer Tom Rosenbury, group leader of the Laboratory's Microwave Impulse Radar Program. "Now we're ready to test the radar system on a real aircraft."

The technology is expected to save up to $45 million in maintenance costs over the life cycle of each $41-million V-22 helicopter.

Placed in the wing beneath a helicopter rotor, the device emits short-duration ultrawideband pulses upward toward the rotating blades. Pulses are reflected by a small section of the blade as it passes over the radar. The transit time of pulses to and from the moving blades is measured, allowing the vertical distance to be calculated with great accuracy. If the rotor blades are not tracking within a required tolerance band, rebalancing may be necessary to prevent damage to the rotor or excessive transmission vibration.

Contact: Tom Rosenbury (925) 423-7510 (rosenbury1@llnl.gov).

Small-scale fusion with big promise

A team of researchers at Lawrence Livermore has created tiny fusion explosions with a compact laser in experiments that could lead to new methods for detecting hidden flaws in materials.

Using a laser so compact that it could fit on a large table, the researchers, led by physicist Todd Ditmire, blasted deuterium (heavy hydrogen) gas generated in a vacuum chamber with flashes of high-intensity laser light. These experiments produce fusion reactions similar to but much smaller than the explosions of hydrogen bombs or in the sun.

According to Ditmire, the experiments offer no path toward the long-sought goal of creating an inexhaustible supply of fusion energy, nor are they related to the sensational and widely discredited cold fusion claims made a decade ago by Utah chemists.

Instead, the experiments are basic physics research into how short, intense pulses of light interact with small clusters of atoms and cause the clusters to collide against each other randomly. The clusters are transformed into highly compressed, superheated exploding balls of electrically charged gas that emit clouds of subatomic particles called neutrons.

The goal of the research, Ditmire says, is to devise ways of increasing the yield of the fusion neutrons so that the particles can be used as probes, much as x rays are, to investigate defects in materials ranging from metals to human tissue.

Contact: Todd Ditmire (925) 422-1349 (ditmire1@llnl.gov).

Squeezing a gas into a solid

In a recent issue of *Science* magazine, Livermore researchers report that they have transformed carbon dioxide into a polymeric solid with a structure like that of quartz by squeezing it at high temperatures and pressures.

Physical chemist Choong-Shik Yoo, leader of a high-pressure physics group at the Laboratory, and his colleagues synthesized the new extended-solid phase by heating carbon dioxide in a diamond anvil cell with a laser to temperatures above 1,800 kelvins and pressures above 40 gigapascals (400,000 times atmospheric pressure).

Spectrographic analysis indicates that each carbon atom is bonded to four oxygen atoms, yielding a three-dimensional network like that of the quartz polymorph of silicon dioxide. Once formed, the quartzlike carbon dioxide remains stable at room temperature and pressures above 1 gigapascal.

The researchers hope to isolate the new material soon at ambient pressures. Its thermal conductivity is expected to be "very high, just like diamond's," says Yoo, noting that it is also "a good candidate for a superhard material."

Contact: Choong-Shik Yoo (925) 422-5848 (yoo1@llnl.gov).

The Future of Atmospheric Emergency Response

LAWRENCE Livermore's Atmospheric Response Advisory Capability (ARAC) is a formally recognized national emergency response service for real-time assessment of atmospheric releases involving nuclear, chemical, biological, or natural hazardous material. Within minutes to hours of a release, ARAC can map the probable spread of contamination and the resulting exposure. Given this information, emergency managers decide what, if any, action is necessary.

As the article beginning on p. 4 reports, ARAC's primary function is to support the Department of Energy and the Department of Defense for radiological releases. Under the Federal Radiological Emergency Response Plan, it also assists several other federal agencies and, with the approval of DOE, it supports local, state, and international agencies' responses to natural and anthropogenic releases. Since 1979, ARAC has supported more than 900 exercises and over 160 alerts, accidents, and disasters involving radiological and chemical releases.

ARAC's expert staff of 40, its validated three-dimensional atmospheric dispersion modeling system, and its state-of-the-art emergency operations center are the leading resources for analyzing and forecasting the fate of nuclear materials inadvertently or intentionally released into the atmosphere. ARAC's operations with their rapid response to real events distinguish it from similar efforts nationally and internationally.

In recent years, national security concerns have expanded beyond nuclear to include chemical–biological releases. Potential ARAC applications range from accident response to countering terrorism threats. Emphasis has been increasingly placed on meeting the needs of the in-field first responder. Desired services and capabilities continue to stress rapid initial response and depth of available backup expertise, but they now also include stand-alone predictions, mobile support teams, and network-based communication.

We have taken several steps to prepare the ARAC program to meet these new challenges. Through reorganization, we have coordinated ARAC and the DOE Chemical and Biological Nonproliferation Program (CBNP) efforts. The CBNP is developing the capability to predict the fate of chemical–biological releases both outdoors and indoors (for example, in buildings and subways). Its main focus is the prediction of airflow and dispersion in an urban environment—an environment where the presence of extremely heterogeneous surface features in a small area makes modeling a challenging problem. The effort is developing computational fluid-dynamics models to simulate the flow and dispersion of releases around and through building complexes. By coordinating this chemical–biological research with the operational ARAC program, we expect to prototype in the coming years a planning, training, and ultimately, emergency-response assessment capability for urban chemical–biological releases.

ARAC modernization is providing additional capabilities to help facilitate the program's current and future roles. To open ARAC services to potential new clients such as additional federal agencies, local emergency managers, and field personnel, we are developing Web-based network communications to the ARAC central system. These will allow simultaneous access by multiple emergency response agencies to ARAC's incident characterization and assessment products during an actual event.

We are also developing an ARAC interface to Lawrence Livermore's high-performance computers to provide real-time local meteorological and dispersion forecasts, detailed vulnerability and mitigation assessments, and accurate predictions of the dispersion and ultimate fate of chemical and biological agents released into the complex urban environment. Finally, to further enhance the value and utility of our plume forecasts, we are developing new visualization tools for analysis and interpretation, including demographic and critical infrastructure displays.

Our vision for the future is simple. We want to be a national center for atmospheric release assessments used by federal, state, and local agencies as they plan for and respond to hazardous atmospheric releases. We expect to realize this vision in collaboration with other organizations offering complementary services and capabilities. In doing so, we will strive to offer the right tools at the right time for users at the local, state, federal, level and international levels, be they research and development experts, emergency managers, or first responders.

■ L. W. Younker is acting Associate Director, Earth and Environmental Sciences.

Forewarnings of Coming Hazards

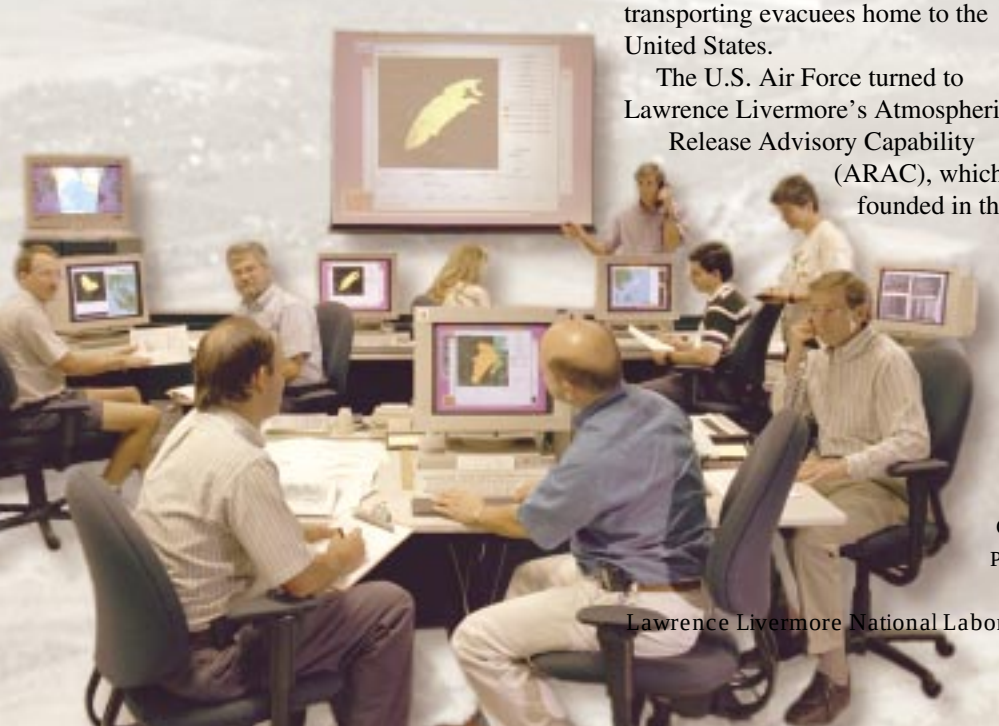
Modeling atmospheric emergencies is the business of Livermore's Atmospheric Release Advisory Capability. As ARAC stands on call to assist with present-day atmospheric threats, it anticipates and prepares for future ones.

THE call for help came from halfway around the world. In the Philippines, Mount Pinatubo was erupting cataclysmically, spewing volumes of ash into the atmosphere. Strong, high-altitude winds were transporting the clouds of ash over the South China Sea into Southeast Asia, India, and beyond. Continuing eruptions darkened the sky over the Philippines, blanketing the area with ash and bringing most activity to a standstill. Worse yet, monsoon storms converted some of that ash into a flood of mud that descended on numerous villages. Evacuating U.S. military personnel and dependents at Clark Air Base and Subic Naval Base became imperative. But first, the volcanic ash plumes had to be tracked, so that safe flight paths could be planned for the military aircraft transporting evacuees home to the United States.

The U.S. Air Force turned to Lawrence Livermore's Atmospheric Release Advisory Capability (ARAC), which was founded in the late 1970s to predict the dispersion of radioactivity into the atmosphere during nuclear accidents, threats, attacks, and terrorist incidents. The Air Force was presenting a problem of quite a different sort, one that fit well within ARAC's capabilities. ARAC scientists expanded three-dimensional atmospheric models up into the jet stream and beyond—to an altitude of over 100,000 feet (Figure 1). For five days, they simulated the complex and divergent ash clouds and predicted its movement two days into the future, thus helping pilots dodge ash clouds that could damage aircraft engines and instrumentation.

Providing Emergency Readiness

ARAC is one of many emergency response organizations sponsored by the U.S. government to counter dangers and threats to the nation. Over the years, its charter to simulate radionuclide dispersion from nuclear incidents has expanded to include working with all manner of toxic and hazardous releases. ARAC today can predict the transport and fate of material released during disasters, whether natural or caused by human activity. ARAC makes



An emergency response team at Lawrence Livermore's Atmospheric Release Advisory Capability's Emergency Operations Center mobilizes to model an atmospheric release. Pictured (clockwise from top right) are: Ron Baskett, Fernando Aluzzi, Connee Foster, Jim Ellis, John Pace, Brent Bowen, Phil Vogt, Mike Bradley, and Brenda Pobanz.

Lawrence Livermore National Laboratory

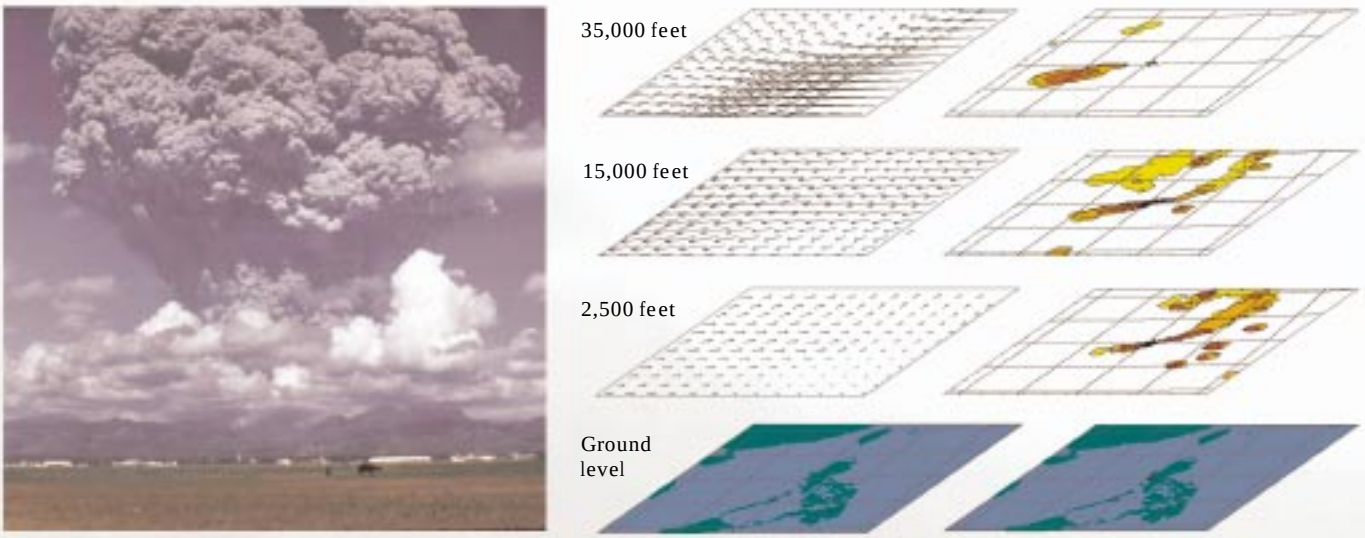


Figure 1. When Mount Pinatubo in the Philippines erupted in June 1991, the complex three-dimensional atmospheric structure of the region produced dramatically divergent ash-cloud patterns. Meteorologists from Livermore's Atmospheric Release Advisory Capability Center developed extensive daily analyses and forecasts of the ash-cloud positions two days into the future.

predictions not only during atmospheric releases but also for contingency planning purposes, before a potential one might occur. ARAC conducts detailed postevent analyses as well.

The organization has evolved considerably since the first atmospheric dispersion estimates were made in the 1960s. Then, scientists at Lawrence Livermore were engaged in the Plowshare Program, an effort to use nuclear technology for civilian and commercial purposes. Projects such as excavating harbors and canals with nuclear explosives required estimates of the path of radioactive particles that could be lofted into the atmosphere.

The first rudimentary Plowshare calculations determined only the speed and direction of radioactive dispersion. But they were enough to cement the idea that tracking radionuclides was a useful and necessary task. In ensuing nuclear-related projects, the Laboratory's atmospheric scientists continued to improve methods and approaches for nuclear dispersion calculations and used the tools as part of efforts to contain radioactivity from underground nuclear tests. The calculations demonstrated a nascent, useful capability and led to funding for an operational system in the late 1970s and ultimately for the organization that is today's ARAC. Fortuitously, ARAC was scheduled to be up and running two days after the accident at Three Mile Island.

The Department of Energy provided ARAC with its first funding. Later, in the mid 1980s, the Department of Defense also became a major funder, enabling a major expansion and automation of the system. Both DOE and DoD wanted the system to be networked so that it could provide aid during atmospheric release emergencies to an increasing number of their facilities around the U.S. By 1988, ARAC served over 70 government sites.

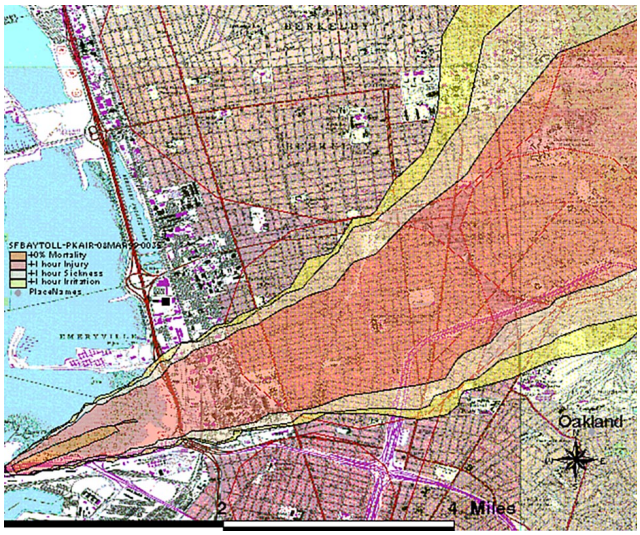
Improving with Experience

For two decades, ARAC has benefited from experience gained during more than 160 alerts and incident responses. For example, in providing assistance during the 1986 Chernobyl accident in the former Soviet Union, ARAC had to enlarge its models to handle continental-to-hemispheric scales. Subsequently, the group expanded its meteorological, terrain, and mapping data to cover Earth. The large volume of data prompted improvements to ARAC's computer systems and software to increase throughput and reduce response time.

ARAC also advances its capabilities through continuous training exercises, simulating emergency atmospheric release scenarios several times a week in cooperation with supported sites and

agencies. In an exercise performed in March 1999, the organization supported the U.S. Navy in its Fleet Battle Experiment—Echo to test new technologies and tactics for combating terrorist attacks. ARAC scientists modeled chemical attack scenarios in Oakland and San Francisco and delivered simulation results in minutes to the command ship, the USS *Coronado*. They collaborated with Livermore's Nonproliferation, Arms Control, and International Security scientists, who created a Web browser interface to allow Navy personnel on board the *Coronado* to tap into the ARAC system easily. With information provided by the *Coronado*, ARAC simulated two attacks: a truck explosion that released chlorine at the San Francisco–Oakland Bay Bridge toll plaza and a release of sarin (a nerve gas) north of Pier 35 from an airplane flying across San Francisco Bay. The results (Figure 2) allowed the *Coronado*'s medical staff to understand the progression and concentration of the chemical plumes and therefore advise where to best deploy emergency services.

(a)



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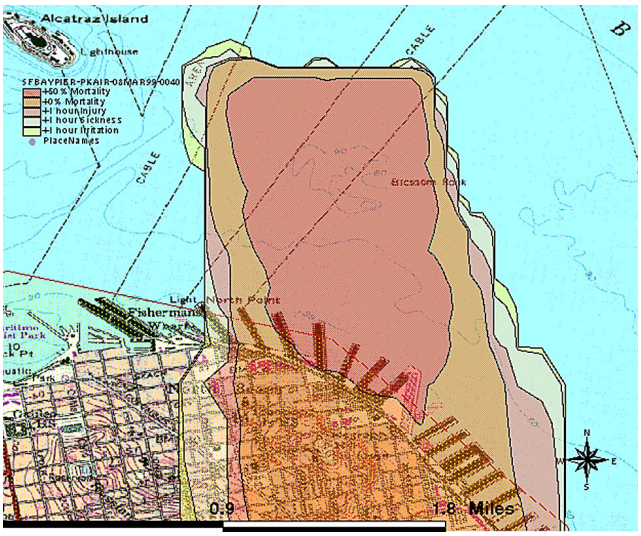


Figure 2. During a recent U.S. Navy emergency response training exercise, ARAC scientists were called on to simulate (a) a chlorine release following a truck explosion at the San Francisco–Oakland Bay Bridge toll plaza and (b) a release of sarin north of Pier 35 in San Francisco from an airplane flying over San Francisco Bay. Simulations such as these tell emergency response personnel where to best deploy emergency medical services.

Dealing with Complexities

Simulations of the atmospheric dispersion of hazardous gases, aerosols, or particulates start with information about the release: its location and time and the initial size of the cloud or mechanism of the release. To this data, atmospheric modelers must add information about the processes that play a role in dispersing, transforming, and depositing the material. Different meteorological factors are important in modeling a release, depending on its magnitude and type.

Initially, the wind speed and direction at the release location control the plume's path. Accurately determining the winds at the accident site is paramount to producing a credible result. If the release involves a powerful explosion or fire, the winds thousands of feet above the ground may determine the plume's transport, and its vertical extent may be limited by a temperature inversion in the atmosphere. As the plume travels downwind, turbulence dilutes the plume by mixing the material vertically and horizontally, which the modeler must estimate. In addition, local wind systems (such as sea breezes) or terrain may change the plume's path. Mountain ridges can block flows, and valleys are channels for winds. Furthermore, material may be removed from the plume by being deposited on the ground or washed out by precipitation.

The ARAC Emergency Response Modeling System (Figure 3) accounts for these effects through the use of a series of codes that represent the third-generation modeling system in ARAC's 20-year history. The first code, GRIDGEN, draws on a terrain database with a 500-meter resolution covering

most of the globe to develop the underlying terrain and numerical grid for the area where the dispersion occurred. The second code, ADAPT, creates three-dimensional wind fields using worldwide meteorological data obtained from on-line links to the Air Force Weather Agency or weather forecasts from the U.S. Navy and the National Oceanic and Atmospheric Administration.

If the event needs to be projected several days into the future, ARAC may run its own version of the Navy's Coupled Ocean–Atmosphere Mesoscale Prediction System model to generate detailed wind data. Based on terrain and weather descriptions, ADAPT approximates the local wind velocities (interpolating more detail when actual measurements are sparse) and then adjusts the winds to account for the influence of the topography. For example, it might show how hills deflect the oncoming wind flow and how wind is channeled through passes.

LODI, the third code, simulates the release, transport, diffusion, and deposition of a release by using numerical marker particles, that is, the positions in space representative of the released material. Finally, a graphics code converts the data to plots of interest, such as doses for radiological accidents, air concentrations for chemical releases, or ground deposition. The plots are displayed on a map of the model domain.

The ARAC system can model problems of any scale anywhere in the world. Versatile and accurate, its models are ranked in the top tier of atmospheric dispersion models in use throughout the world. But the models must be supplemented by scientific expertise and experience. The variety, complexity, and data limitations of atmospheric dispersion problems challenge all modeling systems. Thus, it takes an experienced atmospheric

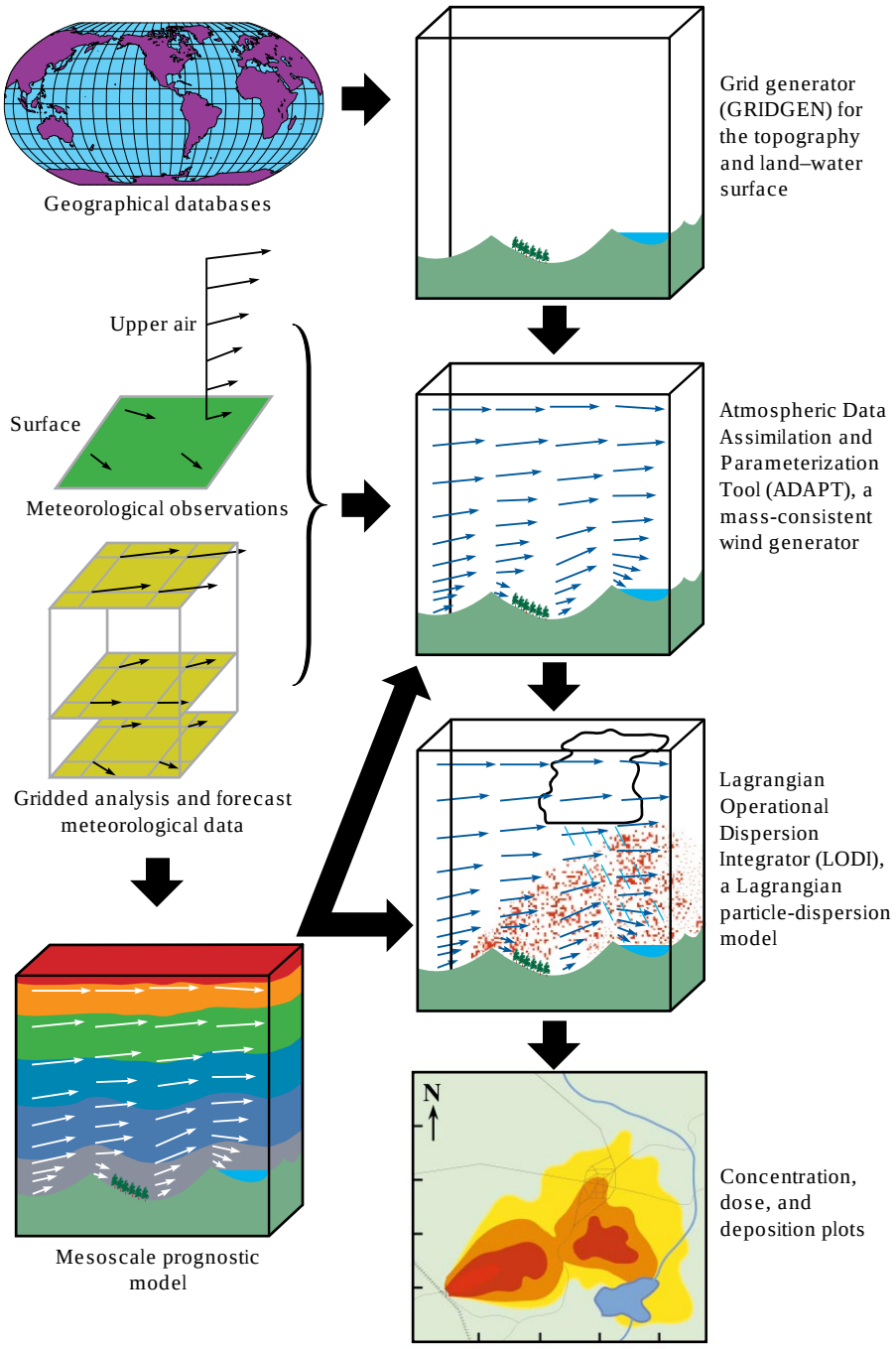


Figure 3. The series of codes in the ARAC Emergency Response Modeling System accounts for physical processes that affect the dispersion of hazardous material in the atmosphere. Taking terrain information from a database, GRIDGEN develops the topographical grid for the area of interest. ADAPT uses observed and forecasted weather data to develop three-dimensional wind fields and adjusts them to account for the influence of topography. LODI simulates the release, transport, diffusion, and deposition of particles.

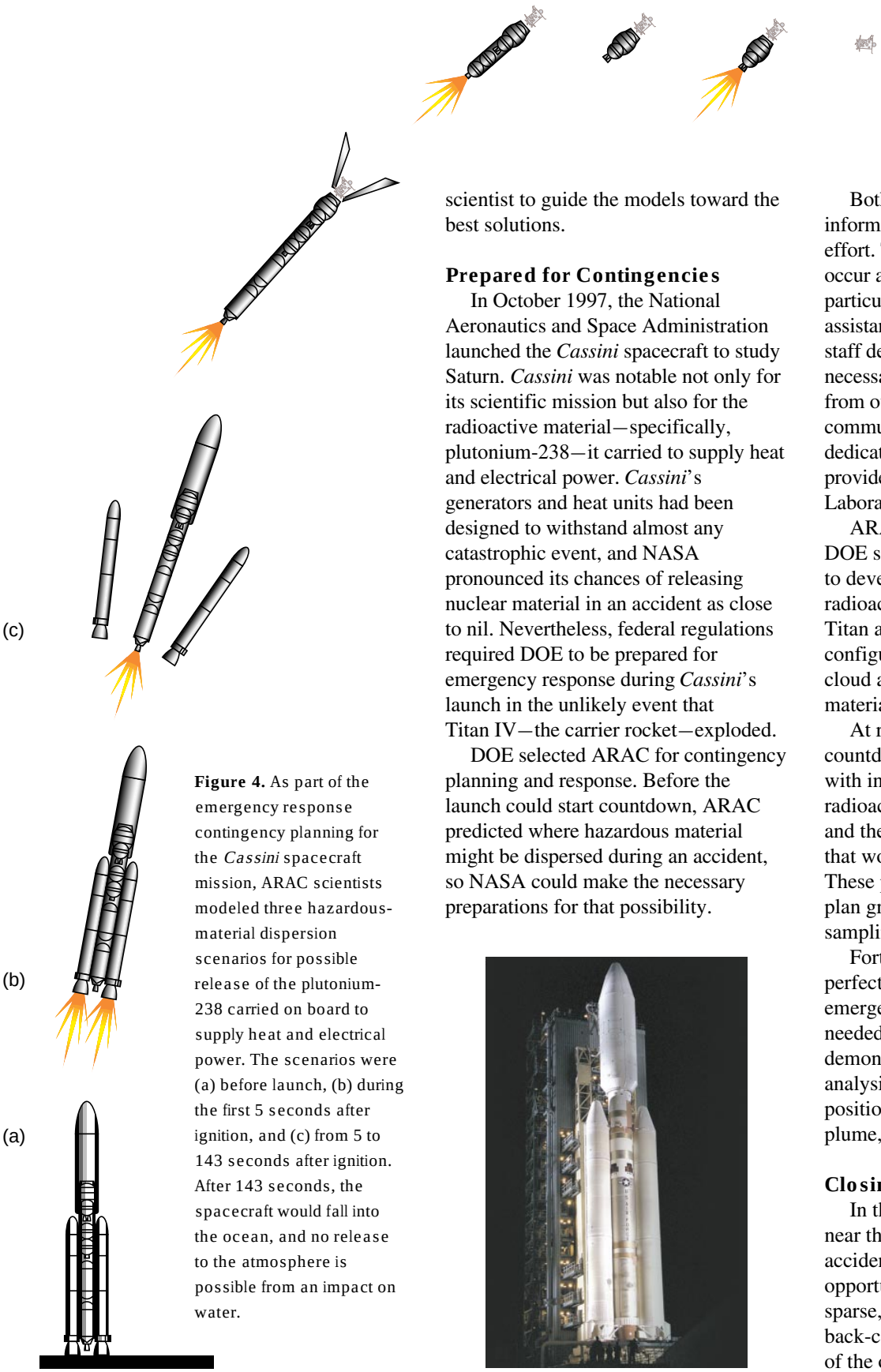


Figure 4. As part of the emergency response contingency planning for the *Cassini* spacecraft mission, ARAC scientists modeled three hazardous-material dispersion scenarios for possible release of the plutonium-238 carried on board to supply heat and electrical power. The scenarios were (a) before launch, (b) during the first 5 seconds after ignition, and (c) from 5 to 143 seconds after ignition. After 143 seconds, the spacecraft would fall into the ocean, and no release to the atmosphere is possible from an impact on water.

scientist to guide the models toward the best solutions.

Prepared for Contingencies

In October 1997, the National Aeronautics and Space Administration launched the *Cassini* spacecraft to study Saturn. *Cassini* was notable not only for its scientific mission but also for the radioactive material—specifically, plutonium-238—it carried to supply heat and electrical power. *Cassini*'s generators and heat units had been designed to withstand almost any catastrophic event, and NASA pronounced its chances of releasing nuclear material in an accident as close to nil. Nevertheless, federal regulations required DOE to be prepared for emergency response during *Cassini*'s launch in the unlikely event that Titan IV—the carrier rocket—exploded.

DOE selected ARAC for contingency planning and response. Before the launch could start countdown, ARAC predicted where hazardous material might be dispersed during an accident, so NASA could make the necessary preparations for that possibility.

Both real-time and forecasted weather information were crucial to the modeling effort. The complex wind patterns that occur around Cape Canaveral are particularly challenging to simulate. With assistance from the Air Force, ARAC staff deployed in Florida obtained the necessary real-time meteorological data from over 40 locations and communicated it to Livermore using dedicated circuits via a field satellite unit provided by DOE's Remote Sensing Laboratory from Las Vegas.

ARAC scientists used NASA and DOE safety studies on rocket explosions to develop the initial conditions for a radioactive release from a potential Titan accident. The studies predicted the configuration of the explosion or fire cloud and the status of the radioactive material (Figure 4).

At regular intervals during the launch countdown, ARAC provided NASA with information on the potential radioactive dose to affected populations and the amount of radioactive materials that would be deposited on the ground. These plots would have been used to plan ground-level and airborne plume sampling, had that become necessary.

Fortunately, *Cassini*'s launch was perfect, and the preparations for emergency response support were never needed. Nevertheless, they demonstrated a timely and effective analysis capability for predicting the position and course of a hazardous plume, should an accident ever occur.

Closing in on the Source

In the extreme southern tip of Spain, near the town of Algeciras, an accidental release of cesium provided an opportunity for ARAC to use actual, if sparse, measurements of a dispersion to back-calculate the magnitude and extent of the original release.

On June 9, 1998, the Swiss government announced that radiation levels up to a thousand times background had been detected by their national monitoring network. The source was unknown. France and Italy also reported measurements.

The next day, a steel mill near Algeciras notified the Spanish Nuclear Security Agency that radiation had been detected in one of its oven filtration systems. The agency, however, had not observed elevated radiation levels in its network. On June 12, the source of the release was identified as a medical radiotherapy device containing cesium-137 that apparently melted in the steel mill's scrap metal furnace. The amount and time of the release were unknown, but the incident was thought to have taken place during the last week of May 1998.

On June 12, the International Atomic Energy Agency also announced the incident and speculated on its possible connection to elevated levels of cesium-137 detected at the end of May and early June in southern Europe.

As ARAC staff became aware of the incident, they assessed gridded meteorological data archived for the area and began acquiring preliminary ambient cesium air concentration measurements from European colleagues. The various countries offering data had collected them with different samplers, using different averaging times (ranging from 1 to 14 days) and different radiological sensitivity thresholds. Having only data of sparse and varying quality, the staff set themselves the challenge of modeling the incident without knowing the exact location of the release. With each successive simulation, they incorporated new data as they were received and made model adjustments based on what they learned from previous simulations.

The first simulation led to an estimate of a 100-curie (370-gigabecquerel) release of cesium-137 over a 12-hour period on May 29, 1998. At that point, ARAC received more data on concentrations of cesium in the air at greater distances downwind, that is, from eastern and central Europe. ARAC enlarged the model domain to include these data. It also decreased the release duration from 12 hours to 30 minutes, based on results from the first model run. By the third simulation, the exact location of the steel plant releasing the cesium became known and was incorporated into the model, as were the parameters of the stack responsible for the release. Once this location was pinpointed, ARAC meteorologists blended observed meteorological data from the area with gridded weather data and produced their final simulation. It led to an estimate of a 50-curie (1,850-gigabecquerel) release, which compared favorably with the 8- to 80-curie (296- to 2,960-gigabecquerel) estimate provided by the Spanish government (Figure 5).

The Algeciras release was too small to produce any measurable health effects. However, the fact that ARAC tracked even this small release for great distances demonstrates the potential of accidental releases to affect substantial geographic

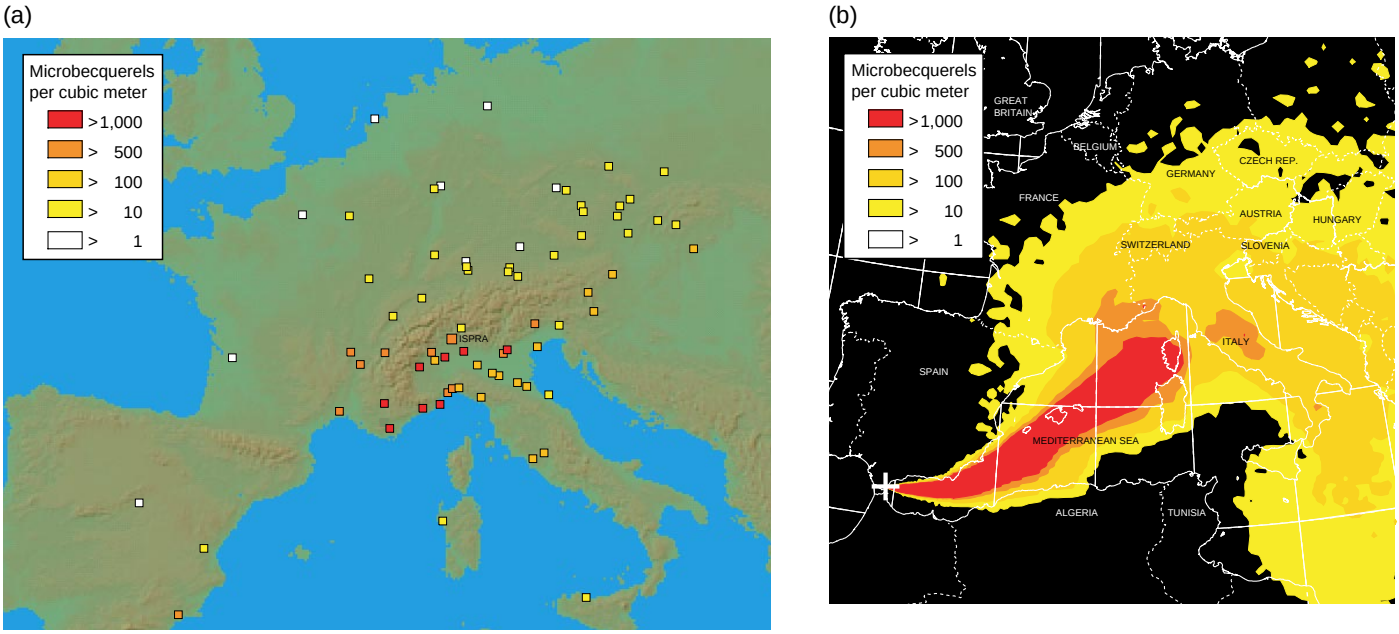
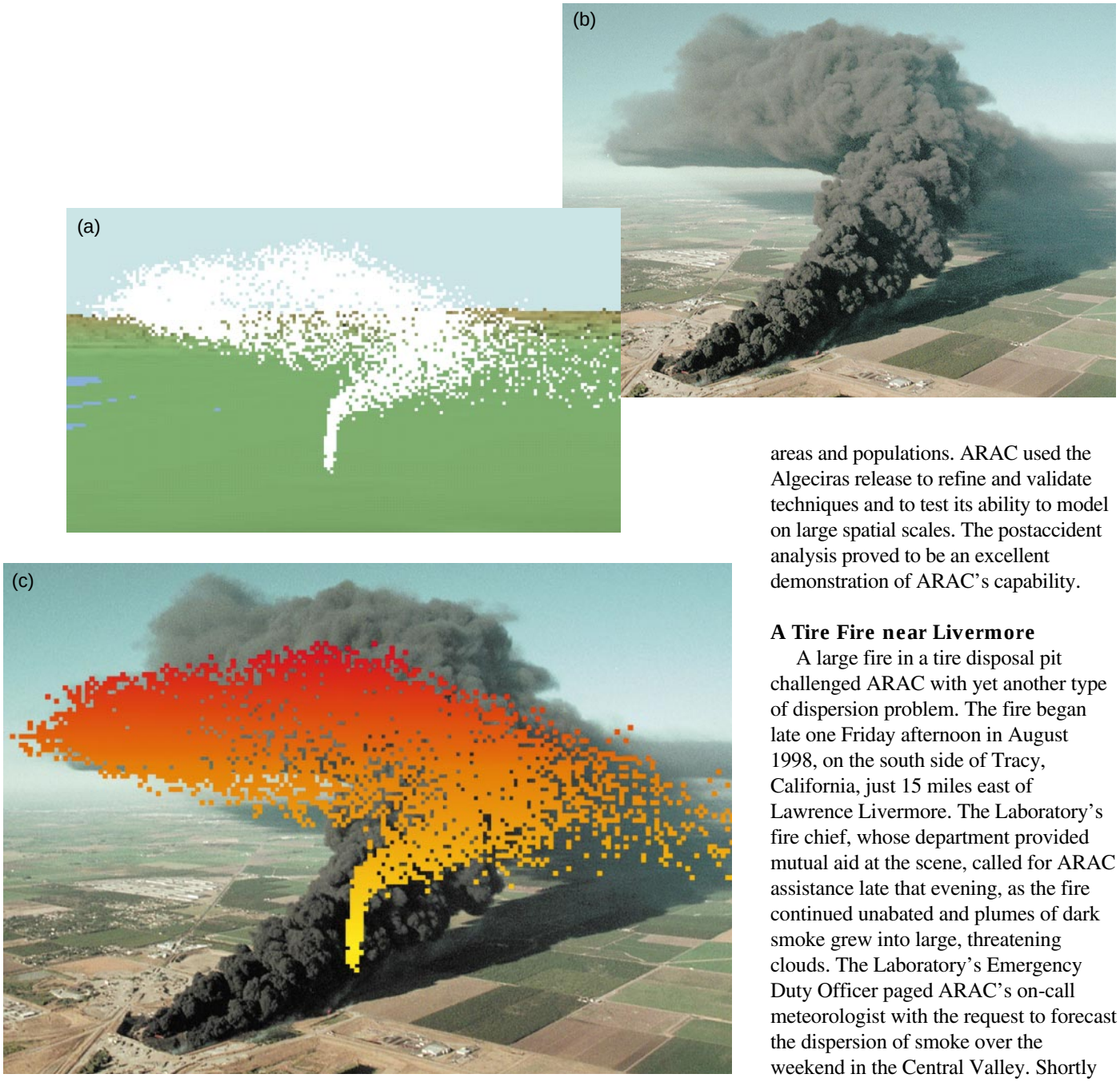


Figure 5. Following a cesium-137 release in southern Spain, ARAC received (a) measurements of elevated radiation levels from disparate European sources, which it superimposed on a terrain map of central and southern Europe. (b) Results from ARAC's third set of simulations for this release show the average air concentrations over a 7-day period. These results led to a good estimate of the original cesium release.



Photograph by: Glenn Moore, *Tracy Press*

Figure 6. (a) ARAC's simulation of smoke dispersion from (b) a large tire fire in Tracy, California, (c) agreed well with an aerial photograph taken a few hours after the fire started.

areas and populations. ARAC used the Algeciras release to refine and validate techniques and to test its ability to model on large spatial scales. The postaccident analysis proved to be an excellent demonstration of ARAC's capability.

A Tire Fire near Livermore

A large fire in a tire disposal pit challenged ARAC with yet another type of dispersion problem. The fire began late one Friday afternoon in August 1998, on the south side of Tracy, California, just 15 miles east of Lawrence Livermore. The Laboratory's fire chief, whose department provided mutual aid at the scene, called for ARAC assistance late that evening, as the fire continued unabated and plumes of dark smoke grew into large, threatening clouds. The Laboratory's Emergency Duty Officer paged ARAC's on-call meteorologist with the request to forecast the dispersion of smoke over the weekend in the Central Valley. Shortly thereafter, two ARAC meteorologists arrived at the ARAC Center, ready to start work on the problem.

The tire pit covered about 20 acres and was estimated to be about 100 feet deep. The burning tires, each containing

the equivalent of about 1 to 2 gallons of oil, caused a massive black cloud to rise about 5,000 to 7,000 feet above ground level. With only this information, ARAC meteorologists assumed that the fire covered an area of about 2.5 acres and that the smoke consisted of fresh combustion particulate products with a median diameter of one micrometer. Their simulation agreed well with an aerial photograph taken a few hours after the fire started (Figure 6). Their models were used to derive the air concentrations of the particulate at ground level over the next three days.

Later, ARAC went on to evaluate the smoke dispersion on a larger scale, from Sacramento to Fresno. State agencies used the larger assessment to alleviate the public's concerns about health effects from inhaling the smoke or drinking surface water downwind of the fire where the contents of the plume were estimated to have been deposited.

Moving Ahead of Emerging Risks

As ARAC embarks on its third decade of support to the nation, its cadre of operational atmospheric scientists is taking advantage of the ever-finer model resolution and ever-greater speed made possible by increasingly powerful computers. Their objective is to continually shorten response time and to increase the breadth of their capabilities and the accuracy of their predictions. Although ARAC's emergency readiness role is formally defined by its sponsors, improved capabilities are required to meet emerging risks. For the sake of national security, ARAC must stay ahead of those risks.

—Gloria Wilt

Key Words: ADAPT (Atmospheric Data Assimilation and Parameterization Tool), Atmospheric Release Advisory Capability (ARAC), ARAC Emergency Response Modeling System, atmospheric dispersion modeling, Coupled Ocean–Atmosphere Mesoscale Prediction System, emergency incident response, GRIDGEN (Grid Generator), LODI (Lagrangian Operational Dispersion Integrator).

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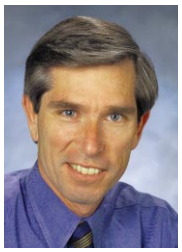
About the Scientist



RONALD L. BASKETT received his B.S. and M.S. in atmospheric science from the University of California at Davis. Throughout his career, he has focused on the use of measurements and models to solve problems of hazardous atmospheric releases, especially in complex terrain and coastal areas.

Baskett began his career with environmental consulting firms as a manager of meteorological and modeling projects to determine how proposed industrial facilities will affect air quality. In 1983, he joined Livermore's Atmospheric Release Advisory Capability (ARAC) program. He helped develop the software for the ARAC modeling system, performed numerous modeling studies, and gained extensive emergency response experience. He has been involved in about 40 emergencies and alerts worldwide, played a key role in several major field exercises, and supported hundreds of drills and assessments of individual facilities. He currently leads ARAC's operations team.

Unraveling the Mystery

Livermore scientists are using the state-of-the-art computational power supplied by DOE's Accelerated Strategic Computing Initiative to increase understanding of high-explosive detonations.

IN the study of weapons, a low explosive burns, but a high explosive detonates—a very different phenomenon. An initial shock compresses a high-explosive material, heating it and causing chemical decomposition. The formation of chemical products releases enormous amounts of energy in just billionths of a second. This process sustains the shock wave, which travels at supersonic velocity. All of this happens almost instantaneously to produce a blast of rapidly expanding hot gases.

In the brief instant of a high-explosive detonation, some remarkable events take place: the shock wave produces pressure up to 500,000 times that of Earth's atmosphere, the detonation wave travels as fast as 10 kilometers per second, temperatures can soar to 5,500 kelvins, and power approaches 20 billion watts per square centimeter.

Scientists at Livermore have been studying high explosives and modeling their behavior since the Laboratory was established because high explosives are an essential ingredient in every nuclear weapon. The first high explosives used in nuclear weapons were relatively easy to model because their detonation occurred virtually instantaneously. For purposes of modeling, detonation was considered instantaneous, and experimental results matched the models very closely. But while these high explosives made the modeler's life easier, they were less safe to work with in the field because of their sensitivity to heat, impact, and other conditions.

About 20 years ago, less sensitive high explosives were developed that have significantly improved the safety and survivability of munitions, weapons, and personnel. TATB (1,3,5-triamino-2,4,6-trinitrobenzene), for instance, is virtually invulnerable to significant energy release in plane crashes, fires, and explosions or to deliberate attack with small arms fire. But this extreme insensitivity has its drawbacks. Initiating a TATB detonation is not easy. Detonation is still fast but by no means instantaneous. The resulting shock wave propagates

Lawrence Livermore National Laboratory

# of Detonation

differently from that of sensitive explosives, and the molecules that detonation produces are different. Using TATB and other insensitive high explosives effectively in weapon systems has required a more sophisticated understanding of the physics and chemistry of initiation and detonation.

Randy Simpson, explosives leader of the Stockpile Stewardship Program at Livermore, is coordinating efforts by several Livermore scientists to learn more about the detonation of these slower, insensitive high explosives. Their collective goal is to be able to model the detonation process as accurately as possible.

Getting Down to Fundamentals

For the Department of Energy's Stockpile Stewardship Program, Livermore is working to vastly improve the modeling of nuclear weapon performance. Without empirical results from nuclear testing, the models must be based on first principles—the fundamental laws of physics—and data that can be gathered from nonnuclear tests. This reliance on developing much more accurate modeling capabilities extends to the high-explosive detonation phase.

The challenge for scientists who study explosive detonation is knowing—for an event that lasts less than a millionth of a second—the physics of each component over a wide range of pressures, densities, and temperatures and the way the components interact. This thermodynamic relationship of pressure, density, and internal energy for a given material is called its equation of state (EOS). Each of the components of a high-explosive detonation—hydrogen, nitrogen, oxygen, carbon, etc.—has its own EOS, as do the molecules that are various combinations of these elements. Behind the detonation front, the EOS of the system is constantly evolving and changing, because the chemical composition is changing.

First-principles research is impossible without high-speed computers to perform the necessary number crunching. The calculations for even the simplest molecules are hugely time consuming. And the number of possible combinations rises rapidly as the number of atoms in the molecules grows or when the molecular changes are looked at over time. It is only with the massively parallel computers of the DOE's Accelerated Strategic Computing Initiative (ASCI) that this first-principles numerical work on high-explosives detonation is possible.

Simpson notes, "We now have the fastest computers anywhere in the world. The detonation properties of high explosives are a mystery, and it is only with the computational power of ASCI that we can hope to unravel the mystery."

Adding Kinetics to the Equation

ASCI is putting a new twist on research that has been under way for years by physicists and chemists at Livermore. Francis Ree, for instance, has been studying the products of high-explosive detonations for over 20 years and has, in the process, helped to develop CHEQ, a thermochemical code used to study the effects of fluid-phase separation on detonation. Larry Fried has been developing another thermochemical code, CHEETAH, which predicts the performance of explosives. CHEETAH specializes in multispecies chemical kinetics. Similarly, Jack Reaugh has been working with hydrodynamic codes for years. (Thermochemical codes use statistical mechanics and intermolecular potentials to provide equations of state of reactive mixtures. Hydrodynamic codes describe material flow by solving the conservation laws of mass, momentum, and energy.)

Experimentalists, the "people who blow things up," look at detonation at the macroscopic level. Ree's and Fried's teams work at the other end of the spectrum where individual molecules and atoms and their interactions are what matter. With his current research, Reaugh is in the middle, doing mesoscale simulations of the initiation process and exploring the effects of changes in the size of voids and grains of high explosives.

With ASCI and other high-powered computational capabilities, all three teams can better understand their data and actually produce better data. In particular, they can address kinetics, including chemical kinetics (chemical changes over time) and mass transport kinetics, which are determined by material flow.

Traditional Chapman–Jouguet thermodynamic theory does not do a good job of modeling slow, or non-ideal, detonation processes. Chapman–Jouguet theory is essentially one-dimensional, which is fine for sensitive high-explosive detonations. It assumes that thermodynamic equilibrium of the detonation products is reached instantaneously and that all products are consumed completely. In fact, detonation of insensitive explosives is much more complicated. For one thing, it is three dimensional. For another, some chemical reactions occur more slowly than others. At the same time, a range of chemical reactions takes place during the decomposition of large high-explosive molecules into simple product molecules. The evolving equation of state for this collection of changing materials must somehow be represented. Adding kinetics to the equation is the key (Figure 1).

With the addition of kinetic information, Livermore's hydrodynamic codes can be tied to its thermochemical codes to fully model the underlying physics and chemistry of a high-explosive detonation. Until recently, computer capabilities were such that three-dimensional hydrodynamic modeling had to be stripped of all chemistry. Now, with ASCI, the evolving chemistry can finally be addressed.

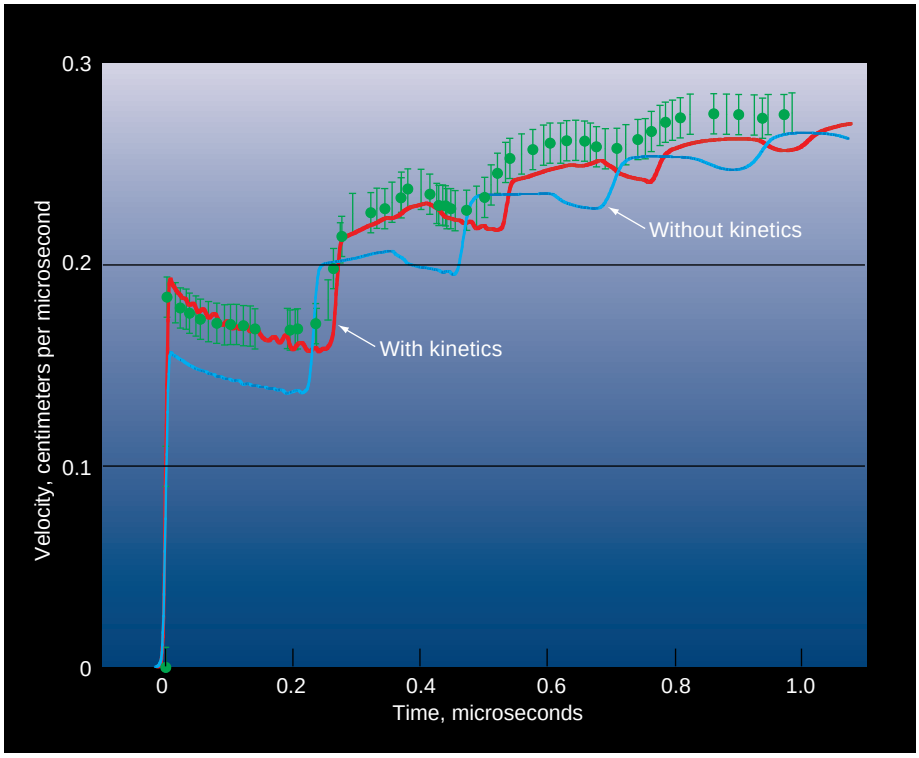


Figure 1. Adding kinetics to the CHEQ thermochemical code improves correlation with experimental results. Results from experiments run at Livermore's Site 300 are shown with error bars, which much more closely match the code when kinetics of carbon coagulation has been incorporated. The velocity is that at the surface of a metal shocked by an explosive.

Complex Products

Francis Ree and his team are examining the molecules that are produced during detonation. An

interesting aspect of this work is the phase changes that these products undergo as detonation proceeds. Last year, the team worked with scientists at the California Institute of Technology in Pasadena in an ASCI alliance. This year, they are collaborating with researchers at the University of North Carolina.

Ree says, "With conventional high explosives such as LX-14, which Livermore developed, the most important products behind the reaction zone are carbon dioxide, water, nitrogen, and carbon residues. But with insensitive high explosives, the product mix is more varied and involves more complex physics and chemistry."

Livermore's insensitive high explosives use fluorine in their binder. During detonation, the fluorine combines with hydrogen to make gaseous hydrogen fluoride (HF), a highly corrosive compound and the strongest hydrogen bonding system occurring in nature. Moreover, insensitive high explosives produce large amounts of condensed carbon, which changes from graphite to diamond and then back to graphite. These explosives ultimately produce gases such as carbon dioxide when temperatures, pressures, and densities fall behind the detonation front. Accurate modeling of insensitive high explosives must consider both the thermodynamics of chemically reactive mixtures and the kinetics of carbon coagulation.

Predicting the performance of a high explosive requires information on all intermolecular potentials, which determine the forces of attraction and repulsion acting between molecules, the dynamics of many possible chemical reactions, and such unusual phenomena as fluid–fluid phase separation (Figure 2). Calculating intermolecular potential is relatively simple in a pure stable gas such as nitrogen or carbon dioxide. In a gaseous mixture, the problem becomes more complex.

To handle the products of detonation, whose composition changes over time, the team developed CHEQ (chemical equilibrium) in 1984 to continually check the composition of a detonating mixture, pick the most stable mixture, and adjust the effective intermolecular potential accordingly.

No experimental data on HF exist at the conditions occurring during detonation because it is such a difficult

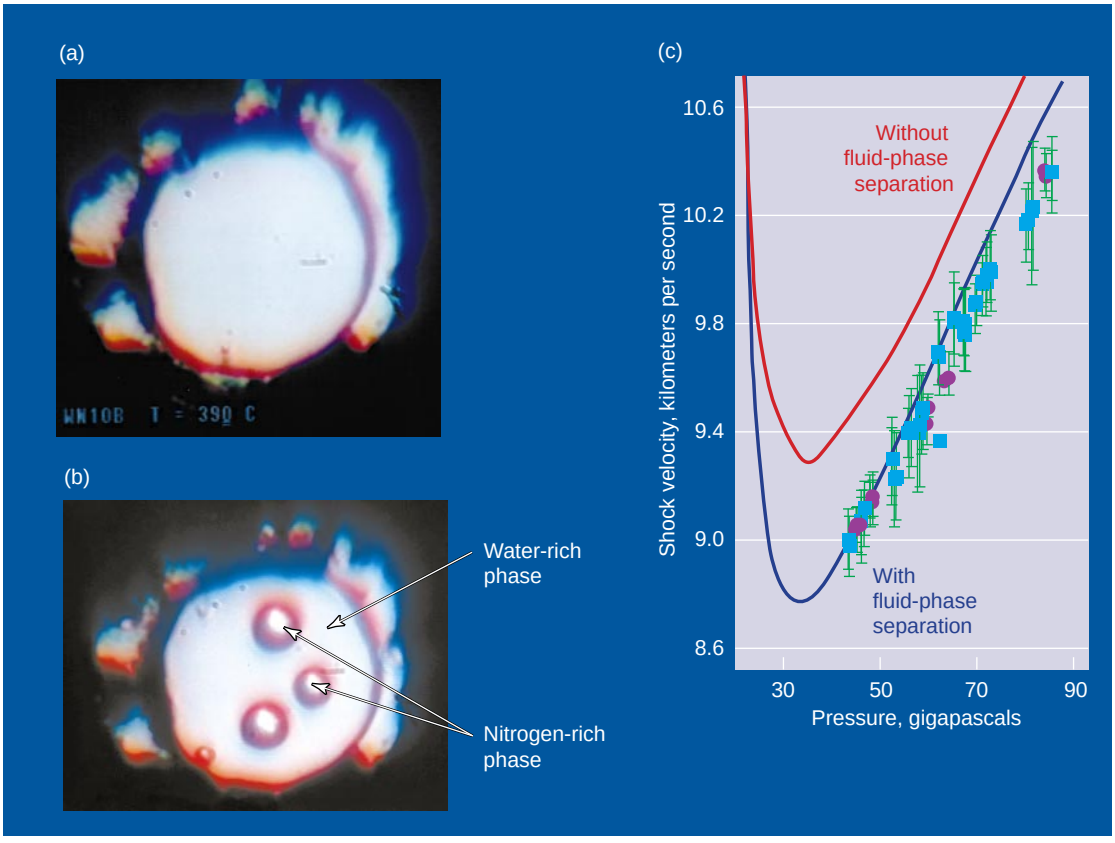


Figure 2. Using Livermore's diamond anvil cell, Marc Costantino has demonstrated fluid–fluid phase separation of water and nitrogen at high pressures and temperatures. (a) At 663 kelvins, a bubble of water and nitrogen may be seen. (b) When the temperature is lowered just slightly to 641 kelvins, the nitrogen and water separate. (c) When this fluid-phase separation is included in the CHEQ code, experimental results (error bars) closely match code predictions.

material to work with. There are, therefore, no data on intermolecular potentials between HF and other detonation products. In addition, there is no experimental information on potentials between nitrogen and carbon dioxide, carbon dioxide and water, and nitrogen and water at the pressures and temperatures relevant to explosive detonation. So, to establish intermolecular potentials between these detonation product species, Ree called in Livermore experts in quantum molecular dynamics Guilia Galli and Francois Gygi, who are using ASCI to perform simulations at high pressures and temperatures (Figure 3). By incorporating these potentials generated by computer into CHEQ, Ree's team will be able to produce reliable EOSs for several insensitive high explosives.

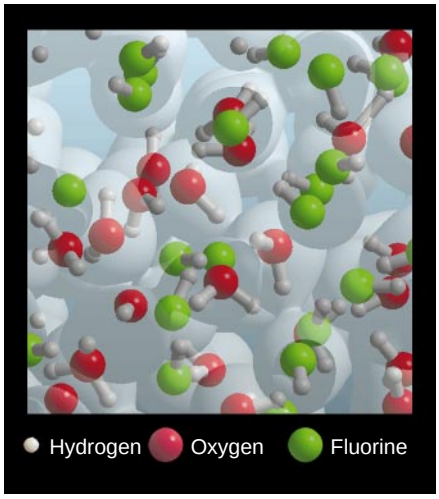


Figure 3. Quantum mechanical molecular dynamics results using Livermore's Accelerated Strategic Computing Initiative computer for hydrogen fluoride and water mixtures at 10 gigapascals and 600 kelvins. Computing 1 picosecond of real-time molecular activity took 372 hours of computing time, even with the most powerful computer in the world.

The relative leisureliness with which insensitive high explosives detonate is apparently caused in part by the slow release of energy from the carbon in them. During detonation, the free carbon coagulates into small clusters, which grow larger by diffusion. Because small carbon clusters have a larger surface area than larger clusters, a greater proportion of their energy is tied up in surface atom bonds. As the clusters agglomerate into larger and larger clusters, the fraction of energy in surface bonds decreases. Studies of carbon kinetics by Ree's team are directed at the slow diffusion kinetics of carbon clusters and the structural changes in the clusters (graphite to diamond and back to graphite).

To date, using molecular dynamics and Monte Carlo simulations, the team has computed the melting line of diamond and the line at which diamond liquefies. They are also studying the stability of diamond and graphite clusters, energy barriers between the two cluster types versus size, and kinetics of the graphite–diamond phase change. One result of this work is a better predictive model of high-explosive performance during detonation.

Multispecies Chemical Kinetics

Larry Fried and the CHEETAH team first incorporated a flexible kinetics capability into their thermochemical code in 1997. The code is particularly useful for dealing with complicated problems in which more than one chemical species is out of equilibrium. (See *S&TR*, November 1997, pp. 21–23.) Kinetic-rate laws were derived by matching dozens of measured curved detonation fronts. The result was the first general-purpose kinetics capability applicable to a broad range of slowly reacting explosives.

Currently, the team is combining kinetics with sophisticated molecular equations of state. The EOSs are based on massive statistical mechanics calculations performed on the ASCI supercomputer and validated with EOS experimental data, including information on static compression and shock. Says Fried, "Our goal is to produce molecular equations of state that are accurate over the broadest range of thermodynamic conditions possible, including relatively cold states of only a few hundred kelvins. Such states have not been well modeled by traditional thermochemical codes." Fried and his coworkers have also developed a way to infer the equation of state of hydrogen fluoride and other difficult molecules from high-pressure shock experiments performed on plastics. Only recently did researchers realize that these experiments contained "keys" to the EOS of hydrogen fluoride and hydrogen chloride, materials that are difficult to study in isolation.

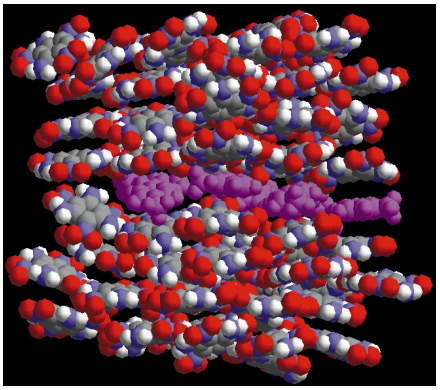
CHEETAH's kinetics calculations offer the most detailed picture possible of chemical compositions through the high-explosive reaction zone. Because this level of detail is difficult to include in large-scale hydrodynamic simulations, the team is producing simplified reactive flow models that incorporate reaction rates calculated with the more detailed CHEETAH. The simplified models will be used in three-dimensional hydrodynamic calculations with billions of zones.

ASCI's computers are being used to produce basic science data for CHEETAH where massive statistical calculations are required. And they will continue to become more powerful. Fried noted that in its current configuration, ASCI computers can handle much more difficult calculations than it could a year ago. This improved capability will allow the team to

develop accurate models for highly charged molecules such as water and hydrogen fluoride.

The team is also interested in understanding how chemical impurities in high explosives affect their detonation, safety, and aging properties. In the past, the effects of impurities on high explosives were not carefully studied.

(a)



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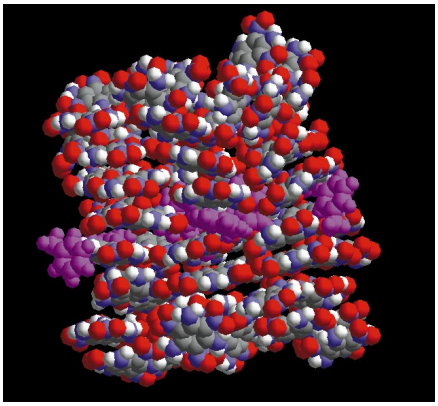


Figure 4. Studies of toluene impurities and the insensitive high explosive TATB are important because toluene is the major volatile chemical released from industrial TATB. (a) At room temperature, the toluene impurities are locked into the TATB. (b) At 500 kelvins, they are released from the TATB lattice. These impurities are especially important in the aging of TATB.

ASCI resources make it possible to study these problems in detail.

Figure 4 shows a simulation of a toluene release from TATB. At room temperature, the simulation indicates that toluene is "locked" in TATB. When heated to 500 kelvins, however, the toluene is released from the TATB lattice. These calculations help explain experiments where large quantities of toluene are released when TATB is exposed to strong sound waves.

In the future, Fried expects to link CHEETAH directly to ASCI's hydrodynamic codes. CHEETAH has been linked to smaller hydro codes, but not to massively parallel codes such as ARES and ALE3D. Fried is also considering developing a version of CHEETAH that would run exclusively on ASCI. For CHEETAH to perform Monte Carlo statistical calculations, ASCI's computing power is essential.

A Look at Initiation

We usually think that perfect things work better. But in high explosives,

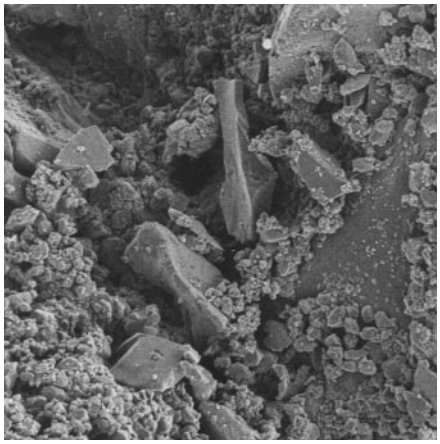


Figure 5. High-explosive materials contain crystalline explosives, binders, plasticizers, and porosity. The voids and other irregularities are necessary for explosives to perform properly.

defects are important to their performance. In some cases, pure, homogenized high explosives do not get sufficiently hot at the shock front to react rapidly enough for detonation. Instead, porosity, impedance mismatches between explosive components, and intracrystalline defects in the high explosive, binder, and other materials are essential. They cause localized hot spots that drive the decomposition reactions (Figure 5).

According to Jack Reaugh, "These temperature spikes are visible in liquid high explosives as bubbles where ignition takes place. With solid high explosives, we know the hot spots are there, but they are not visible. So simulations are necessary to 'see' the phenomenon."

If the voids are too small, heat diffuses too quickly, and the mixture will not ignite. Reaugh's challenge is to quantify what size is best, both for voids and for the particles around them, to maximize the accuracy of reactive flow models.

His work started in early 1999, and his focus initially is on modeling small parts of a detonation's initiation at the grain scale. Some of his first results are illustrated in Figure 6, which shows a block of high-explosive particles and the binder between them at three points just after initiation. As the shock front moves through the block, it compresses the mixture.

For these pictures to be meaningful, Reaugh must first develop models of all materials involved prior to ignition, that is, the EOS of the unreacted high explosive, binder, and air that fills the voids. Then he must incorporate such information as temperatures, the thermal conductivity of the unreacted materials, heat transfer, and chemical reactions that take place as initiation is occurring. Each of these processes has a model associated with it, and at the moment, not all the

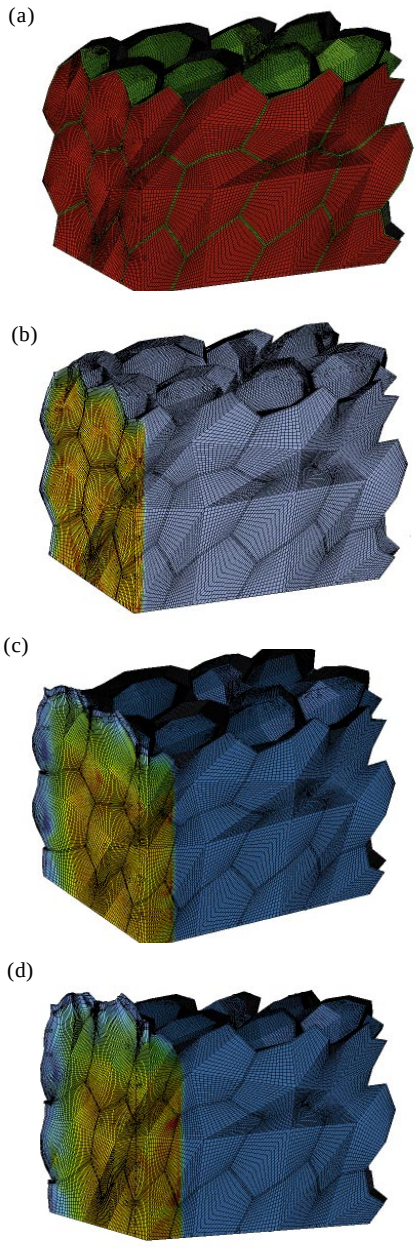


Figure 6. (a) A tiny block of high explosives, just four by three by three particles, with binder locking the particles together, prior to detonation. (b), (c), and (d) The block of high explosive shown at three moments immediately following initiation. The shock wave compresses the particles as it moves through the material.

information needed is available. For the time being, he is making do with bare-bones models that use available data and is running his simulations on Livermore's three-dimensional hydrodynamic code ALE3D.

Unlike Ree, who is looking at the products of detonation, Reaugh is studying the front end. According to Reaugh, "The really interesting stuff goes on in the first moments after detonation." His work will give the closest look yet at how initiation occurs, how long it takes, how reactions occur, whether full reaction occurs, and so on.

His simulations are just now getting big enough that he needs to use ASCI. When they include just a few particles, a smaller computer is adequate. ASCI makes possible larger, more complex simulations that show "the really interesting stuff."

With Even Faster Computing

Says Simpson, "ASCI's computational power is enormous. It allows us to simulate high-explosive detonation to a level of detail unimaginable even a few years ago. By effectively incorporating kinetics into our models, we will not only be able to describe what is occurring in a high-explosive detonation, but will also be able to predict what will happen over time. That is a huge improvement over current modeling capabilities." With better models will come increased performance, safety, and reliability of the high explosives on which stockpiled weapons rely.

—Katie Walter

Key Words: Accelerated Strategic Computing Initiative (ASCI), CHEETAH, CHEQ, detonation, equation of state (EOS), high explosives, hydrodynamic codes, initiation, insensitive high explosives, multispecies chemical kinetics, thermochemical codes.

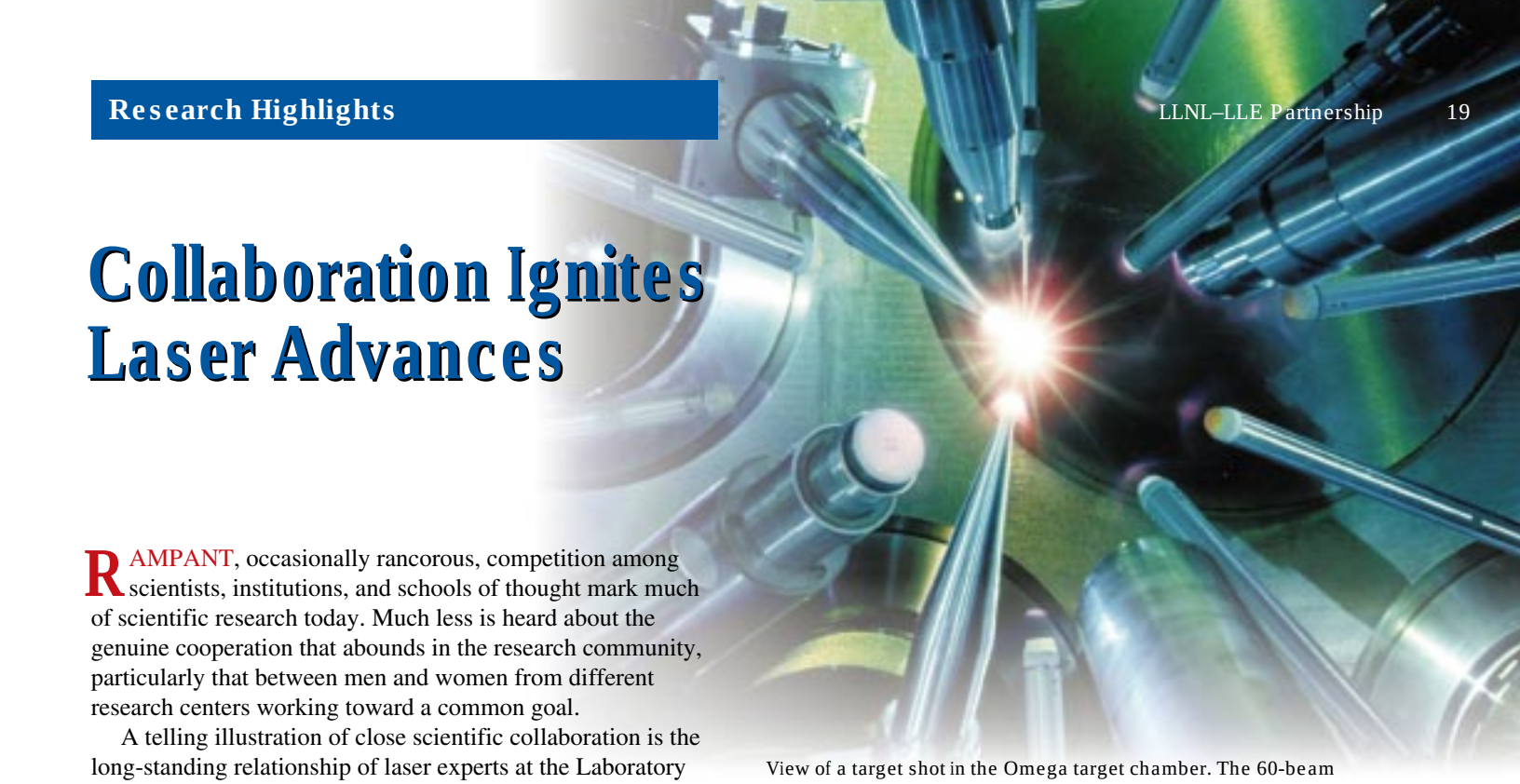
For further information contact Randy Simpson (925) 423-0379 (simpson5@llnl.gov).

About the Scientists

Like all science done at Lawrence Livermore, modeling the details of slower, insensitive high explosive detonations requires a multidisciplinary team. Leading this work is **RANDY SIMPSON** (left), explosives leader of the Stockpile Stewardship Program at Livermore. Other principals include chemist **LARRY FRIED** (second from right), one of the primary developers of the CHEETAH code, which Fried and his colleagues are developing to accurately model the molecular equations of state of explosive materials over a broad range of thermodynamic conditions.

Physicist **FRANCIS REE** (right) and his team are refining the physics models in the CHEQ code to study the products of insensitive explosives as they are generated and change during detonation. Physicist **JACK REAUGH** (second from left) and his associates are concentrating not on the products of detonation but on the process of initiation. They are simulating the imperfections of an explosive's components during the first moments of detonation to determine how the interactions of these imperfections drive the detonation.

Collaboration Ignites Laser Advances



View of a target shot in the Omega target chamber. The 60-beam Omega laser system is a 40-kilojoule, direct-drive laser located at the Laboratory for Laser Energetics (LLE) at the University of Rochester. Collaborations between LLE and Livermore's Laser Programs have been of mutual benefit to both organizations.

RAMPANT, occasionally rancorous, competition among scientists, institutions, and schools of thought mark much of scientific research today. Much less is heard about the genuine cooperation that abounds in the research community, particularly that between men and women from different research centers working toward a common goal.

A telling illustration of close scientific collaboration is the long-standing relationship of laser experts at the Laboratory for Laser Energetics (LLE) of the University of Rochester and at Lawrence Livermore National Laboratory. Their common goal has been to harness the potential of the laser as a future energy source and as a tool for revealing the secrets of matter at extreme temperatures and pressures.

Involved in inertial confinement fusion (ICF) research since the late 1960s, LLE today operates the only fusion research program jointly supported by the federal government, state government, industry, utilities, and a university. The U.S. Department of Energy has designated LLE as the National Laser Users' Facility to enable academic institutions, industrial research establishments, and government laboratories to have access to its facilities.

Showcasing the Omega Laser

LLE's showcase facility is its 60-beam Omega laser, which can deliver more than 40 kilojoules of energy on a target less than 1 millimeter in diameter. (By comparison, the 192-beam National Ignition Facility [NIF], now under construction at Lawrence Livermore, will produce 1.8 megajoules of energy.)

Completed in 1995, Omega is the nation's principal direct-drive laser fusion research facility. With direct drive, laser light strikes a minuscule capsule directly to compress it. In the other approach to inertial fusion—indirect drive—laser light first strikes the inner wall of a metal cylinder called a hohlraum, causing the production of x rays that symmetrically implode a capsule located inside.

Omega is the latest achievement of LLE's laser program, which has paralleled Lawrence Livermore's for nearly four decades. During that time, researchers at each institution have readily adopted the breakthrough technologies developed by the other, often collaborating to improve them or modifying them to suit unique experimental goals. "Such shared technologies translate to a 'national win,'" says LLE director Bob McCrory.

Sharing Improves Technologies and Reduces Cost

When Omega was upgraded from 24 to 60 beams, it married technologies pioneered by both Livermore and LLE. Livermore scientists advised their LLE colleagues about disk amplifier technology they had developed, recalls Howard Powell, Livermore physicist and program leader for Laser Science and Technology. "We told them everything we knew about how to use flashlamps to pump disk amplifiers and how to cool the amplifiers," he says.

Although NIF will use nitrogen gas as a flashlamp coolant, Omega scientists decided to use water. This new technology has paid off—the Omega laser beams have only a 45-minute turnaround time. "The fact that flashlamp cooling works so well for them means we're very confident about using flashlamp cooling techniques for NIF," says Powell.

Livermore laser scientists point to two key developments by their LLE colleagues. The first, achieved in 1980, uses crystals of KDP (potassium dihydrogen phosphate) to efficiently convert a laser's infrared wavelengths to ultraviolet to better couple the laser energy to the target. Early generations of Livermore's neodymium-doped glass lasers—Janus, Cyclops, Argus, and Shiva—produced successively higher peak power and output energy at 1,050-nanometer wavelengths. This wavelength was not short enough to produce effective implosions. Livermore researchers took advantage of the LLE breakthrough in 1985 to convert the laser light on their 10-beam Nova laser to the 351-nanometer wavelength.

McCrory points out that until the Omega upgrade began operation, Nova was the world's most powerful laser. Because of technology advances, Omega was built for roughly one-third the cost of Nova. Further advances make NIF's cost per unit of output energy even lower. NIF has about 60 times the output energy of Omega at roughly 20 times the cost, continuing the trend of advancing technology from Nova to Omega to NIF.

The second major LLE breakthrough was smoothing by spectral dispersion (SSD). This technology shimmers the beam on the target to get rid of speckling and intensity variation, thereby avoiding destructive hot spots. Although it was originally developed for direct-drive experiments, Livermore researchers discovered it was also useful for indirect drive. As a result, SSD was modified and implemented on Nova; it will also be used on NIF.

"The real contest," says McCrory, "is the quality of the laser beam." In that respect, he says, SSD is comparable in importance to Livermore's development of spatial filters in the late 1970s. These filters prevent damage to laser glass by smoothing the shape of and eliminating the high-frequency noise in the beam. At the time, says McCrory, spatial filters were the "salvation" of solid-state lasers.

Omega Stands in for Nova

When Nova was decommissioned in May 1999, Omega became the only facility in the nation doing laser fusion implosion experiments. Although it was designed to do direct-drive experiments, it is working well as a facility for Livermore's indirect-drive experiments.

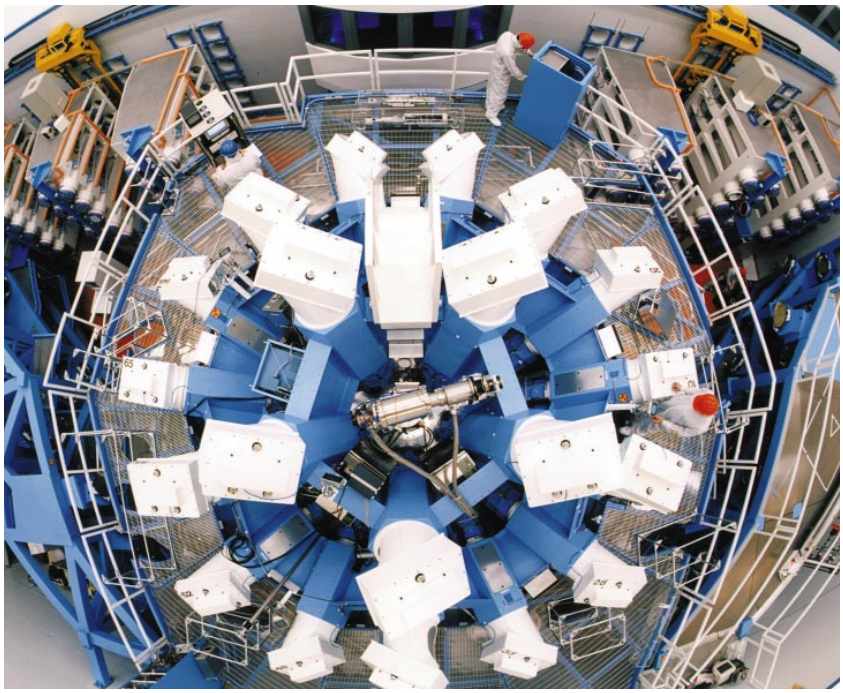
The decision to close Nova and transfer experiments to Omega until NIF begins operation in 2002 was not made lightly. Livermore physicist Ted Perry notes that because Omega was designed as a direct-drive facility, it can use only about 40 of its 60 beams for the indirect-drive targets used on Nova and NIF.

"Omega had to demonstrate that it could do the experiments. It passed all the tests," says Perry, who credits the ingenuity of Livermore and Rochester scientists working together to optimize the facility for indirect drive.

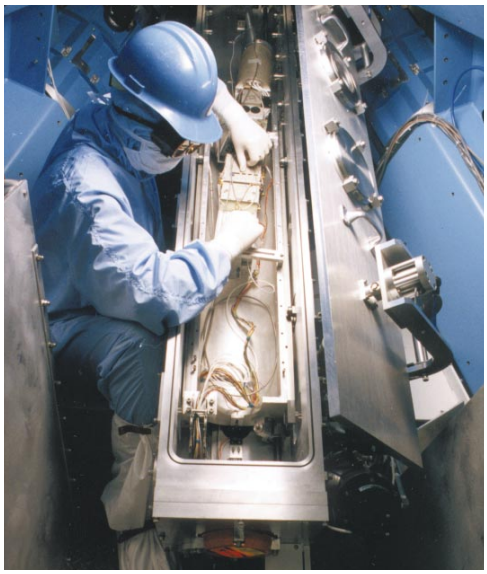
Omega Contributes to Stockpile Stewardship

Most of Livermore's planned shots on Omega for 1999 are earmarked as part of DOE's science-based Stockpile Stewardship Program to ensure that the nation's nuclear weapon stockpile remains safe and reliable. Small Livermore teams travel to Rochester with their laser targets and stay for about a week-long "campaign" of 20 to 30 shots. (Omega averages 10.5 shots per day.)

Most experiments are unclassified, especially fundamental hydrodynamics experiments that can be applied as much to



A view of the Omega target bay from high above the target chamber shows critical components associated with the ultraviolet transport system.



Livermore scientist Ted Perry adjusting a gated x-ray imager on the Omega target chamber. While the National Ignition Facility is being built, teams of Livermore scientists travel to Rochester regularly to do experiments on Omega in support of stockpile stewardship and to advance their understanding of laser target physics.

astrophysics as to understanding nuclear weapons. Diagnostic instrumentation originally built for Nova works well on Omega, thanks to what McCrory calls "shared modularity." In turn, instruments built for Omega can be readily adapted to work on NIF.

Livermore physicists have been impressed with the precision of Omega's 60 beams. "Omega is more precise than Nova because it has more modern technology," says Powell. "Precision is everything in laser fusion."

Livermore physicist Kim Budil points out that Omega's 60 beams give experimenters more flexibility to design experiments than Nova did. What's more, she says, working with the complicated geometry of the beams is good preparation for NIF's 192 beams.

For ICF, it is important that the spherical target stays round as it is squashed by the x rays in the hohlraum. It is relatively easy to detect sausage- and pancake-shaped deviations from spherical implosions, but more complicated deviations from roundness, such as a cross, are harder to measure. A team led by Livermore physicist Nino Landen recently concluded experiments on Omega that demonstrate the detection capability for these subtler deviations, so-called high-order asymmetries, which were difficult, if not impossible, to isolate on Nova. The control of these high-order asymmetries is important to achieving highly spherical implosions and eventually ignition on NIF.

Some Key LLE Accomplishments

1975 to 1976	First direct experiments of compressed fuel density in laser-driven targets.
1975 to 1976	First detailed measurements of ablation and preheat using x-ray line emission.
1975 to 1976	First comprehensive measurements of harmonic and subharmonic emission from spherical targets.
1980	Invention of high-efficiency third-harmonic generation schemes for high-power glass lasers.
1980	First extensive laser–matter interaction experiments with ultraviolet irradiation.
1988	First demonstration of compressions in excess of 100 to 200 times liquid deuterium–tritium density (greater than 20 to 40 grams per cubic centimeter) in thermonuclear fuel using cryogenic targets.
Late 1980s	Pioneering use of SSD (smoothing by spectral dispersion) beam-smoothing technique to produce uniform beam profiles.
1995	Construction of the 60-beam, upgraded Omega laser completed.

In addition to supporting stockpile stewardship experiments by Livermore and Los Alamos personnel, LLE scientists are preparing for direct-drive experiments. McCrory says that LLE is facing the same kinds of technical challenges to make direct-drive work that Nova experimenters faced in the mid-1980s proving indirect drive.

Direct drive is an attractive option to indirect drive because of the potential for higher energy gain, says Charles Verdon, head of the Livermore group that designs laser targets and LLE deputy director from 1994 to 1997. "As Rochester solves its technical issues, such as handling cryogenic targets, the results will help Livermore scientists prepare for NIF," Verdon says. In addition, he says that as a multiuser facility, Omega is serving as a model for how best to operate NIF as a stockpile stewardship facility for all three weapons laboratories.

Omega after NIF

Verdon says that Omega will continue to be an important facility to Livermore even after NIF begins operation. Lawrence Livermore will use Omega to scope out scientific ideas more easily and cheaply. High-power or high-energy experiments, however, will require NIF.

The strong LLE connection to NIF is evident in other areas. LLE optics experts are applying essential multilayer coatings to several NIF optical components, such as the polarizers that form part of the giant laser's optical switches and the deformable mirrors used to control beam quality.

Looking beyond NIF, Livermore and LLE researchers are collaborating on a proposal to develop a DOE "virtual laboratory" to design a diode-pumped solid-state laser for inertial fusion energy. The laser would fire some 10 times per second with 10 percent efficiency. A similar virtual laboratory for a heavy-ion laser facility was formed last year as a collaboration between Livermore and Lawrence Berkeley National Laboratory.

"The ICF program has worked synergistically. There is always pride in ownership, but there haven't been a lot of 'not invented here' roadblocks," says Verdon.

"We compete," adds Powell, "but it's a healthy competition."

—Arnie Heller

Key Words: diode-pumped solid-state laser, direct drive, flashlamp cooling, indirect drive, inertial confinement fusion (ICF), KDP (potassium dihydrogen phosphate) crystals, Laboratory for Laser Energetics (LLE), Lawrence Berkeley National Laboratory, National Ignition Facility (NIF), Nova laser, Omega laser, smoothing by spectral dispersion (SSD), spatial filters.

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Predicting Material Behavior from the Atomic Level Up

MICROSTRUCTURAL features in metals profoundly affect what happens on a larger scale, particularly when systems are pushed to their limits. For example, jet aircraft turbine blades can fail if small concentrations of particular impurities cluster at the boundaries between the individual crystalline grains of the metal. Even in the absence of impurities, the strength and plastic deformation of a metal are controlled by extended crystal defects called dislocations. Such features also affect the performance of nuclear weapon systems, where materials are pushed to extremes of temperatures and pressures.

Modeling macroscopic mechanical properties such as strength and failure at different length scales—that is, multiscale modeling—is of major interest at Lawrence Livermore because of its relevance to the Department of Energy's Stockpile Stewardship Program. With the cessation of underground nuclear testing, weapons scientists must be able to predict with confidence the properties of materials in stockpiled warheads and their effect on weapons performance.

This need to predict performance has put a high premium on understanding materials behavior. In this respect, the mechanical properties of nuclear weapon materials are uniquely complex. Unlike thermodynamic properties, such as the equation of state, which are fully determined at the atomic length scale, mechanical properties are inherently multiscale, depending on phenomena at all length scales. Thus, multiscale modeling is a huge scientific challenge as well as a critical necessity for successful stockpile stewardship. To meet these demands, Livermore's multiscale-modeling effort involves some 25 researchers from a variety of disciplines (theoretical and weapons physics, engineering, and chemistry and materials science) as well as many outside collaborators, including the Massachusetts Institute of Technology, Stanford University, the University of California at Los Angeles, the University of Illinois, Brown University, Yale University, Carnegie–Mellon University, and IBM.

Making Connections among Scales

In the multiscale program, scientists are creating and validating computer models to predict and explain the mechanical properties of metals at dimensions ranging from a fraction of a nanometer to meters. The focus is on three major length scales—the atomic scale (nanometers), the microscale (micrometers), and the mesoscale (millimeters and above) (Figure 1). What sets this effort apart from previous ones is that fundamental physical and mathematical principles are rigorously applied to the modeling at each scale, and data are then passed to the next scale up. In the past, such efforts were hampered by the lack of computational power needed to simultaneously model the individual and collective behavior of a large number of atoms and defects. Now, by combining a multiscale-modeling strategy with spectacular advances in computational technology, scientists are shedding light on the fundamental mechanisms that determine how materials deform and fail.

John Moriarty, a leading physicist in Livermore's multiscale-modeling effort, notes, "In the days of underground weapons testing, hydrodynamic computer codes relied on purely phenomenological models of mechanical properties based upon limited experimental data obtained at or near ambient conditions. In the multiscale-modeling program, we are developing a predictive capability based on first principles. That is, the predictions we make at the everyday macroscopic level will be based on fundamental quantities and rules derived from the atomic scale and microscale."

The program is currently focused on the prototype problem of strength and plastic deformation in body-centered-cubic (bcc) metals, such as molybdenum and tantalum (Figure 2). These metals are of special interest because of their physical and structural similarity to stockpile materials. Tantalum, in particular, is predicted to remain a bcc metal to extremely high pressures. In addition, notes Moriarty, the thermodynamic and mechanical properties of metals such as tantalum are of long-standing interest to both the high-pressure and materials physics communities.

Over the years, the materials scientists have accumulated substantial data on the yield strength and other mechanical properties of bcc metals at or near ambient pressure, and more detailed and accurate data are being obtained as part of the multiscale program. Theoretical corroboration has been lacking, however, as has information on tantalum's mechanical properties at high pressures. Rigorous

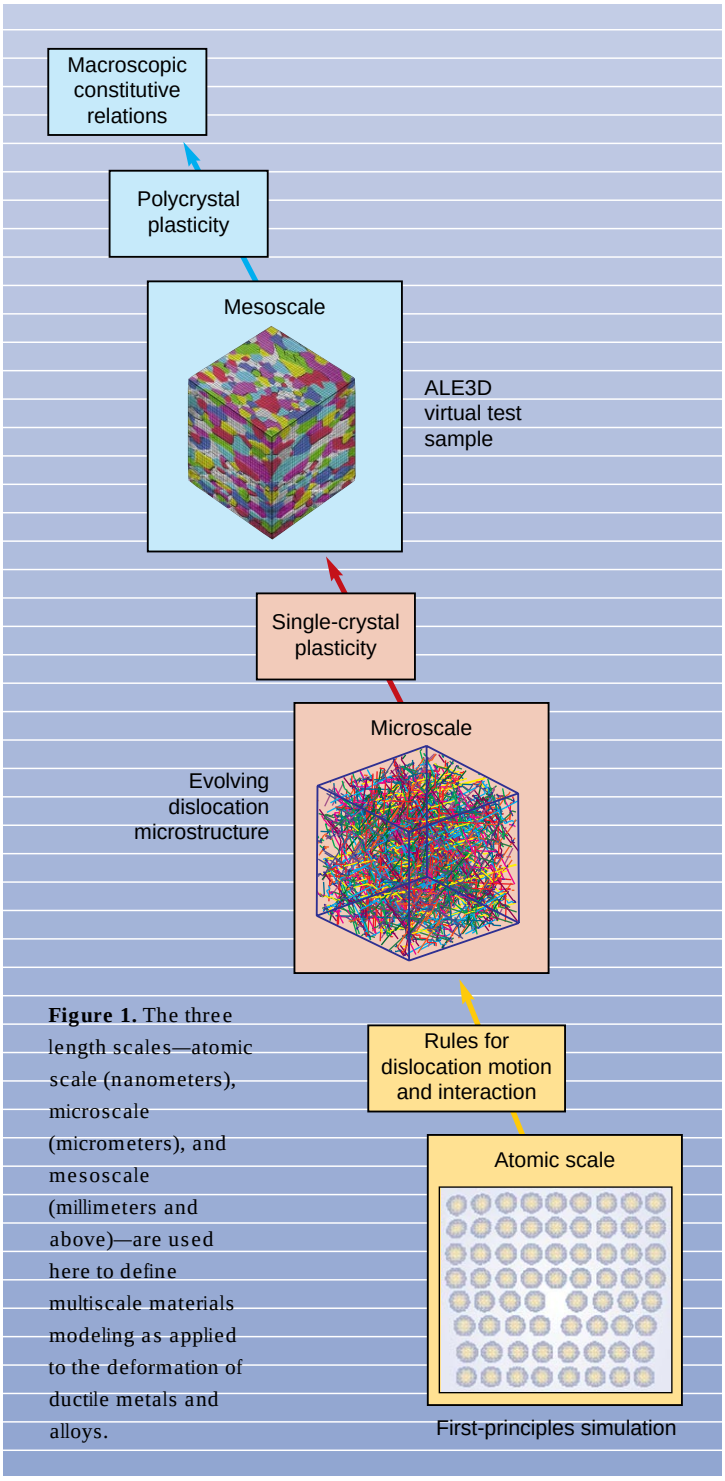

Figure 1. The three length scales—atomic scale (nanometers), microscale (micrometers), and mesoscale (millimeters and above)—are used here to define multiscale materials modeling as applied to the deformation of ductile metals and alloys.

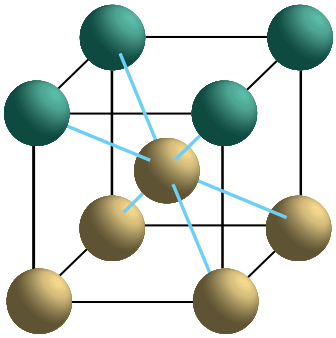

Figure 2. A body-centered-cubic (bcc) crystal. Tantalum and molybdenum are examples of metals with a bcc crystal structure.

mathematical answers are difficult to come by because mechanical properties depend on phenomena at all length scales. The advent of the Department of Energy's Accelerated Strategic Computing Initiative means that the computational power is now available to bridge the different length scales and accurately model the mechanical properties of tantalum and other metals from first principles.

Climbing the Multiscale-Modeling Ladder

To define the plastic deformation problem in detail, multiscale modelers use a top-down strategy to pose questions and a bottom-up strategy to obtain solutions. Modeling at each length scale helps pose critical questions to be addressed at the next lower scale. To achieve the corresponding solution, appropriate simulations at the atomic scale, for example, provide input at the microscale.

For tantalum, Moriarty and others start with its fundamental atomic properties, using rigorous quantum-mechanical principles and first-principles calculations to develop accurate interatomic force laws that can be applied to atomistic simulations involving many thousands of atoms. From these simulations, they derive the properties of individual dislocations in a perfect crystal and then, with new microscale simulation techniques, look at the behavior of large collections of interacting dislocations at the microscale in a grain-sized crystal. They model the grain interactions in detail with

finite-element simulation codes, and from those simulations, they finally construct appropriate models of properties such as yield strength in a macroscopic chunk of tantalum. At each length scale, the models are experimentally tested and validated with available data. Once validated, the models can be used to predict behavior in regimes not achievable in the laboratory.

The challenge at the atomistic level is to learn how individual dislocations move and interact in the presence of an applied stress. Dislocations—which appear as extra or displaced planes of atoms inserted into the regular latticelike structure of a metal crystal—allow otherwise crystalline material to deform plastically without brittle fracture or failure. Figure 3 shows examples of edge and screw dislocations. Edge dislocations resemble an extra sheet of paper slipped part way into a stack of sheets. In a screw dislocation, the atomic planes are twisted like the steps of a spiral staircase.

The energy of a dislocation is stored largely as strain in the surrounding lattice. The important property of a dislocation is its ability to move easily through the lattice, allowing slip to propagate rapidly. (Slip, or the movement of one atomic plane over another, is the primary way that plastic deformation occurs in a solid.) In bcc metals, screw dislocations limit plastic flow because they are much less mobile than edge dislocations, especially at low temperature or under high strain-rate deformation conditions.

Progress So Far

To date, the team has calculated a wide range of deformation and defect properties for tantalum, validated those calculations, and carried them up to extremely high pressures for many of those properties, including bcc elastic constants. At ambient pressure, the elastic constants agree with measured values. Experiments are under way to measure these quantities at high pressure. Atomistic simulations have been used to predict the atomic structure of selected grain boundaries in niobium, molybdenum, and tantalum. The predicted structures in niobium and molybdenum were confirmed by high-resolution electron microscopy (HREM) experiments, and additional experiments on tantalum are in progress.

The team has also used atomistic simulations to study fundamental properties of screw and edge dislocations in molybdenum and tantalum at ambient pressure. The simulations predicted atomic core structures with unique threefold spreading for the screw dislocations; for molybdenum, this spreading was recently confirmed by HREM experiments in Germany. The minimum, or Peierls, stress required to move these screw dislocations has also been studied as a function of the orientation of the applied stress. This minimum stress can be further reduced by forming local excitations called kinks along the dislocation line, and a study of kink energetics leading to dislocation mobility is in progress.

Bridging Length-Scale Worlds

Microscale modeling bridges the atomic and mesoscale worlds. At the microscale, researchers are developing entirely new three-dimensional, dislocation-dynamics (DD) simulation techniques to model single 15-micrometer-long crystals. In these simulations, dislocation structures are resolved, but individual atoms are not, and the basic building blocks are small segments of individual dislocations. In DD simulations, dislocations move and interact according to linear elasticity laws as well as rules established by atomistic simulations and fine-grained DD simulations of small numbers of dislocations.

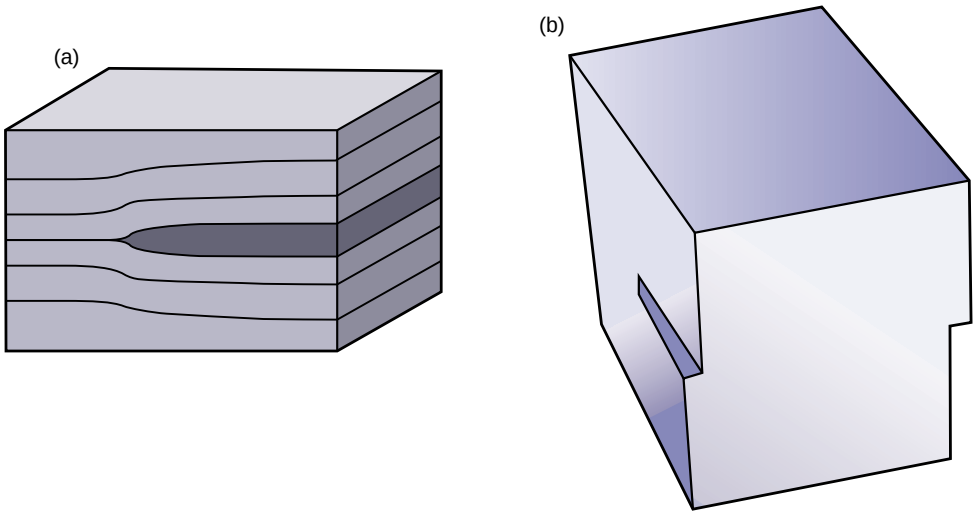

Figure 3. Representation of (a) an edge dislocation and (b) a screw dislocation.

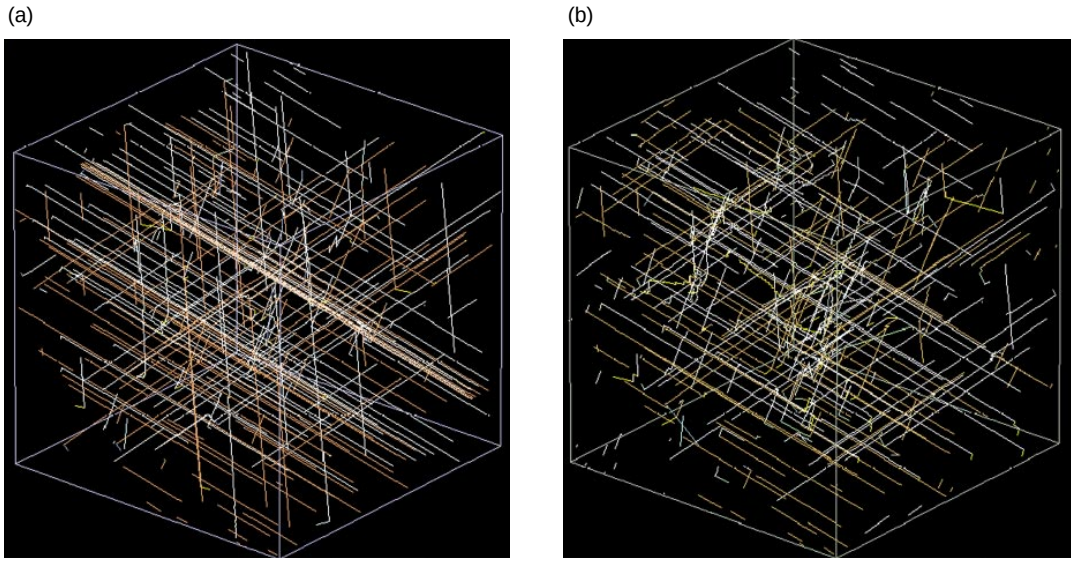

Figure 4. Three-dimensional simulations of dislocation structures in body-centered-cubic tantalum at (a) 197 kelvins and (b) 300 kelvins. The long, straight segments are screw dislocations, while the majority of short segments are edge dislocations.

Developing these rules rigorously is one of the most difficult aspects of the multiscale program. A complementary experimental program is examining dislocation microstructures with transmission electron microscopy and providing stress–strain data on well-characterized, high-purity samples.

The DD simulations provide insights and detailed information about the collective behavior of large numbers of interacting dislocations. They also simulate the evolution of a complex dislocation microstructure under an applied stress (Figure 4). Adds Moriarty, "Dislocations and their distribution are an essential part of plastic deformation. But never before has there been such a powerful tool to model this phenomenon." In the multiscale strategy, the goal at the microscale is to provide a full quantitative description of single-crystal plasticity, including the yield stress and stress–strain relationships. With currently available phenomenological input, the DD simulations have provided accurate results for the single-crystal yield stress in tantalum, including its temperature dependence.

The derived laws of single-crystal plasticity will ultimately be used in mesoscale-modeling simulations to predict the deformation of millimeter-sized tantalum polycrystals, that is, multiple single crystals with different orientations packed together into a single specimen. In mesoscale modeling, the individual crystals and their boundaries are resolved, but microstructures and individual dislocations are not. At this scale, scientists are using finite-element simulation codes such as NIKE3D and ALE3D to examining how a system of randomly arranged, computer-generated single crystals—a virtual test sample—deforms in response to an applied stress. The mesoscale-modeling results will finally be used to derive constitutive relations that describe macroscopic plasticity.

The multiscale-modeling program expects to complete its task in about eight more years, linking quantum-based atomistic models all the way up to finite-element-based mesoscopic simulations. When complete, the models will help stockpile stewardship scientists confidently predict the performance of stored weapons and changes that might occur in the stockpile, as well as provide basic information about material behavior of interest to the nation's industrial products manufacturers.

—Ann Parker

Key Words: atomic scale modeling, body-centered-cubic (bcc) crystal structure, dislocation dynamics (DD), edge dislocation, mesoscale modeling, microscale modeling, multiscale modeling, polycrystals, screw dislocation, stockpile stewardship, transmission electron microscopy.

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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

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Arthur W. Molvik Albert R. Ellingboe	**Helicon Wave Excitation to Produce Energetic Electrons for Manufacturing Semiconductors** U.S. Patent 5,824,602 October 20, 1998	A means of controlling a helicon plasma source by varying the axial magnetic field or radio-frequency power controlling the formation of the helicon wave. An energetic electron current is carried on the wave when the magnetic field is 90 gauss (G), but there is minimal energetic electron current when the magnetic field is 100 G in one particular plasma source. Similar performance can be expected from other helicon sources by properly adjusting the magnetic field and power to the particular geometry. This means of control for adjusting the production of energetic electrons can be used in the semiconductor and thin-film manufacturing process. It is especially advantageous in multilayer semiconductor manufacturing because trenches can be formed that are in the range of 0.18 to 0.35 millimeters or less.
William P. Chandler Christine L. Hartmann–Siantar James A. Rathkopf	**Calculation of Radiation Therapy Dose Using All Particle Monte Carlo Transport** U.S. Patent 5,870,697 February 9, 1999	A means of calculating the actual radiation dose absorbed in the body using the three-dimensional Monte Carlo transport method. Neutrons, protons, deuterons, tritons, helium-3, alpha particles, photons, electrons, and positrons are transported in a completely coupled manner, using this Monte Carlo all-particle transport method. The major elements include computer hardware, radiation source description, physical databases, Monte Carlo transport method, and output of dose distributions. Dose distributions are estimated for neutrons, photons, electrons, positrons, and heavy charged particles incident on any biological target, with resolutions ranging from micrometers to centimeters. Calculations can be extended to general-geometry (non-Cartesian) grids for other media.
David J. Erskine	**Noise Pair Velocity and Range Echo Location System** U.S. Patent 5,872,628 February 16, 1999	An echo-location method for microwaves, sound, and light capable of using incoherent and arbitrary waveforms of wide bandwidth to measure velocity, range, and target size simultaneously at high resolution. Two interferometers having very long, nearly equal delays are used in series with the target interposed. The first interferometer imprints a partial coherence on an initially incoherent source. The second interferometer performs autocorrelation on the reflected signal to determine velocity. A coherent cross-correlation subsequent to the second interferometer with the source determines a velocity-discriminated range.
Steve P. Swierkowski	**Micromachined Chemical Jet Dispenser** U.S. Patent 5,877,580 March 2, 1999	A dispenser for precisely ejecting chemical fluid samples. The dispenser is a microelectromechanical system (MEMS) device fabricated in a bonded silicon wafer and a substrate, such as glass or silicon, using integrated circuitlike fabrication technology amenable to mass production. Dispensing is actuated by ultrasonic transducers that produce a pressure wave in capillaries containing chemicals. The 10- to 200-micrometer-diameter capillaries can be arranged to focus in one spot or can be arranged in a larger dense linear array (about 200 capillaries). The dispenser, analogous to a computer ink-jet print head, does not heat up, so damage of certain samples does not occur. Applications are in biological sample handling and analytical chemical procedures.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Clifford B. Dane Lloyd A. Hackel	**All Solid-State SBS Phase Conjugate Mirror** U.S. Patent 5,880,873 March 9, 1999	A simulated Brillouin scattering (SBS) phase conjugate laser mirror uses a solid-state nonlinear gain medium instead of the conventional liquid or high-pressure gas medium. The concept has been effectively demonstrated using common optical-grade fused silica. An energy threshold of 2.5 megajoules and a slope efficiency of over 90 percent were achieved, resulting in an overall energy reflectivity of greater than 80 percent for 15-nanosecond, 1-micrometer laser pulses. The use of solid-state materials is enabled by a multipass resonant architecture that suppresses the transient fluctuations that would damage the SBS medium. This all-solid-state phase conjugator is safer, more reliable, and more easily manufactured than those based on prior designs. It allows nonlinear wavefront correction to be implemented in industrial and defense laser systems whose operating environments preclude the introduction of potentially hazardous liquids or high-pressure gases.
M. Allen Northrup Conrad M. Yu Norman F. Raley	**Porous Silicon Structures with High Surface Area/Specific Pore Size** U.S. Patent 5,882,496 March 16, 1999	Fabrication and use of porous silicon structures to increase surface area of heated reaction chambers, electrophoresis devices, thermopneumatic sensor–actuators, chemical preconcentrates, and filtering or control-flow devices. In particular, such high-surface-area or specific-pore-size porous silicon structures will be useful in significantly augmenting the adsorption, vaporization, desorption, condensation, and flow of liquids and gases in applications that use such processes on a miniature scale.
Anthony F. Bernhardt	**Electrochemical Formation of Field Emitters** U.S. Patent 5,882,503 March 16, 1999	A method of electrochemical formation of field emitters that is particularly useful in the fabrication of flat-panel displays. Fabrication involves field-emitting points in a gated field-emitter structure. Metal field emitters are formed by electroplating, and the shape of the formed emitter is controlled by the potential imposed on the gate as well as on a separate counter electrode. The method allows sharp emitters to be formed more inexpensively and easily than they can be by the vacuum deposition processes used currently. The fabrication process involves etching of the gate metal and the dielectric layer down to the resistor layer and then electroplating the etched area and forming an electroplated emitter point in the etched area.
Robert Chow Gary E. Loomis Ian M. Thomas	**Optical Coatings of Variable Refractive Index and High-Laser-Resistance from Physical-Vapor-Deposited, Perfluorinated Amorphous Polymer** U.S. Patent 5,882,773 March 16, 1999	A method of making variable-index optical single-layer, optical multilayer, and laser-resistant coatings from a perfluorinated amorphous polymer material by physical vapor deposition. A vapor of polymer material, such as bulk Teflon AF2400, is deposited on a substrate to form thin layers that have an extremely low refractive index (about 1.10 to 1.31), are highly transparent from the ultraviolet through the near-infrared regime, and maintain the low refractive index of the bulk material. The refractive index can be changed by varying either the deposition rate or the substrate temperature. The coating can be used in antireflectors and graded antireflection coatings as well as in optical layers for laser-resistant coatings at optical wavelengths of less than about 2,000 nanometers.

(continued)

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Richard F. Post	**Method for Leveling the Power Output of an Electromechanical Battery as a Function of Speed** U.S. Patent 5,883,499 March 16, 1999	A method of leveling the power output of an electromechanical battery during its discharge while maximizing its power output into a given load. The method employs the concept of series resonance, using a capacitor, the parameters of which are chosen optimally to achieve the desired near flatness of power output over any chosen charge–discharge speed ratio. Capacitors are inserted in series with each phase of the windings to introduce capacitative reactances that act to compensate the inductive reactance of those windings. This compensating effect both increases the power that can be drawn from the generator before inductive voltage drops in the windings become dominant and acts to flatten the power output over a chosen speed range. The values of the capacitors are chosen to optimally flatten the output of the generator over the chosen speed range.
Thomas E. McEwan	**Ultra-Wideband Impedance Sensor** U.S. Patent 5,883,591 March 16, 1999	The ultrawideband impedance sensor (UWBZ sensor, or Z sensor) is implemented in differential and single-ended configurations. The differential UWBZ sensor employs a subnanosecond impulse to determine the balance of an impedance bridge. The bridge is configured as a differential sample-and-hold circuit that has a reference impedance side and an unknown impedance side. The unknown impedance side includes a short transmission line whose impedance is a function of the near proximity of objects. The single-ended UWBZ sensor eliminates the reference side of the bridge and is formed of a sample-and-hold circuit having a transmission line whose impedance is a function of the near proximity of objects. The sensing range of the transmission line is bounded by a two-way travel time of the impulse, thereby eliminating spurious Doppler modes from large distant objects that would occur in a microwave continuous-wave impedance bridge. Thus, the UWBZ sensor is a range-gated proximity sensor. It senses the near proximity of various materials such as metal, plastic, wood, petroleum products, and living tissue. It is much like a capacitance sensor, yet it is impervious to moisture. It has broad application in the replacement of magnetic sensors, particularly where nonferrous materials need to be sensed and in sensing full/empty levels in tanks, vats, and silos.

Awards

Michael MacCracken has been named a **fellow** of **the American Association for the Advancement of Science**. He was cited for "leadership of modeling of climate and air quality, for studies of natural and anthropogenic effects on climate, and for coordination of national and international research activities." A former leader of the Laboratory's Global Climate Research Division, MacCracken credits the collective efforts of his colleagues in the Earth and Environmental Sciences Directorate for the honor. Their projects include work to develop the Bay Area air quality model and contributions to the region's successful air quality maintenance plan; model development and studies of the climatic effects of greenhouse gases, volcanoes, and nuclear war; assessment of ozone concentrations at all levels of the atmosphere; and work with the Atmospheric Release Advisory Capability and international collaborations.

MacCracken is currently on assignment in Washington, D.C., as executive director of the U.S. Global Change Research Program's National Assessment Coordination Office.

Abstracts

Forewarnings of Coming Hazards

The Atmospheric Release Advisory Capability (ARAC) at Lawrence Livermore is an emergency response organization chartered to aid Department of Energy and Department of Defense sites when radioactive or toxic material is released into the atmosphere. Developed from studies beginning in the 1960s, it became a funded operational program in the late 1970s. Using an emergency response modeling system now in its third generation, ARAC scientists predict how atmospheric releases that could affect public health and safety will disperse. The ARAC system has evolved through experience gained during regular training exercises and in over 160 alerts and emergency responses to date. The work of ARAC scientists described in the article demonstrates the different modeling challenges they encounter in preparing for and responding to a variety of atmospheric emergencies.

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Unraveling the Mystery of Detonation

Laboratory experts in the detonation of high explosives are putting the computational power of the Accelerated Strategic Computing Initiative (ASCI) to the test. Their research centers on insensitive explosives, whose behavior during detonation is slower and more complex than that of sensitive explosives. The article features three research projects, which are exploring detonation from different angles: the initiation phase, the molecules produced during detonation, and further development of CHEETAH, a thermochemical detonation code. All research teams are using ASCI supercomputers, which have increased their ability to simulate the detonation process by a factor of 100,000.

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Coming Next Month

On Target: Designing for Ignition

A report on the laser targets being designed for fusion experiments at the National Ignition Facility.

Also in July–August

- Adaptive optics improve telescopic views of the skies.
- Atomic-scale simulations of complex systems.
- Developing small, agile service satellites.

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