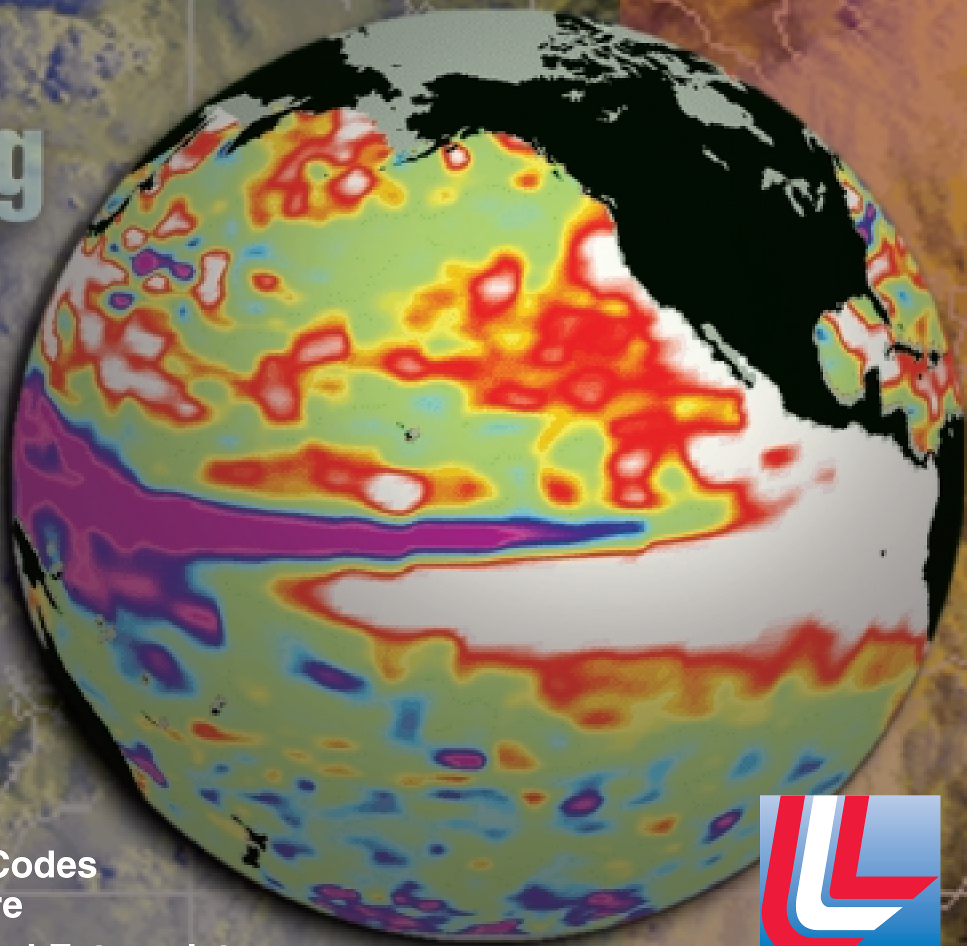
Science & Technology REVIEW

July/August 2002

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

Clearer Look at Global Warming



Also in this issue:

- Experiments Help Codes Predict Metal Failure
- Mathematical Method Extrapolates More, Better Information
- 50th Anniversary Highlight: Anticipating and Countering Ever-Changing Threats

Lawrence Livermore
National Laboratory

Making History
Making a Difference

1952-2002

About the Cover

Natural phenomena affect temperatures on Earth and are part of the mix of effects that climatologists must understand before they can come to any definitive conclusions about global warming. In the foreground, a globe shows sea surface height measurements, taken by satellite, during El Niño conditions. In the background is the volcanic ash cloud from the 1991 eruption of Mount Pinatubo in the Philippines. Accounting for the effects of these events is helping climate researchers to better understand what is happening to global climate. That accounting, along with other work to steadily improve climate models, is described in the article beginning on p. 4. (Globe image courtesy of National Aeronautics and Space Administration; Mount Pinatubo image courtesy of National Oceanic and Atmospheric Administration.)

Cover design: Kitty Tinsley

About the Review

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

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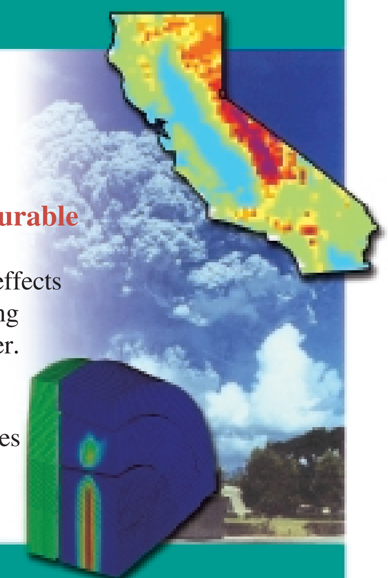

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Interim measures to save the Salton Sea

California has long been using more than its allotment of Colorado River water and now is under mandate to reduce that usage. One way the state plans to achieve the reduction is to save on agricultural water usage.

In the Imperial Valley agricultural region of southern California where such saving is being proposed, one concern has to do with the effects of conservation on the aquatic ecosystem at the Salton Sea, which depends on agricultural runoff to keep its salt levels down. If runoff were decreased, dilution would decrease, the Salton Sea's salt levels would rise, its fish would die, and the migratory birds—for which the sea is a key stop—would have no food.

At the request of California Representative Duncan L. Hunter, Livermore researchers conducted studies to come up with recommendations on how to stave off increased salinity in the Salton Sea. The researchers recommended that irrigation canal water that has seeped into the ground, on the order of some 145,000,000 cubic meters per year, be reclaimed and fed into the Salton Sea. They also proposed the construction of evaporation ponds to extract salt from the sea. And they are looking at ways to use geothermal energy to desalinate Salton Sea water and then pump it back in.

Dave Layton, division leader for the Laboratory's Health and Ecological Assessment Division and one of the researchers on this project, said that the proposal requires more study and drilling of test wells to see if it is worthwhile to pump water into the Salton Sea. He added, "In any event, the use of groundwater would only constitute an interim measure and would have to be linked to management actions regarding other potential mitigation measures for the Salton Sea."

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Bioterrorism detectors also protect food supplies

Livermore biomedical scientist Paula McCready told her audience at a meeting of the American Society for Microbiology last May that "The tools we use to develop DNA signatures for the detection of bioterrorist agents could also be used to search out food-borne pathogens."

DNA signatures, the regions of DNA unique to specific organisms, are being identified much more quickly as a result of advances in DNA sequencing. What used to take years to find has been condensed to a period of weeks or months. This is important because now DNA signatures can be quickly developed for new strains of pathogens.

And using those signatures in another application—to find the bacteria that cause food poisoning—allows laboratories to more rapidly identify their presence in food and in the environment. The diagnostic tests to identify such food bacteria have been lessened from hours and days to under one hour because scientists no longer need to culture and prepare samples before analysis.

"We can tailor our tests to distinguish harmful forms of different organisms from the benign forms," says McCready. Among the bacteria that could be identified, according to her, are *Camphylobacter*, a bacterium present in undercooked chicken, or *Salmonella*, a bacterium that can be found in eggs, juice, fruit, or vegetables.

Livermore researchers and other biomedical scientists have developed highly accurate DNA signatures for the bacteria that cause plague and anthrax as well as for other organisms. This work has been performed in collaboration with Los Alamos National Laboratory researchers and the Bioterrorism Rapid Response and Advanced Technology Laboratory of the Centers for Disease Control and Prevention in Atlanta.

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Osmium has it over diamonds in stiffness

Stiffness is the measure of a material's compressibility. The stiffest materials also tend to be the hardest ones. But in the case of diamonds and osmium, the former is still the hardest, even though the latter is stiffer. This surprising information was discovered by Laboratory physicist Hyunchae Cynn, who decided to look at osmium because its stiffness had never been accurately measured. "It caught my eye," he said.

When the bulk modulus—resistance to compression—of osmium turned out to be higher than that of diamond, no one really believed it. So Cynn crushed the osmium under 60 gigapascals of pressure in a diamond-anvil device and looked at the resulting x-ray diffraction patterns to determine the spacing between crushed osmium atoms. The data gave osmium a bulk modulus of 462 gigapascals compared with the 443 gigapascals for diamond.

Because osmium is so different from other materials with high bulk modulus, Cynn says that researchers should take a closer look at metals and other materials to see if they might have missed discovering any properties simply because the properties were unexpected.

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Integration Is Key to Understanding Climate Change

IN March 2001, President George W. Bush chose to delay support of the Kyoto Protocol, which recommends that industrialized nations reduce their emissions of carbon dioxide. The Kyoto Protocol is a product of the 1997 United Nations Framework Convention on Climate Change. Although the protocol addresses environmental issues, implementing it will affect the nation's industries and economy. The President reasoned that the contribution of human-made carbon dioxide to climate change is not yet understood well enough to form the basis for a national policy.

More recently, the administration sent a report to the United Nations indicating that human activity may be affecting global climate change. As a leader in research on climate change, Livermore plays an important role in developing needed understanding of the complex causes behind our changing climate.

A recent organizational change at Livermore has simplified the framework for that research. The Energy and the Environmental and Earth Sciences directorates have been combined into a single Energy and Environment Directorate, allowing Laboratory research to more easily link environmental factors to technologies related to energy production and use.

In this new directorate, research focuses on three interrelated issues: energy technologies (which may release carbon), management of human-made carbon (which may reduce carbon's effects on climate), and global climate–carbon modeling. Understanding the complex interactions between Earth's system and human activities in the biosphere requires that all three issues be examined as an integrated package.

The article beginning on p. 4 is an example of this integrated approach. In examining the climate record to detect climate change, Livermore scientists separated, for the first time, the effects of volcanic eruptions and El Niño from the effects of human activity. Concurrently, they evaluated the practical effects of the interplay of human activities and the regional environment to reveal that while climate phenomena may be global, the effects can vary from location to location.

Over the next century, fossil fuel will remain the primary avenue for energy production and use. Energy emissions, especially carbon dioxide, will be the impetus behind a more comprehensive focus on the management of excess carbon. At Livermore, our climate modeling capabilities will be used to evaluate the effects of emission-producing energy technologies; carbon processes in the biosphere; aerosols, weather, and air quality; and water resources and their management.

An important technology option being examined at Livermore and elsewhere for managing excess carbon is carbon sequestration, which would collect emitted carbon and pump it into the ocean or into rock formations to be stored for thousands of years. Understanding the science behind carbon sequestration will bring us one step closer to being able to manage our climate.

As a national laboratory, Livermore does not make policy. Instead, it provides the scientific understanding that enables policy makers to make informed decisions. By integrating our disciplines and program activities, we are better able to clarify complex scientific issues. Presenting an integrated scientific position for those who do make policy helps to solve challenges of enduring national and global importance.

■ C. K. Chou is associate director of Energy and Environment.

The Outlook Is for Warming, with Measurable Local Effects

Our planet's climate is warming up. The effects are, for the first time, visible on a regional scale.

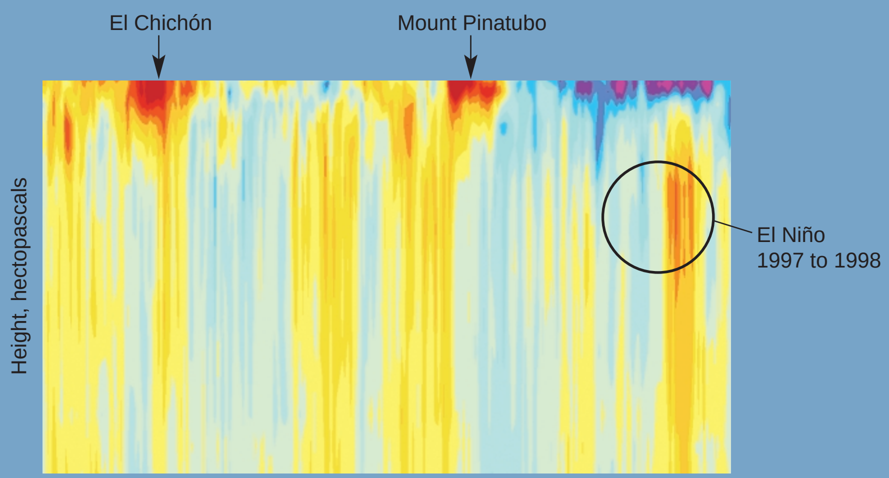
GLOBAL warming. Few phrases elicit so much controversy today. But is our climate truly changing? And if it is, do we know why it is changing?

At the United Nations, the Intergovernmental Panel on Climate Change (IPCC) certainly thinks the world is getting warmer and puts much of the blame on human activity. In its 2001 *Third Assessment Report*, the IPCC projects that average global temperature will increase by 1.6° to 6°C by 2100.

The report indicates that, globally, the 1990s were the warmest decade on record, with 1998 the single warmest year. Accompanying this global-scale temperature increase were changes in other climate variables, such as precipitation, snow cover, glacier extent, and sea level. The changes in these variables are broadly consistent with the IPCC's estimate that Earth's surface warmed by roughly 0.6°C over the 20th century. The 2001 IPCC report concluded that "there is new and stronger evidence that most of the warming observed over the last 50 years is attributable to human activity."

Atmospheric carbon dioxide and other trace gases help keep our planet warm by absorbing some of the Sun's heat that the Earth would otherwise emit back into space. This natural greenhouse effect makes Earth's surface about 34°C warmer than it would be without greenhouse gases. But human activities, such as the burning of fossil fuels, have added greenhouse gases to the atmosphere. Atmospheric carbon dioxide levels, for example, have increased by about 30 percent since the beginning of the Industrial Revolution. This human-caused enhancement of the natural greenhouse effect has contributed to the warming of the planet over the last century.

Climate change can occur even in the absence of human activities. The climate system is like a bell that rings in a certain way. One form of "ringing" is



Globally averaged temperatures have changed at different levels in Earth's atmosphere. This profile is from close to Earth's surface through to the stratosphere. Temperatures are in the form of departures (anomalies) from long-term monthly means computed from 1979 to 1999 and are in degrees Celsius. The stratospheric warming caused by the El Chichón and Mount Pinatubo volcanic eruptions is clearly evident, as is the cooling of the lower atmosphere after Pinatubo. Results are from the so-called reanalysis project jointly performed by the National Center for Environmental Prediction and the National Center for Atmospheric Research.

the ocean warming phenomenon known as El Niño or its cooling sister, La Niña. Such changes are thought to be due to the internal variability of the climate system. But external events can also cause natural climate changes. Large volcanic eruptions can pump massive quantities of dust into the upper atmosphere (the stratosphere). The dust may remain in the stratosphere for years, cooling Earth's surface by absorbing and reflecting some of the incoming sunlight. Natural changes in the Sun's energy output and slow changes in Earth's orbit can also influence climate.

Carbon dioxide and other greenhouse gases get the most press, but there are other human influences as well. Changes in land use can be a concern. For example, Livermore scientists recently showed that human-caused changes in land-use patterns (especially conversion of forests to farm land) may have caused a gradual global cooling of approximately 0.25°C, mostly before the 20th century.

Large-scale burning of rain forests sends particulate matter into the lower atmosphere, warming us. At the same time, with fewer trees, less carbon dioxide can be absorbed from the atmosphere, which warms us further. Land surface changes also affect Earth's reflectivity, or albedo.

If Earth is getting warmer, is it possible to expose individual factors causing climate change? And what will global warming mean on a regional level? Two Livermore research teams are searching for—and finding—answers.

Atmospheric scientist Ben Santer, a 1998 John A. and Catherine T. MacArthur Foundation Fellow, has used sophisticated climate models to separate the effects of recent major volcanic eruptions and El Niños from other causes of climate change. The motivation for this research was to shed light on one of the outstanding puzzles in climate science: why Earth's surface has apparently warmed faster than the lower atmosphere.

At the same time, a team led by physicist Philip Duffy has brought the highest resolution yet to global climate modeling, revealing a wealth of regional effects for the first time. Instead of a 300-kilometer grid—the previous state of the art—Duffy's team has been able to perform global simulations using models with grid cell sizes of 75 and even 50 kilometers. These are the finest-resolution global climate simulations performed to date. The figure on p. 6 compares these resolutions.

Duffy's work would not be possible without Livermore's massively parallel supercomputers, which can quickly perform the computationally demanding calculations inherent in global climate modeling. The first simulations using the 50-kilometer grid ran on the Advanced Simulation and Computing (ASCI) White computer during its initial, unclassified testing period in December 2000. Because the ASCI White computer is now used exclusively for classified computations, models used by Duffy's group are being run on other supercomputers at Livermore and at Lawrence Berkeley National Laboratory.

A 1-year simulation of global climate using the 300-kilometer grid can now be accomplished in 4 or 5 hours. Five years ago, it would have taken over a day to complete a comparable simulation. For the 50-kilometer grid, "At best, we can do about a month of simulated climate in a day," says Duffy. A 50-kilometer grid for climate modeling was the stuff of dreams 5 years ago.

Why the Controversy?

Much of the controversy about global warming results from two apparent contradictions. One relates to observed temperature data and the other to the issue of how well computer models of the global climate system can represent such observations.

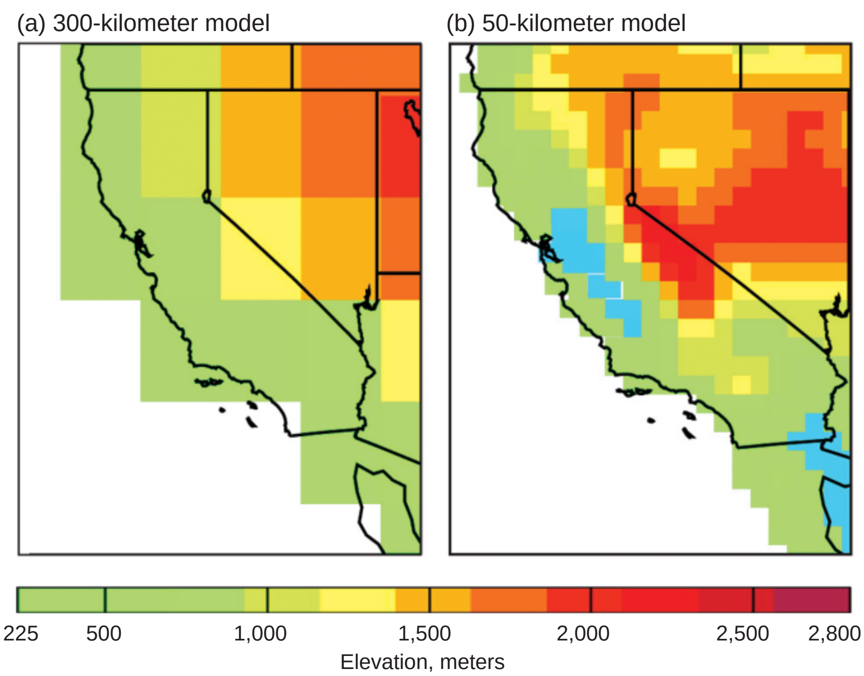
While Earth's surface has warmed by about 0.15° to 0.2°C per decade since 1979, temperatures in the troposphere (the layer of the atmosphere extending from Earth's surface to 8 to 16 kilometers above it) have shown little warming, and even a slight cooling.

The apparent lack of tropospheric warming from 1979 to the present has been used to cast doubt on the reality of strong surface warming. It is important to understand whether this difference between surface and tropospheric warming rates is real or is an artifact of data problems. If this difference is real, what factors might be causing it?

The second puzzle relates to the inability of many climate models to simulate the apparent difference in surface and tropospheric warming rates. This inconsistency is sometimes used to bolster arguments that models are inappropriate tools for making projections of future climate change.

Recent work by Santer and his colleagues has addressed both of these puzzles. They have learned that at least some of the differential warming of Earth's surface and lower troposphere is real and attributable to the combined effects of stratospheric ozone depletion, volcanic eruptions, and natural climate variability. Differences in the geographic regions sampled by the surface thermometer network and the satellite-based tropospheric temperature measurements also explain some of the divergent temperature changes of the surface and troposphere.

"But," Santer concedes, "accounting for these effects still does not fully explain the different rates of temperature change. Nor does it explain why models don't reproduce this differential behavior accurately."



The topography of California and Nevada is simulated in models with (a) 300-kilometer and (b) 50-kilometer grids. Models that use the 300-kilometer grid have been the state of the art, but Livermore has developed a 50-kilometer-grid model. Even with 50-kilometer grids, the topography of California and Nevada is not represented. The Coast Range mountains are not visible in (b), and the data smoothing process lowers the elevation of the Sierra Nevada mountains.

A Search for Resolution

For several years, Santer has been working with other investigators at Livermore and research institutions around the world to reconcile the apparent contradictions in actual data and global climate models. In one study of climate between 1979 and 1998, they discovered that a model including anthropogenic (human-caused) factors and volcanic aerosols produced surface–troposphere temperature differences that were the closest yet to actual observed data.

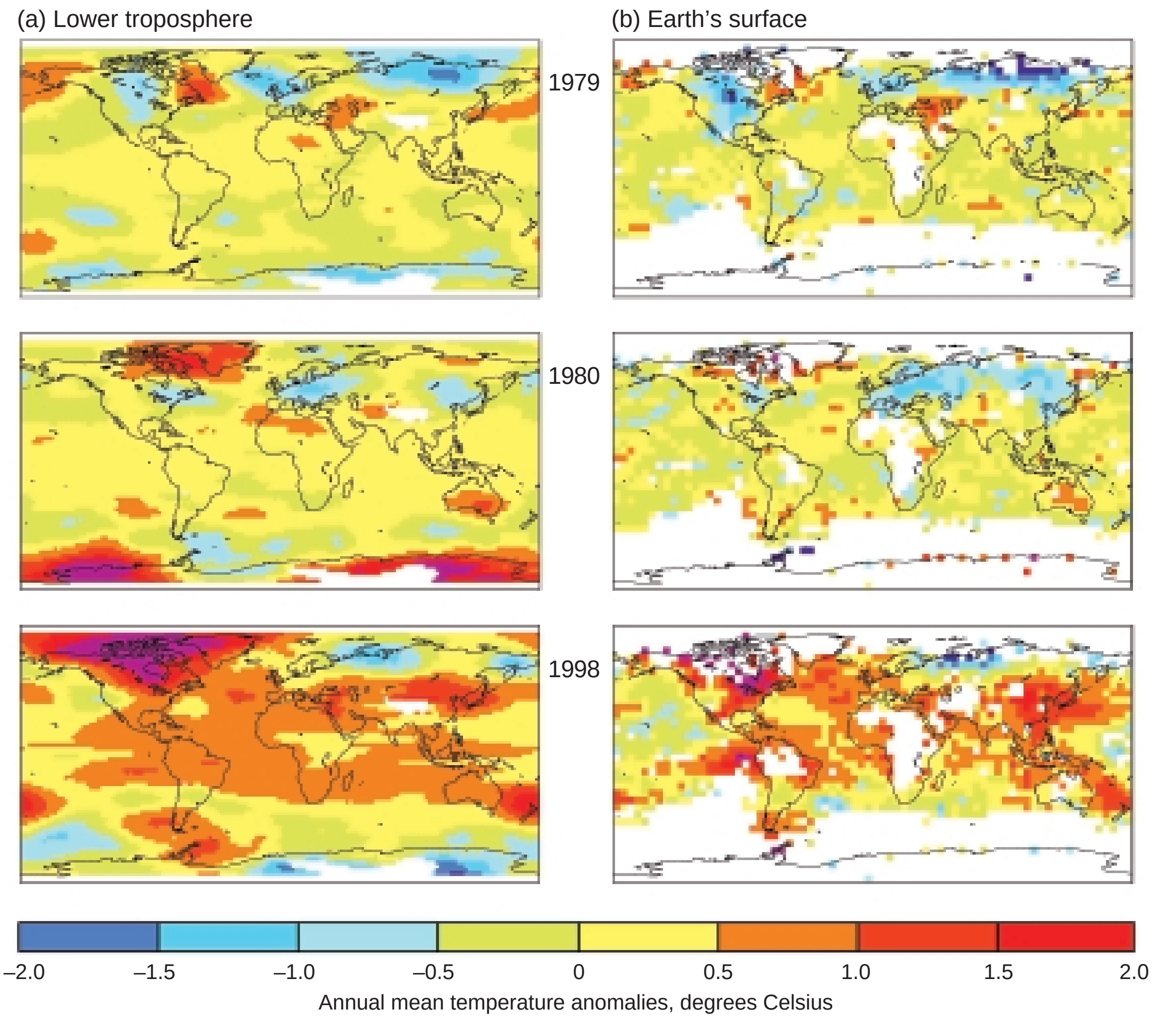
As a follow-up, they wanted to examine the influence of volcanoes alone. But, says Santer, "We had a bit of bad luck. Nature made our lives difficult. There was a major El Niño in

1982, at the same time as the eruption of El Chichón in Mexico. A smaller El Niño coincided with the 1991 eruption of Mount Pinatubo in the Philippines. This made it tough to disentangle the effects that volcanoes and El Niños had on surface and tropospheric temperatures."

Santer and his Livermore colleagues had been doing similar work for the past 10 years. For the first half of that time, they were trying to identify human-caused climate signals in observed temperature records. This involved using both model and observational climate data to understand the characteristic fingerprints of the many natural and anthropogenic influences on climate. (See the figure on p. 8.)

Previous researchers had attempted to remove the effects of explosive volcanic eruptions and El Niños from surface and tropospheric temperatures so they could obtain better estimates of the underlying human component of climate change. But Santer's team was the first to deal fully with the correlation of volcanic eruptions and El Niños, known in statistical problems as collinearity.

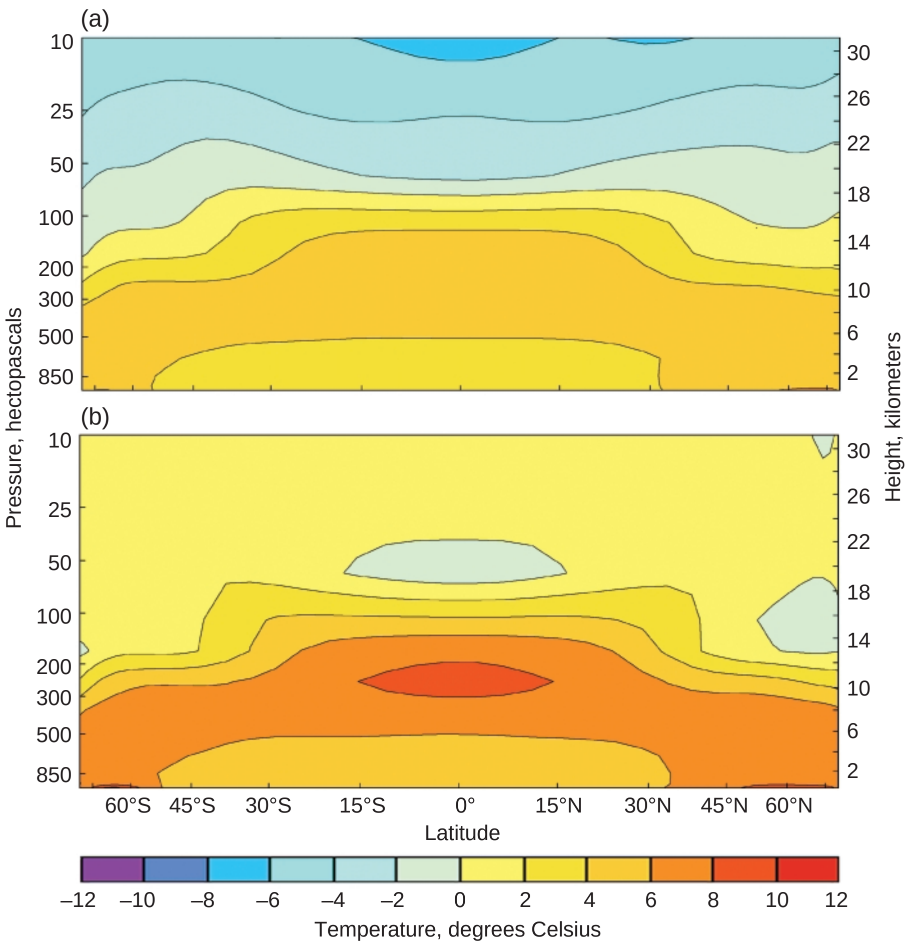
The team's observational data were land and ocean surface temperatures compiled at the Climatic Research Unit in Norwich, England, together with satellite-based tropospheric temperature measurements. Their model data came from a number of different sources: the Max Planck Institute for Meteorology in Hamburg, Germany, the Goddard Institute for Space Studies in New York, and the National Center for Atmospheric Research in Boulder, Colorado. Researchers from all of these organizations participated in the team. Other team members were with Livermore's Program for Climate Model Diagnosis and Intercomparison,



Geographic patterns of annually averaged temperature anomalies in (a) the lower troposphere and (b) at Earth's surface. Tropospheric temperature measurements are from polar-orbiting satellites, and surface measurements were made by thermometers. White areas denote missing data. Although the satellites have near-global coverage, the surface data have large gaps. Comparing satellite and surface data over areas of common coverage helps to explain some of the differential warming of the surface and troposphere. Anomalies are expressed relative to annual mean temperatures averaged over 1979 to 1998.

which routinely develops methods and tools for the diagnosis, validation, and intercomparison of global climate models.

The team first dealt with observed data. They found that removing El Niño and volcanic effects always led to larger warming trends in the residual surface and lower tropospheric data than in the raw observational data (where these effects were left in). Although El Niños caused a small net warming from 1979 to 1999, the El Chichón and Mount Pinatubo volcanic eruptions caused a larger net cooling during the same period. Removing both El Niños and volcanoes more clearly revealed the underlying warming trend in surface and tropospheric temperatures. It also helped to explain some of the differential warming of the surface and troposphere.



(a) Atmospheric temperature changes predicted to occur in response to a doubling of preindustrial levels of carbon dioxide. (b) Projected temperature response to a 2-percent increase in the Sun's energy output. Each factor that influences our climate has a characteristic "fingerprint." Scientists typically use computer models of the climate system to gain information on these fingerprints. In a model, it is possible to study the climatic effects of a single influence only, such as changes in atmospheric carbon dioxide. This is not feasible in the real world, where multiple factors that influence climate are changing simultaneously. Both (a) and (b), which are clearly dissimilar, show annual mean changes (in degrees Celsius) as a function of latitude and altitude.

"It's clear that if the Mount Pinatubo and El Chichón eruptions had not occurred, the lower troposphere would have experienced more pronounced warming," says Santer.

The team then removed volcanic and El Niño effects from model output and compared the results with observations. It is important to do this because even in a model with "perfect" representation of El Niño variability, the simulated El Niños would not necessarily occur at the same time that they happened in the real world. Also, some model experiments include the effects of well-observed volcanoes (such as Mount Pinatubo) but exclude other eruptions where less is known about the properties of the volcanic aerosols. Removing volcano and El Niño effects from both models and observations allows a fairer comparison of the underlying simulated and observed responses to human-caused changes in greenhouse gases.

The general conclusion from such comparisons was that removing volcano and El Niño effects from atmospheric temperature data improves the correspondence of the modeled and observed differential warming of the surface and troposphere over the last several decades. It does not, however, fully reconcile models and reality. The remaining differences are probably caused by problems with the observational temperature data; missing or inaccurately specified "forcings" in the climate model experiments, such as the neglect of land use changes or aerosol particles from biomass burning; and errors in the climate responses that the models predict.

Santer and his colleagues are actively investigating these possibilities. "We hope we've showed that this is a complex scientific issue," says Santer. "It can't be reduced to a one-minute sound bite. This issue is important, because it relates to our ability to evaluate climate models and to determine whether these models are useful tools for predicting climate change over the next century."

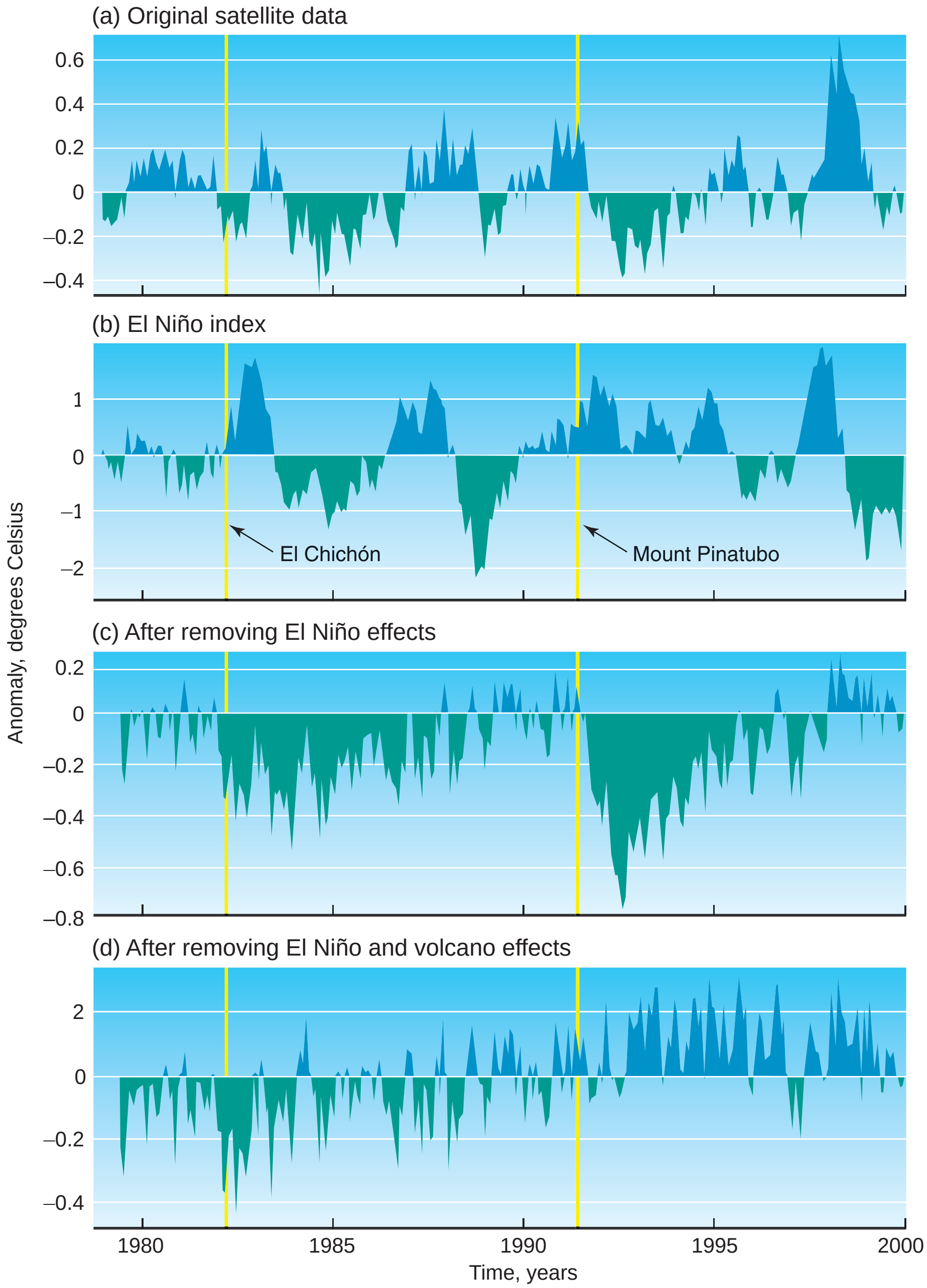
An Up-Close Look

The IPCC's prediction that mean global temperatures will increase from 1.6° to 6°C by the end of this century isn't especially useful for farmers and others whose livelihoods depend on the weather. They need more specific information on temperature increases expected in their area, whether it be Kansas or Kenya. They also need to know about changes in temperature extremes and in other important quantities such as precipitation. By providing improved simulations of climate change on regional scales, Livermore's high-resolution climate simulations should allow for more accurate assessments of the effects of climate change on society.

Grids of 50 kilometers and less are already used in numerical weather prediction, which is much less computationally intensive than climate modeling because it requires much shorter forecasts (days rather than decades). For long-term climate modeling with resolution this fine, scientists had to await the arrival of huge computers with hundreds of processors operating simultaneously.

Duffy's team is using the Community Climate Model 3, or CCM3, an atmospheric model developed by the National Center for Atmospheric Research (NCAR) in Boulder, Colorado. CCM3, the fourth-generation CCM model, is used at coarse resolutions in climate modeling centers around the world.

"For every change in horizontal resolution, there's the problem of retuning the model," says Duffy. Several physical processes such as convection, cloudiness, and precipitation are too small to be represented explicitly in climate models and are therefore treated using semiempirical parameterizations.



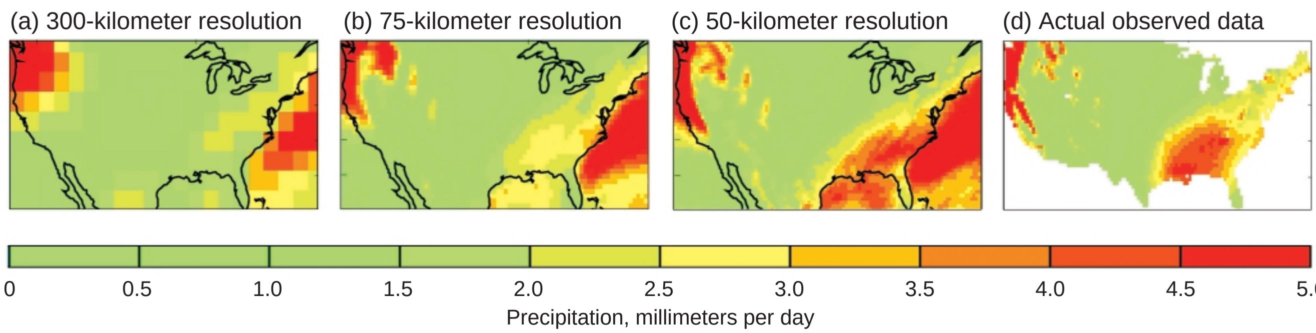
Some of the problems involved in removing the effects of El Niño variability and explosive volcanic eruptions from tropospheric temperature data. (a) In the original satellite-based temperature data, the cooling signal of the 1983 El Chichón eruption is masked by (b) one of the strongest El Niño events of the 20th century. After using an iterative method to successively refine estimates of El Niño and La Niña effects on tropospheric temperatures, these effects are removed from the original temperature data in (a). The cooling effects of the El Chichón and Mount Pinatubo eruptions are now more easily seen in (c). It is clear in (d) that removing both volcanoes and El Niño effects yields a pronounced warming trend that was not apparent in the original temperature data.

For example, although clouds may be too small to be represented directly in a grid cell, they must be accounted for because cloud cover affects the flow of radiation in the atmosphere. “So we parameterize their effects by modifying the optical properties of that layer of the atmosphere,” says Duffy.

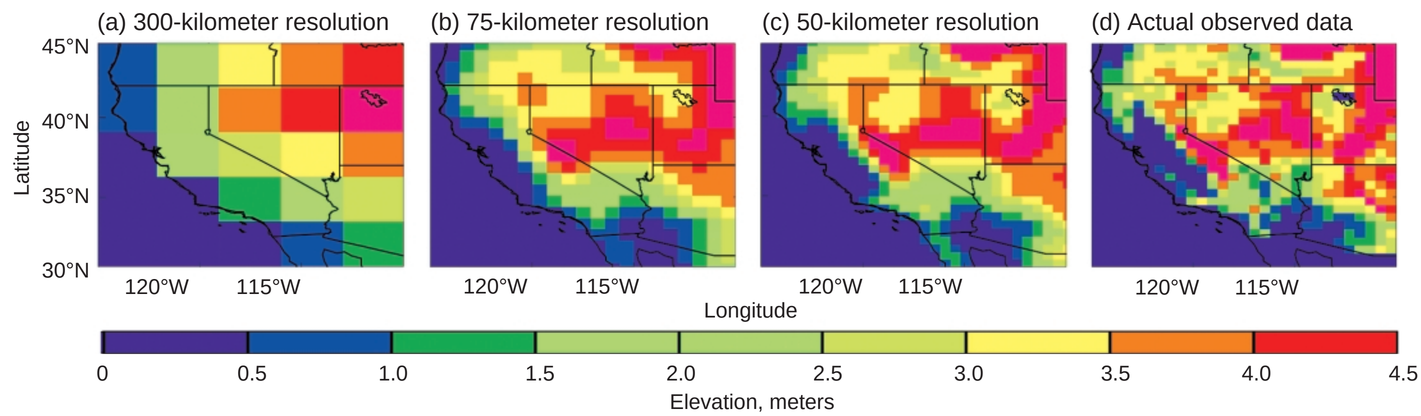
Because these parameterizations are not based on first-principles physics, they must be tuned carefully at each resolution. Tuning is done by adjusting parameter values to make the model’s results agree as closely as possible with observations. The 300-kilometer model has already been carefully tuned at NCAR to optimize results at that resolution. In collaboration with researchers at NCAR, Livermore researchers retuned their 75-kilometer model. Thus far, tuning done for the 75-kilometer model has also worked reasonably well with the 50-kilometer grid.

The team’s proof of principle with the 50- and 75-kilometer models was to compare their modeling results to observed data. Although, as Duffy notes, “the 50-kilometer model actually has better resolution than most of our observational data.” Perhaps not surprisingly, simulations using the 50-kilometer model agreed better with observed data than either a 75- or 300-kilometer grid. In some cases, there were substantial improvements.

When the team examined results in more localized regions of interest, the results were striking. The upper figure below shows simulated precipitation over the U.S. in December, January, and February using 50-, 75-, and 300-kilometer grids and compares all three to observed data. As the grid size shrinks, both small-scale and large-scale simulated precipitation features converge toward observations. This example shows



The representation of December, January, and February precipitation over the U.S. improves as the resolution increases. Simulations using (a) 300-kilometer, (b) 75-kilometer, and (c) 50-kilometer resolution are compared with (d) actual observed data. Both fine- and large-scale aspects of the simulation improve as spatial resolution shrinks.

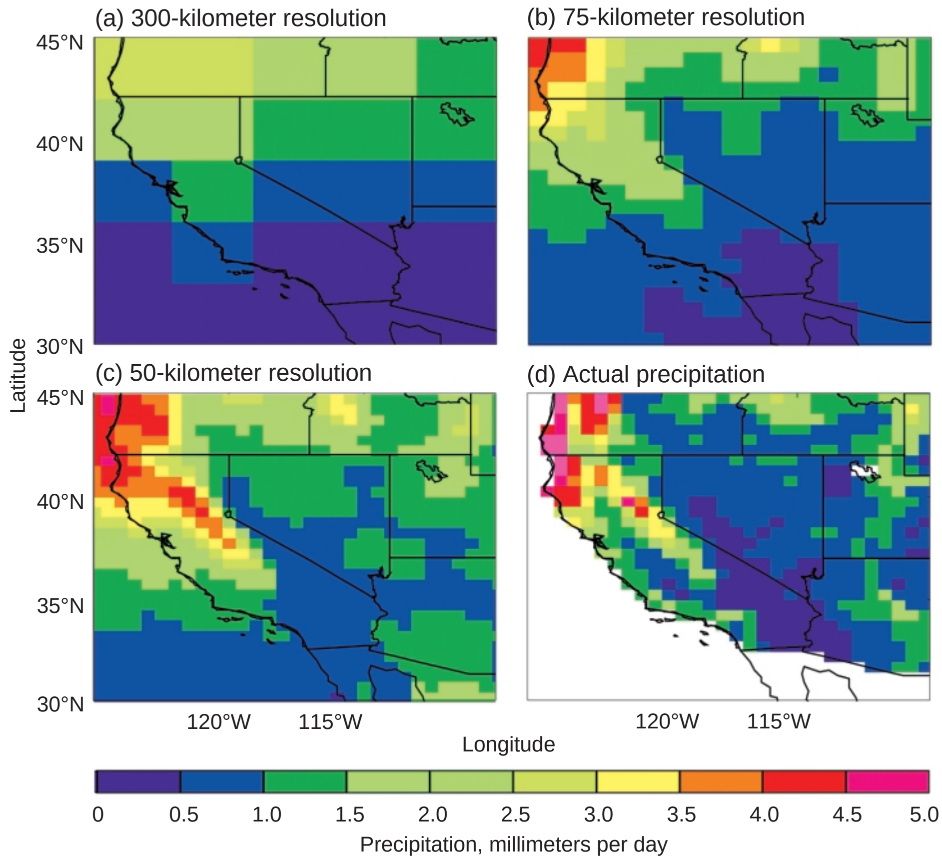


A comparison of elevations in California, as represented in models having (a) 300-kilometer, (b) 75-kilometer, and (c) 50-kilometer resolution, with (d) actual elevations at 50-kilometer resolution. Elevations in the models are lightly smoothed—evened out—to prevent sudden changes that cause numerical noise and contaminate the results. Even at 50-kilometer resolution, California’s Coast Range mountains and the Central Valley are not well represented.

that as spatial resolution becomes finer, not only is fine-scale detail added to the model results, but the large-scale aspects of the solution also become more realistic.

Simulations of California climate are a real test of climate models because of the great variability in climate that occurs within the state's relatively small area. Much of this variability results directly or indirectly from the state's major topographic features: the Coast Range, the Central Valley, and the Sierra Nevada. The figure at left, bottom, compares actual elevations at 50-kilometer resolution with topography as represented in models having 300-, 75-, and 50-kilometer resolutions. Although the topography is more realistic as the model resolution becomes finer, neither the coastal mountains nor the Central Valley are adequately represented in even the 50-kilometer model.

In part because of improved representations of topography, the model's ability to simulate precipitation in California improves dramatically as the resolution becomes finer. Nonetheless, 50-kilometer resolution is still not adequate to represent the state's Coast Range and Central Valley; even at this resolution, the simulation of precipitation differs noticeably from observations.



A comparison of precipitation over California, as represented in models at (a) 300-kilometer, (b) 75-kilometer, and (c) 50-kilometer resolution, with (d) actual precipitation at 50-kilometer resolution.

Simulations of Arctic climate similarly improve dramatically with finer resolution, but further improvements are nonetheless needed. Most coarse-resolution ocean–atmosphere–sea ice climate models produce poor simulations of the pattern of sea-level pressure in the Arctic region. Poor data for sea-level pressure result in unrealistic simulated atmospheric circulation, which in turn produces unrealistic distributions of sea ice thickness and concentrations and other problems. Accurate predictions of sea ice and of changes in sea ice because of global warming are essential. Sea ice strongly affects the climate not only in polar regions but also in far-flung regions through influences on the large-scale ocean circulation and on Earth's radiation balance.

In addition to these simulations of the present climate, Duffy's team has simulated the effects of increased greenhouse gases (that is, global warming) with the 75-kilometer-resolution model. This is the finest-resolution simulation of global warming performed to date and shows very different results from comparable simulations performed at coarser resolutions. Although the globally averaged responses of temperature and other variables to increased greenhouse gases are quite similar in the 75-kilometer model and in coarser-resolution models, the regional responses can be very different. For example, the figure on p. 12 shows predicted wintertime temperature changes between 2000 and 2100 in the U.S. The finer-resolution model shows regions of strong warming in the western U.S. and southeastern Canada, which are not predicted by the coarser-resolution model. In at least some cases, it seems clear that the results of the finer-resolution model are more believable.

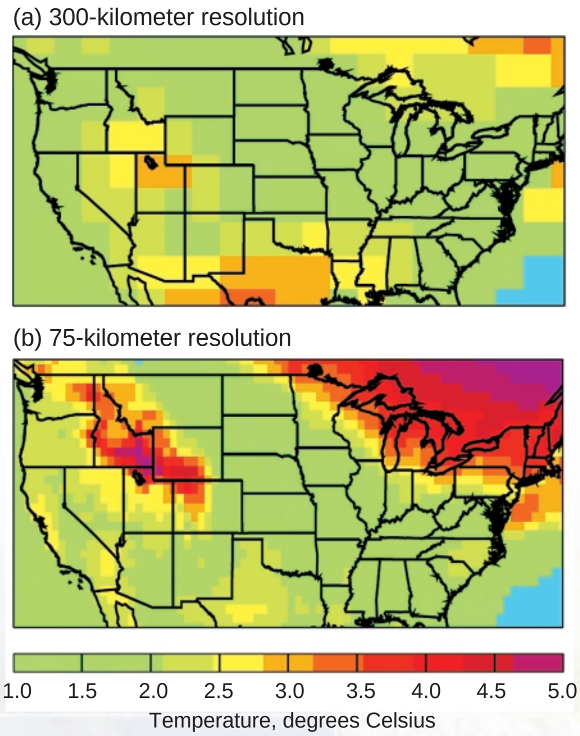
Duffy's group has already fielded inquiries from experts interested in the effects of localized climate change on crop diseases, human health, water resources, and the like. Although the finer-resolution models are far from perfect, they may represent the best tools available today for assessing the regional effects of global warming.

Getting It Right

A few months ago, a chunk of ice larger than Rhode Island collapsed on the east side of Antarctica. It was the largest single event in a series of ice shelf retreats there extending back 30 years. Temperatures at the Antarctic Peninsula have increased by 2.5°C over the last 50 years, much faster than the global average. Getting Arctic and Antarctic models right is crucial for determining what may happen to sea levels around the world as temperatures continue to rise.

Closing in on how much humans are responsible for the changes in our planet's climate is equally important. Getting it right matters to us all.

—Katie Walter



Predicted temperature increases from 2000 to 2100 for December, January, and February at resolutions of (a) 300 kilometers and (b) 75 kilometers. The predicted data from the model with finer resolution are much more specific and useful.

Key Words: climate modeling, Community Climate Model 3 (CCM3), global warming, National Center for Atmospheric Research (NCAR).

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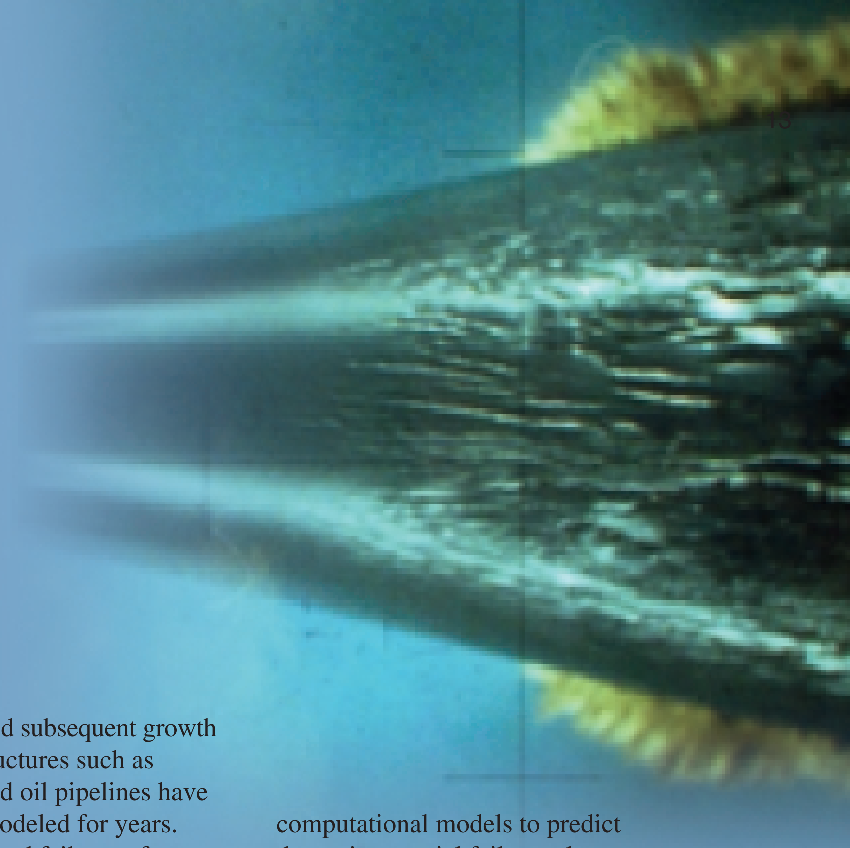
For information about the Intergovernmental Panel on Climate Change:

www.ipcc.ch/

For information about Livermore's Program for Climate Model Diagnosis and Intercomparison:

www-pcmdi.llnl.gov/



How Metals Fail

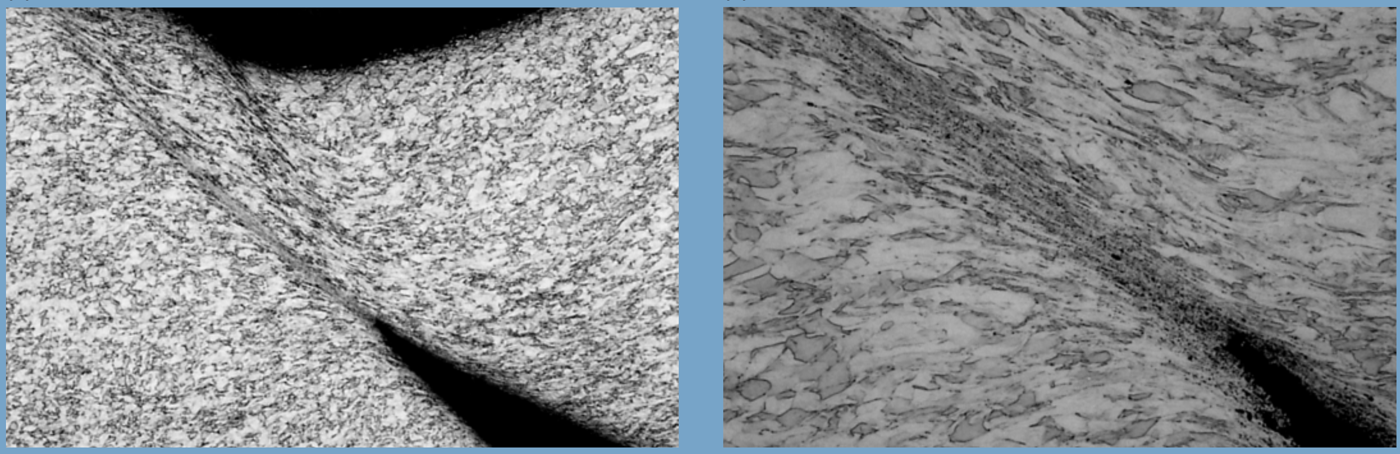
Laboratory experiments point the way to a new generation of computer codes for predicting metal failure.

THE initiation and subsequent growth of cracks in structures such as bridges, aircraft, and oil pipelines have been studied and modeled for years. In contrast, cracks and failures of parts driven by high-explosive detonations are less well understood and poorly modeled. Much more complete information is needed in these cases because the Laboratory's defense-related mission requires an understanding of how metals respond to the sudden shock waves and subsequent high-strain-rate deformations caused by high explosives.

In particular, one of the challenges facing the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program is using computational models to predict dynamic material failure relevant to nuclear weapon safety and reliability. Changes in material properties caused by aging nuclear warheads must be represented in computer simulations that accurately reflect the particular metal's internal structure.

"Our ability to account predictively for dynamic material failure is inadequate and, in some cases, primitive," says Livermore engineer Richard Becker. "We want our computational models to reflect in detail how cracks form, evolve, and

(a) (b)



(a) This micrograph of a tantalum–tungsten alloy cylinder driven by a gas gun shows that the material breaks along shear bands (darker diagonal line). (b) The crack tip at a higher magnification. (Micrograph produced by Anne Sunwoo.)

lead to the failure of a part," he says. Becker is a member of Livermore's code development team that supports NNSA's Advanced Simulation and Computing (ASCI) program. He is using results from experiments conducted at Livermore and elsewhere to construct advanced computer models of how metals crack and ultimately fail.

The new models will help to assure nuclear weapon safety and reliability as well as to advance nonnuclear military applications used to design equipment such as shaped charges and armor-defeating projectiles. The new models will also likely benefit a number of industrial processes, such as explosive welding and shock processing, which use high explosives.

Physicist Elaine Chandler, an associate division leader in the Laboratory's Defense and Nuclear Technologies Directorate, was the original architect of the combined modeling and experimental effort on dynamic failure, which now spans several Livermore directorates. The goal, she says, is to couple theory, simulation, and experiments to yield a much better predictive capability for the behavior of ductile metals—metals such as copper and aluminum that bend before breaking—under extreme conditions of high pressures and high strain rates (deformation). "We need real physics underpinnings for models of how materials fail," she says.

The experimental effort consists of several multidisciplinary projects, some supported by Laboratory Directed Research and Development funds, that investigate different aspects of dynamic failure.

The experiments use well-characterized ductile metals, experimental tools such as gas guns and scanning and transmission electron microscopes, and advanced facilities such as the Laboratory's Janus laser and High Explosives Applications Facility, the University of Rochester's Omega laser, and the Stanford Synchrotron Radiation Laboratory. Together, the experiments cover a wide range of strain rates and pressures. An important focus of the experimental effort is the development of novel diagnostics to illuminate the microsecond-by-microsecond details of material fracture and failure.

The experimental results are being incorporated into Becker's advanced computational models. Becker says that traditional codes provide only simple characterizations of the dynamic fracture behavior of ductile metals. Often, they prescribe just the minimum pressure at which the metal fails. "We need to more accurately capture the complex underlying processes so that we can better account for the influence of microstructure, strain rate, and pressure on the failure of ductile metals. We also need to simulate the orientation of cracks and the recompression of material that is possible following severe cracking."

Becker sees a significant drawback to current models in that they do not take into account a metal's microstructure, which is known to control its mechanical properties. Metals are composed of microscopic grains that have different orientations and, inevitably, contaminants. Some aspects of the subgrain microstructure change dramatically when subjected to a strong shock from a high-explosive detonation. In particular, a strong shock induces numerous dislocations within a metal's crystalline lattice, which changes the metal's mechanical properties such as its strength, ductility, and resistance to cracking.

In addition, shocked ductile metals are known to develop cracks by nucleation (formation), growth, and linking up of microscopic voids, and a metal's microstructure also affects void nucleation and growth. For example, impurities and inclusions often act as void nucleation sites. What makes the current suite of Livermore experiments so important, says Becker, is that the metals under investigation have their microstructure characterized both before and after being subjected to different strain rates and pressures.

Shocking Samples with Lasers

Materials scientist Geoff Campbell is looking at the connection between shear (displacement across a narrow band of material) and fracture in shocked metals. He notes that when metals fail at high rates, the behavior is often associated with shear that is confined within narrow bands. These shear bands are typically precursors to the formation of cracks. The metal deforming within the shear bands becomes hot and softens, which makes it susceptible to failure.

To gain a fundamental understanding of shear localization and fracture, Campbell conducts experiments in which he determines the mechanical properties of shocked metals. He creates the shocked microstructure with laser-shock processing, a method that is considerably easier and less expensive than high-explosives-driven methods. The solid-state, high-energy (50-joule), neodymium-doped glass laser was developed at Livermore as part of a method, now commercialized, to improve the fatigue performance of metals by imparting intense shocks. (See *S&TR*, March 2001, pp. 26–28.)

In Campbell's experiments, the laser pulses the metal sample several times to achieve conditions similar to explosively shocked material. Each laser shot lasts only 20 to 50 nanoseconds, compared to a high-explosive detonation that typically lasts about 1 microsecond.

Campbell's focus is on three metals: copper, tantalum, and a tantalum–tungsten alloy. "These are popular, well-understood materials at the Laboratory, and they allow different experimental teams to compare results," he says.

Following laser shocking, Campbell determines traditional mechanical properties and the degree to which the metals are susceptible to crack propagation and ultimate failure, information that is critical to the development and calibration of Becker's computational models. The information is obtained with tests that measure the material's strength as it is being deformed and the strain energy release required to propagate a crack. The same tests are also performed on unshocked samples as controls.

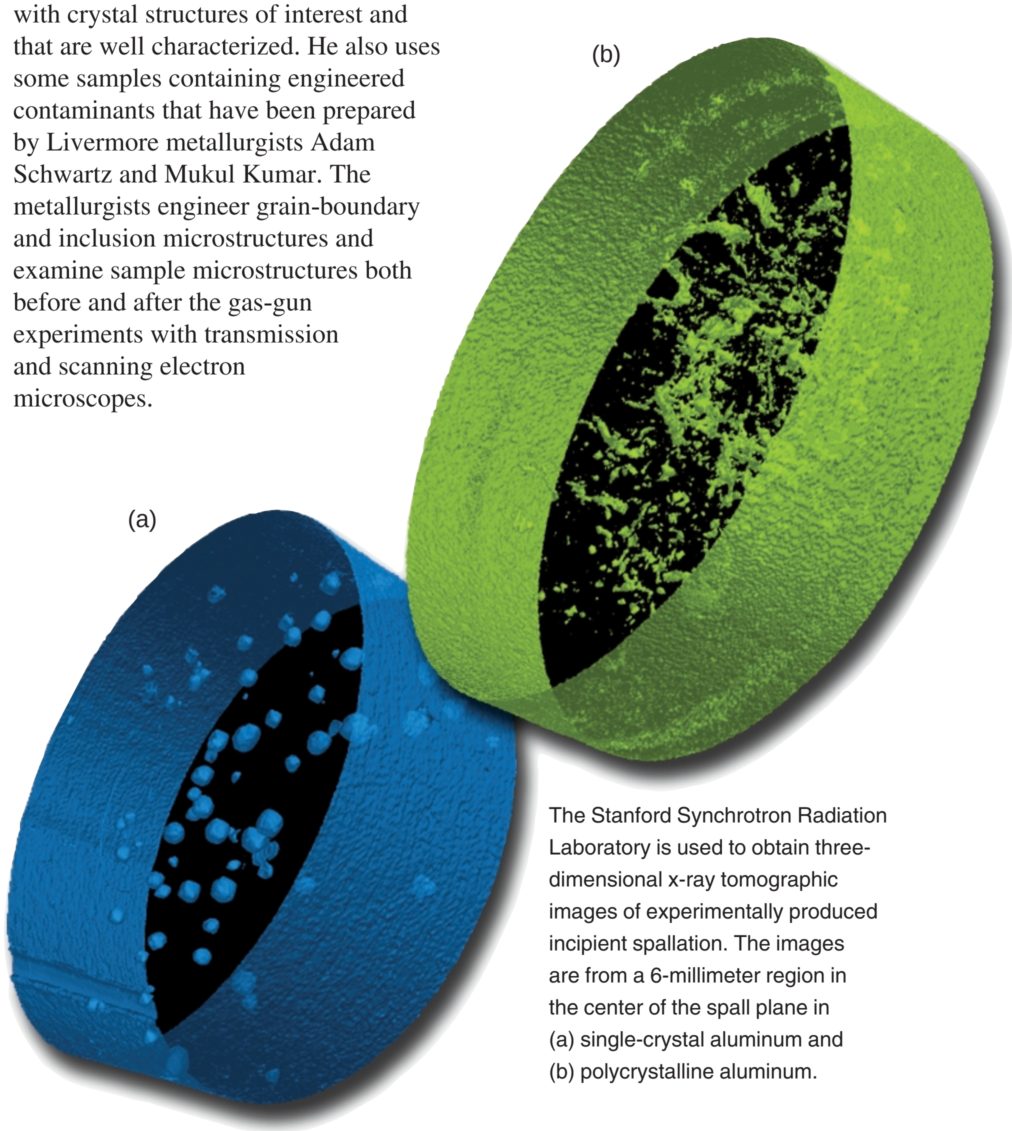
Campbell notes that understanding the real response of materials has always been important to national security as well as industry. During World War II, Liberty Ships were manufactured using welds for the first time instead of rivets. It was not appreciated at the time that the welds could become brittle below a certain temperature, and several ships broke in two. Some sank right after launch, while others were lost suddenly at sea.

Gas Guns Create Spall

Physicist Jim Belak is looking at the microstructural origins of dynamic fracture in ductile metals to obtain a better understanding of beginning damage from spallation, the scab that forms near the metal surface during high-explosive detonations. "We lack a detailed model of spall fracture," says Belak. He explains that spall fractures occur when a shock wave reflects from a surface and produces extreme tension inside the solid. When this tension exceeds the material's internal rupture strength, the solid fails by rapidly nucleating voids, which quickly link to form fractures. The origin of the voids is tied to the solid's microstructure, especially weak points such as inclusions and boundaries between metal grains. Improving our understanding of spall requires correlating the observed incipient damage with the well-characterized microstructure.

Belak and colleague James Cazamias use the Livermore gas-gun facility to create spall in samples of aluminum, copper, titanium, and vanadium, metals with crystal structures of interest and that are well characterized. He also uses some samples containing engineered contaminants that have been prepared by Livermore metallurgists Adam Schwartz and Mukul Kumar. The metallurgists engineer grain-boundary and inclusion microstructures and examine sample microstructures both before and after the gas-gun experiments with transmission and scanning electron microscopes.

The gas gun shoots a metal flyer at velocities ranging from 150 to 210 meters per second. Though higher velocities are possible, the slower velocity is used to create incipient damage. The flyer hits a 25-millimeter-diameter thin metal target of the same material. The target has outside rings that reduce unwanted effects associated with the specimen's edges. At impact, the rings break off, and the 16-millimeter-diameter center of the target flies into a catch tank, where it is recovered with minimal additional deformation.



The Stanford Synchrotron Radiation Laboratory is used to obtain three-dimensional x-ray tomographic images of experimentally produced incipient spallation. The images are from a 6-millimeter region in the center of the spall plane in (a) single-crystal aluminum and (b) polycrystalline aluminum.

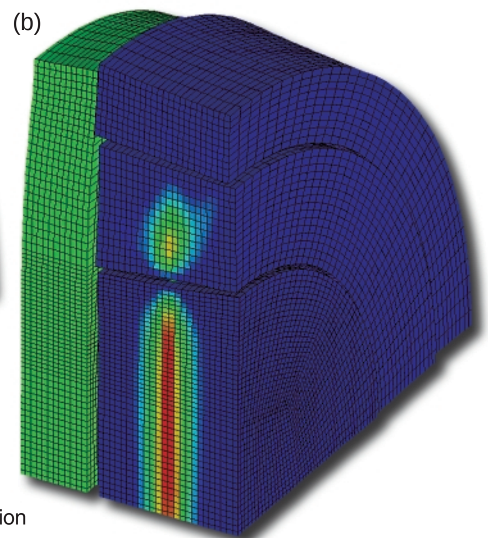
Belak and physicist John Kinney take the target pieces containing incipient spall to the Stanford Synchrotron Radiation Laboratory to obtain three-dimensional (3D) x-ray tomographs in 700 orientations. The images, which have a resolution of about 5 micrometers, are combined to compute the 3D size and space distribution of the voids that have been created during spallation fracture. The data are essential input to spallation models. After the tomographic data are taken, the samples are sectioned to make detailed comparisons with traditional two-dimensional microscopy.

"The synchrotron imagery that Jim is obtaining is quite a breakthrough," says Chandler. "We obtain data of the 3D void distribution just from the images and without having to take thin slices of the material and count the number of voids in each slice."

Belak and physicists Robert Rudd and Eira Seppälä are also performing 3D simulations at the atomic level that track how voids grow and link. The simulations feature 1 to 10 million atoms representing the crystal structure of aluminum or copper. When tensile forces are applied in different directions, the simulations reveal the dislocation mechanism by which microscopic voids grow. The spall recovery experiments using single-crystal copper and aluminum will enable direct validation of these dislocation mechanisms.

(a)

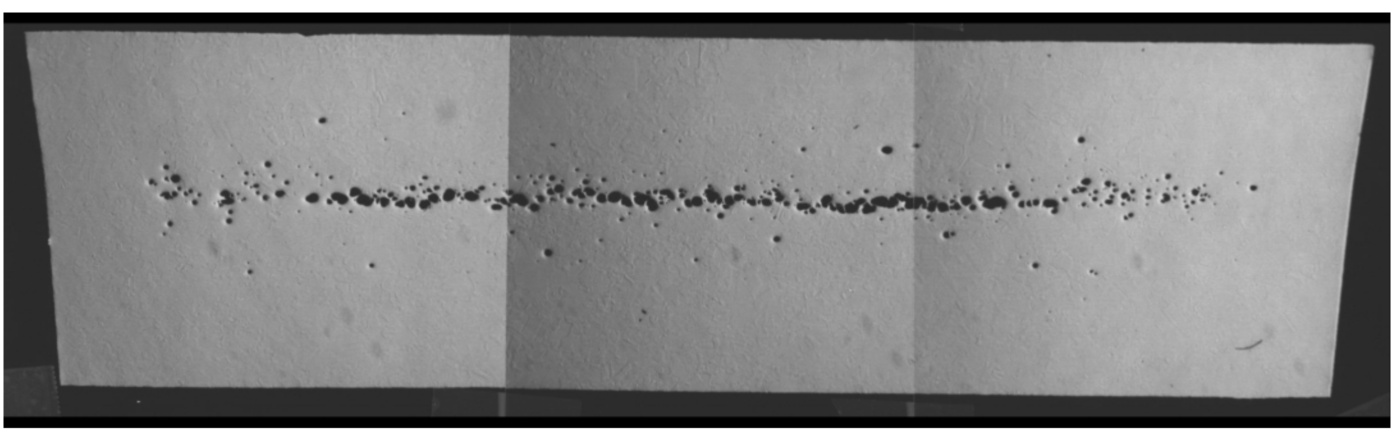
(b)



In this simulation of a gas-gun experiment, (a) is the initial configuration of aluminum striking a copper target, and (b) shows formation of spall. The green area on the left is the aluminum plate that strikes a 5-millimeter-thick cylindrical disk target. The target's two spall rings can be seen on the disk. The formation of voids (red) is seen in the center of the disk.

Closing Up Voids

In some cases, layers of a spalled material can collide as the pressure from the high explosive continues to drive one of the surfaces. The result can be recompression of the spalled material, which closes the voids created by the original shock. Under these conditions, the damaged material could jet out from pores, continue deforming, have localized heating, and even melt.



This photomicrograph of a copper disk used in a gas-gun experiment shows the formation of voids in the spall layer.

Currently, simulations do not include experimentally based models of recompression behavior. Including such models is necessary for accurate stockpile stewardship calculations, says Becker. “We want to determine the material response as these two pieces meet, obtain estimates for the strength of the recompressed region, and insert a recompression model in our ASCI code.”

Becker and his colleagues are performing recompression experiments on recovered metal disks that contain well-characterized spall damage. They use a gas gun and copper targets the same size and shape as those used in Belak’s experiments.

The targets are soft-recovered—that is, captured using soft materials that do not further damage them—and small specimens containing spall are excised from them. The samples are then compressed at various rates to close the voids. Becker monitors the microstructure evolution and the manner in which the damage is being closed. Then the targets are sectioned and micrographs taken of them to examine the recompressed microstructure and track the evolution of the voids.

The data obtained from these experiments will be used to construct a model describing the material behavior during recompression and the residual strength in the damaged samples. The recompression component of an overall model will provide a more accurate representation of material behavior for explosively loaded materials.

“This is a first-cut model based on limited data, but it is a major step along the way toward developing an accurate and robust simulation capability for recompressed damaged materials for stockpile stewardship,” says Becker.

Probing with X Rays

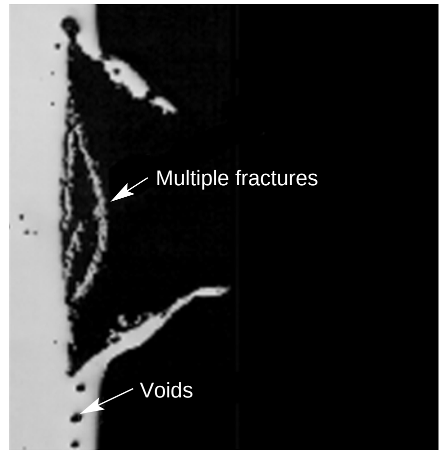
Using lasers, physicist Dan Kalantar has also demonstrated the recovery of shocked single-crystal copper samples about 500 micrometers thick. The experimental results are helping to refine the development of models of void growth and spall formation.

The laser experiments provide pressures—in some cases exceeding 100 gigapascals—greater than those produced by related laboratory experiments using high explosives. The laser pulse lasts 2 to 5 nanoseconds and exerts a maximum pressure at the driven side of the sample. The pressure wave decays as it propagates into the material, resulting in a range of pressures accessed in a single experiment.

One series of experiments is devoted to developing a technique called time-resolved, dynamic x-ray diffraction. This technique uses a high-intensity laser beam focused on a thin metal foil (such as vanadium or iron) to create a source of x rays. The x rays diffract from a single-crystal sample that is shocked by direct laser irradiation with a separate laser beam.

The diagnostic x rays provide a means for recording the response of the metal’s lattice as the shock from the laser pulse passes through. The x rays are diffracted simultaneously from multiple planes within the metal’s crystalline lattice. Kalantar has developed a large-angle film detector that records the diffracted x rays. In addition, optical and electron microscopes are used on recovered shocked targets to determine the metal’s altered microstructure.

Kalantar has also demonstrated, with the Omega laser, the recovery of shocked single-crystal copper samples about 500 micrometers thick. Direct laser irradiation generates a high-pressure shock that causes the formation and coalescence of voids, and this void formation and coalescence in turn create spall. Optical and electron microscopy are used on thin slices of the targets to investigate the final structure. The effect of the dislocation microstructure on the x-ray diffraction pattern is compared with the dynamic x-ray diffraction pattern.



Example of void formation and spall fracture in a copper sample after the passage of a powerful shock wave from the Janus laser at Livermore. Direct laser irradiation generates a high-pressure shock that causes the formation and coalescence of voids, which in turn create spall.

Kalantar is working to extend the dynamic diffraction experiments using the two beams of the Janus laser. In addition, to expand the experiments that Becker is performing, he is designing two-beam experiments to shock materials, create voids and incipient spall with one beam, and then recompact them with the second beam.

Putting It All Together

As experimenters across the Laboratory acquire data, Becker incorporates them into his evolving models of how materials fracture and fail under extreme conditions. “The data from material characterization, metallurgical analysis, and dynamic experiments are helping to constrain and guide our 3D code development,” says Becker. In particular, the code development effort is being aided by

Exploding Metal Cylinders Solve Part of the Puzzle

Physicists Ted Orzechowski, Omar Hurricane, and colleagues are exploding cylindrical samples of metals and monitoring how they fracture and then fly apart. The researchers analyze the failure of the metal cylinders through high-speed images and characterize the fragments that are explosively produced. "We're missing a fundamental understanding of material failure. Just having a big computer, without the correct physics models, is not going to help," says Hurricane.

Hurricane, in collaboration with Lalit Chhalabildas and his group at Sandia National Laboratories, is looking at the failure of metals at high strain rates caused by 2.5-centimeter-long, Lexan™ flyers fired from a gas gun and traveling at about 2 kilometers per second. The flyer slams into another piece of Lexan inside a metal cylinder about 5 centimeters long, with an inner diameter of 1.2 centimeters, and 1, 3, or 5 millimeters thick. The cylinder materials are 1045 steel (a common steel formulation), nitinol (nickel–titanium alloy), and tantalum–tungsten alloy. "Upon impact, the Lexan behaves a bit like a 'working fluid,' driving the cylinder radially outward," says Hurricane.

The gas-gun experiments are more controlled and compact than high-explosives experiments, and researchers do not have to contend with smoke obscuring the high-speed cameras. The shock wave from the Lexan–Lexan impact sweeps through the surrounding metal cylinder with a pressure of about 2.4 gigapascals. "Although there is a shock, it is the rapid radial expansion that causes the material to fracture," says Hurricane.

The experiments are heavily monitored with diagnostics that record the strain rate at different positions on the cylinder. Optical cameras allow Hurricane to watch stop-action movies as cracks form, spread, and quickly tear apart the cylinder. In the case of the tantalum–tungsten alloy, the cracks are associated with shear bands, which tend to form at 45-degree angles from one another.

In what Hurricane likens to a forensic examination, metallurgist Anne Sunwoo cuts up the soft-captured fragments (that is, fragments captured with light materials to prevent further damage) and examines them with a transmission electron microscope to study the metal's altered microstructure.

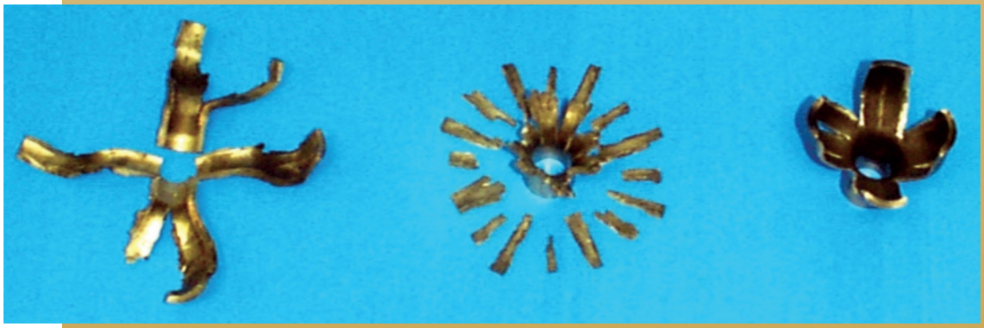
The gas-gun cylinder experiments provide a direct way to document differences in failure according to the changing microstructure of the metal cylinder. Although identical Lexan projectiles are used, there are obvious differences in cracks, fragment size and number, and microstructure of the failed pieces, depending on the metal.

High Explosives Increase the Pressure

Orzechowski and colleagues are conducting experiments similar to Hurricane's, but they are using high explosives to study the dynamics of fragmenting cylinders. These "pipe bomb" experiments involve pressures some 10 times greater (about 20 gigapascals) than those generated in the gas-gun experiments, but the different pressure regimes complement each other, Orzechowski says.

The experiments are providing the data required to develop, improve, and validate material failure models for different kinds of weapons. "We want to improve the understanding of failure and fragmentation of metals and alloys subjected to explosive force," Orzechowski says. In addition to stockpile stewardship applications, the research is relevant to understanding material failure in conventional weapons. The research is funded by Laboratory programs and a Memorandum of Understanding with the Department of Defense's Office of Munitions.

The cylinders measure about 5 centimeters in outside diameter and 20 centimeters long. Preliminary experiments were conducted by John Molitoris at Livermore's High Explosives Applications Facility. Physicist Peter Bedrossian is continuing the experiments at the Laboratory's remote Site 300. The cylinders, made from 1045 steel, Aermat 100 steel, or a uranium alloy, are detonated from one end. The high-explosive

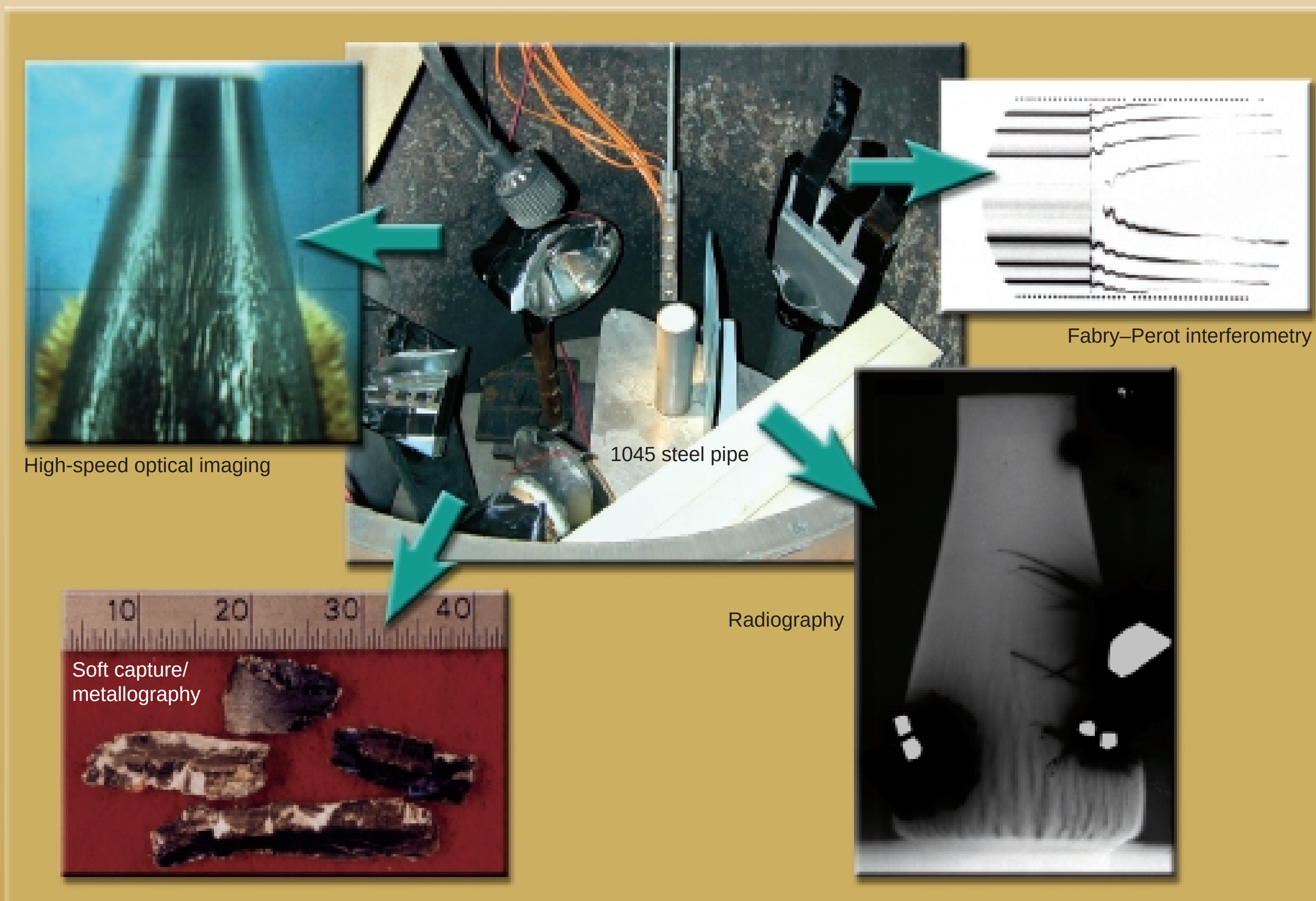


Gas-gun cylinder experiments provide a direct way to quantify differences in material failure. Even under identical drives, differences in cracking and failure are obvious.

detonation front sweeps along the axis, with the shock lasting for several microseconds. The metal fragments that are violently produced are soft-captured with glass wool or other light materials.

A wealth of information is provided by diagnostics, including Fabry–Perot interferometry (which provides time-dependent surface velocity measurements), high-speed optical imaging, and conventional radiography. In addition, a series of proton radiograph experiments, using smaller scale pipes, was conducted at the Los Alamos National Laboratory Neutron Science Center by Livermore physicists Bedrossian and Hye-Sook Park. The proton radiography provides sequential radiographs that show the details of cracks evolving and the cylinder disintegrating into many fragments. (See *S&TR,* November 2000, pp. 12–18.) Metallurgist Sunwoo also characterizes the cylinder metal before the experiment and examines the recovered fragments to help determine their mode of failure.

Like the gas-gun experiments, shear bands are found where the cylinder rips apart. As with the experiments conducted by other researchers, the tests show that a material's microstructure may affect its performance. For example, the experiments reveal differences between steel cylinders that are heat-treated to increase hardness and those that are untreated.



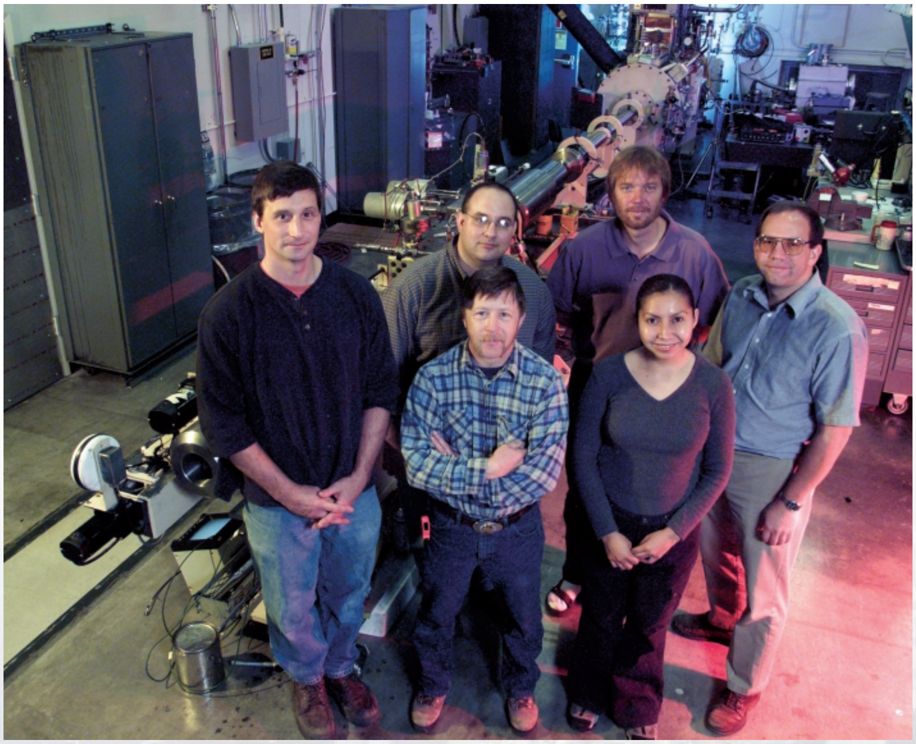
Experiments using high explosives to study the dynamics of fragmenting cylinders are well-diagnosed. Diagnostic instruments include high-speed optical imaging, metallography, radiography, and Fabry–Perot interferometry.

insights gained from examining different material microstructures both before and after experiments. Initial simulations employing the advanced models are encouraging, but much work remains to be done.

Becker notes that the modeling effort is aided by simulation advances made by other Laboratory researchers. Geophysicists such as Lew Glenn have long sought to accurately model the way rocks fracture. Because rocks are brittle, simulations of their fractures are not directly applicable to ductile metals, but methods to account for crack orientation and certain numerical techniques can be applied to modeling ductile metal fractures. Also, some metals important to stockpile stewardship, such as beryllium, are brittle. And glass, a highly brittle material, is vitally important to scientists preparing to operate the National Ignition Facility, now under construction at Livermore to serve the stockpile stewardship mission.

Becker is looking forward to offering scientists a robust, flexible model that can simulate different metals under a wide range of extreme pressures and strain rates. The payoff will be increased confidence in the nation's nuclear stockpile.

—Arnie Heller



Researchers at the gas-gun facility. In the front row, from left, Keith Lewis, Sam Weaver, and Erica Nakai. In the back are James Cazamias, Jim Belak, and Rich Becker.

Key Words: Advanced Simulation and Computing (ASCI), Fabry–Perot interferometry, gas gun, high explosives, High Explosives Applications Facility, Janus laser, Office of Munitions of the Department of Defense, Omega laser, proton radiography, Site 300, spall, Stanford Synchrotron Radiation Laboratory, stockpile stewardship, three-dimensional x-ray tomography.

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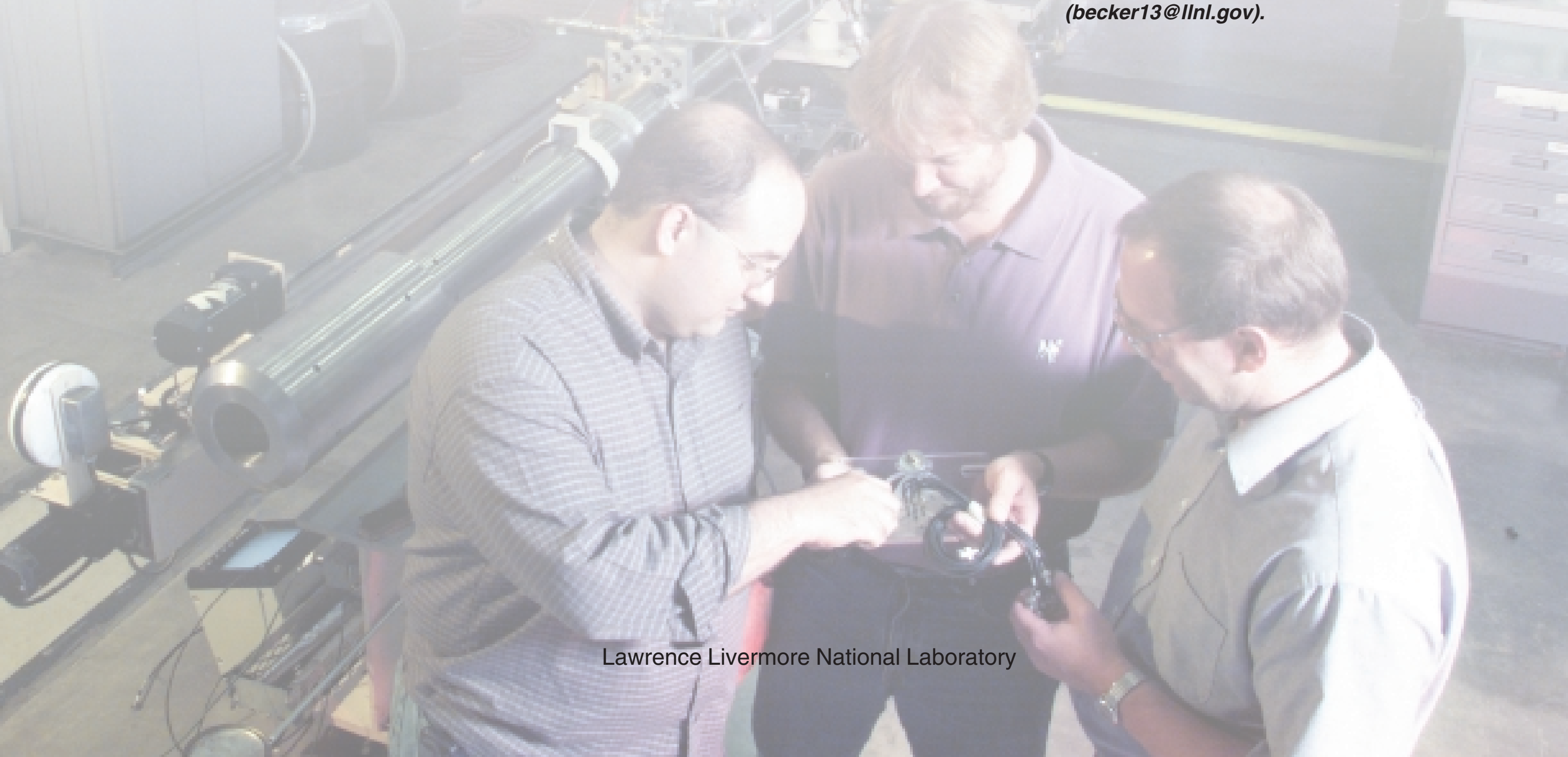


Converting Data to Decisions

ENVIRONMENTAL data aren't easy to obtain, and once obtained, they are often hard to interpret. For example, drilling into the earth to determine what kind of soil exists at any given spot in the substrate is not only expensive but also gives scientists just piecemeal information. Computer analysis with this information can be equally piecemeal. But earth scientists are learning that computer models can be made more meaningful when they are stochastic, meaning that they are based on a certain amount of probability. Now, with the capability of high-performance supercomputers in the National Nuclear Security Administration's Advanced Simulation and Computing (ASCI) program, Livermore scientists are exploring groundbreaking ideas in statistical theory that will help them use stochastic descriptions quantitatively and obtain a much more complete picture of soil composition.

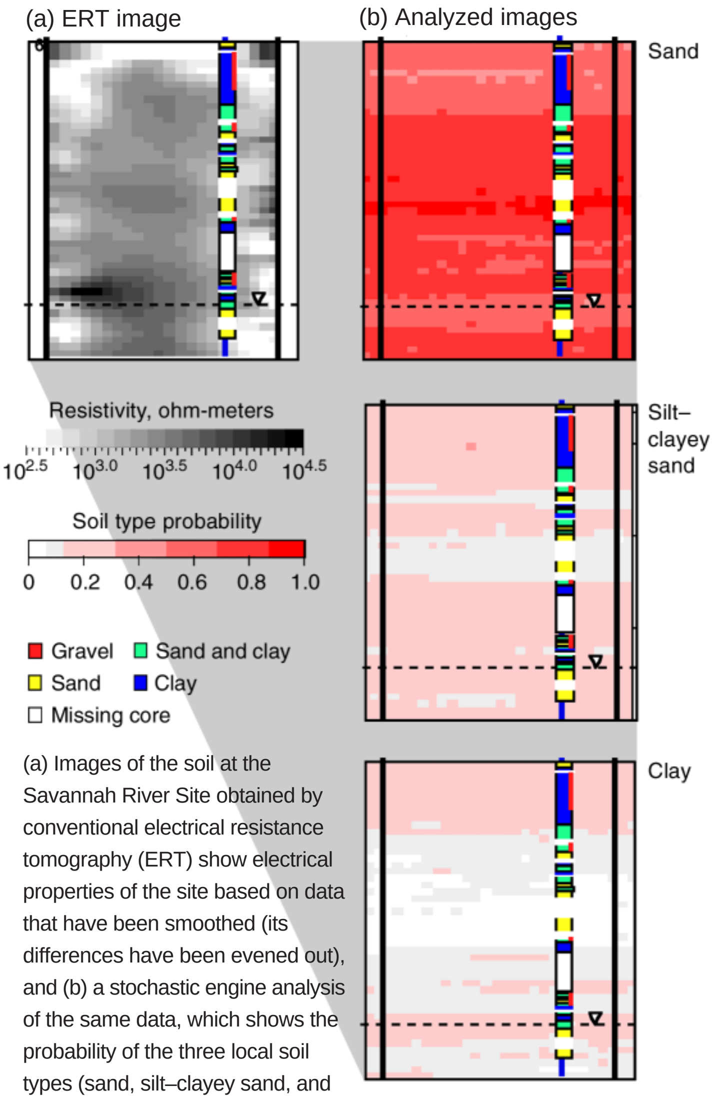
This new technology, called a stochastic engine, is a process that links predictive models, advanced statistical methods, and refined search methods. Using this technology, scientists can incorporate a proposed soil configuration into a computer model and produce a geophysical simulation. The simulated result is compared to actual data. If the result is consistent with observed data, then the simulation is boosted to the next phase of analysis.

The stochastic method is a powerful technique that is now in use. Livermore scientists are consulting on a project with the Westinghouse Savannah River Company in which the stochastic engine will assist in a major cleanup operation at the Savannah River Site in South Carolina. The method could also be applied to problems in stockpile stewardship, atmospheric dispersion, seismic velocities, and intelligence collection.

Cleanup Site Yields New Tool

The stochastic engine concept uses techniques developed at Livermore and was motivated by an innovative steam remediation cleanup being conducted by Southern California Edison at a Superfund site in Visalia, California, in which Laboratory scientists also participated. (See *S&TR*, January/February 1996, pp. 6–15.) During the project, more than 46 million pieces of data were obtained pertaining to the way steam, water, and contaminant flowed through the groundwater plumbing system. These data included temperatures, flow rates, pressures, and electrical resistance tomography (ERT) measurements. ERT, a technology developed at Livermore in

1993 and now available commercially, is similar to a computed tomography scan. It images soil resistivity, and that gives scientists information on soil properties such as temperature, soil type, and saturation. While the data collected from Visalia were rich and invaluable for Edison's operational decisions, the various data types could only be used independently. Observations and simulations could not be linked to provide the kind of cohesive understanding that would dramatically improve site operations and, most importantly, optimize the final outcome of the cleanup work.



(a) Images of the soil at the Savannah River Site obtained by conventional electrical resistance tomography (ERT) show electrical properties of the site based on data that have been smoothed (its differences have been evened out), and (b) a stochastic engine analysis of the same data, which shows the probability of the three local soil types (sand, silt–clayey sand, and clay) at each location.

The work at Visalia, while highly successful overall, is representative of a frustration that Livermore environmental scientists experience whenever they attempt to characterize soil compositions at cleanup sites: how to apply the powerful predictive capabilities of Livermore's supercomputers to complex, real situations. For the past year, Roger Aines and a multidisciplinary team have been discussing how to apply modern computational power and statistical search methods to extract maximum information from sparse initial data and then to improve the analysis on the fly as more data become available.

More Than One Right Answer

The power of the stochastic engine comes from its ability to refine a model by successively narrowing down the possible configurations of a hypothetical model. The refinement is done over progressive layers of data. In this process of model improvement through iteration, the stochastic engine uses an advanced statistical method called a hybrid Markov Chain Monte Carlo (MCMC)–Bayesian analysis.

In the MCMC analysis, a chain (or sequence) of configurations is considered. Each configuration undergoes a probability calculation that compares observed data to corresponding model predictions. If the predictions are acceptable (that is, probable for the configuration), the result of that calculation becomes the basis of the next configuration. This allows the process to rapidly search for good configurations in very complex situations. The Bayesian statistical method, based on the work of English mathematician Thomas Bayes, performs its part in the stochastic engine by comparing the probability calculations with real information to guide the statistical inference process.

Suppose a volume of soil is known to be composed of seven layers that could be either sand or silt, and an ERT measurement of that volume gives a value of 11. The stochastic approach calculates which configurations of silt and sand, and in which positions, give values close to 11. Each case with a value near 11 is passed on to the next stage of analysis. There, the model will continue to restrict possible configurations but base its decisions on other data types, such as water, temperature, or pressure.

For the simple case cited here, it is easy to calculate and compare all the possible configurations, but for a large area, such as the Visalia cleanup site, the possibilities are far too numerous. At Visalia, the MCMC–Bayesian method could help by performing an efficient intelligent search through the collection of possible soil configurations, rapidly identifying the configurations that most closely match all the data.

"It's not about trying to find the single best answer, but all of the good answers," says Aines. "In underground problems, there are usually multiple solutions that are consistent with the data."

The stochastic engine's ability to choose system configurations that are consistent with observed data allows much more tightly constrained (better restricted) answers than conventional methods. Only the ways the system can possibly exist are considered. Using the stochastic technique, for example, researchers can interpret ERT images to derive characteristic soil types for a site, rather than simply provide the electrical properties of the ground. The stochastic engine allows the available information to be used more effectively. It also allows the user to incorporate known constraints, such as the presence of a gravel layer observed in a well, to further guide the statistical inference.

It Doesn't Have to End with Dirt

The stochastic engine method has tremendous potential for use in disciplines that need to combine data and simulation. Currently, the team is working with a number of scientists from other Livermore directorates to identify unknown sources of toxic contaminants in the atmosphere, locate flaws in buildings, evaluate intelligence data, and expand tomography and x-ray imaging data.

The Savannah River Site project illustrates how the engine is being used in industrial partnerships. Livermore has been consulting with Westinghouse's Savannah River Company to clean up organic solvents from the soils and groundwater at the South Carolina site.

Since 1983, the company has been performing environmental cleanup of a site where, over time, solvents became a solvent plume that extended over 5 square kilometers. Now, Westinghouse is ready to present its cleanup results to regulators and assure the community that the remaining plume will not affect surface water bodies. The stochastic engine will be used to evaluate the effectiveness of source cleanup and to predict the ultimate effect of the remaining plume.

Challenges Ahead

Why hasn't the stochastic method been used before? For one thing, the complexity of the method has required robust computer power that simply has not been available until recently. For another, even with the power available on ASCI computers, some scientists are still skeptical of the method. Aines says that because underground problems are so complex, many people are displaying a "show me first" attitude toward the technology. "No one has done this before, so some believe it can't be done." The Savannah River Site project may prove that the engine is a feasible and valuable tool for environmental cleanup and more.

—Laurie Powers

Acknowledgments: The stochastic engine work described in this article was developed by a multidisciplinary team from Livermore's Energy and Environment, Engineering, and Computation directorates, including computational geoscientists John Nitao and Steve Carle; engineering statisticians Bill Hanley, Ron Glaser, and Sailes Sengupta; geophysicists Robin Newmark and Abe Ramirez; and computational scientist Kathy Dyer.

Key Words: Bayesian statistics, electrical resistance tomography, Markov chain, Monte Carlo method, Savannah River Site, stochastic engine, Superfund, Visalia cleanup.

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The sewer at Savannah River Site, South Carolina, that has been the source of solvents soaking into the soil. At the far right, geoscientist Steve Carle is shown at the sewer outfall. He was examining soil just below the outfall, looking at the silt layers that tend to control the migration of the solvent.

Knowing the Enemy, Anticipating the Threat

In a way, Lawrence Livermore was founded as a result of the nation's not knowing—or at least, underestimating—"the enemy." In August 1949, U.S. reconnaissance planes detected radioactive debris near Japan, proof that the Soviets had detonated an atomic bomb. In *Memoirs*, physicist Edward Teller writes, "Until the fall of 1949, our intelligence community, most of the leading scientists, and general public opinion held that the Soviet Union could not develop an atomic bomb before the 1960s." Within days, Ernest O. Lawrence, Nobel laureate and head of the University of California's Radiation Laboratory, met with federal officials to press for a strong hydrogen bomb effort to hold the Soviets in check. Teller, a leading theorist on the hydrogen bomb, also pushed for a vigorous U.S. hydrogen bomb project. The surprise of the Soviet atomic test and the looming threat of a Soviet hydrogen bomb spurred the creation of a branch of Lawrence's Berkeley Radiation Laboratory in Livermore as a second U.S. weapons laboratory.

"If you know the enemy and know yourself, you need not fear the result of a hundred battles."

Sun Tzu, The Art of War
Circa 400 B.C.

As the 1950s progressed, *Sputnik*'s launch in 1957 and the perceived "missile gap" strengthened the drive for improved U.S. strategic forces and better understanding of Soviet capabilities. Over time, this need has expanded to include understanding the nuclear weapon capabilities, intentions, and motivations of other countries or groups hostile to the U.S. Intelligence analysis efforts at the Laboratory grew in response. With the end of the Cold War in 1992, Livermore Director John Nuckolls merged these efforts into the Nonproliferation, Arms Control, and International Security (NAI) Directorate. This new organization focused on the threat

posed by the proliferation of nuclear, chemical, and biological weapons—collectively called the weapons of mass destruction, or WMD.

Today, NAI researchers address the full spectrum of WMD proliferation issues—prevention, detection and reversal, response, and avoiding surprise.

Avoiding Surprise

After the Soviet Union's initial atomic bomb test, monitoring the Soviet weapons program became a paramount concern of U.S. intelligence agencies. In 1965, a formal relationship with the intelligence community was drawn up in a memorandum of understanding between the Central Intelligence Agency (CIA) and the Atomic Energy Commission (predecessor to the present-day Department of Energy). Livermore's Special Projects Group, known as Z Division, was established to provide the intelligence community with technical assessments of foreign nuclear programs and weapons capabilities. According to Dale Nielsen, the first Z Division leader, the division's initial charter was twofold. "We looked at the weapons fired by Russia, and later by China, to see what they were shooting, and we developed intelligence-related equipment as requested."

Z Division scientists gathered radiological samples from Soviet and Chinese nuclear tests, using technologies developed for collecting and analyzing atmospheric samples from U.S. tests. (See *S&TR*, June 2002, pp. 24–30.) They also developed new technologies for monitoring tests and collecting data that allowed analysts to tell what kind of weapons—atomic or thermonuclear—were being tested. Among the many intelligence-related systems, Nielsen recalls a clever "bug sniffer" designed by physicists and electronic engineers for detecting minute electronic monitoring devices. "The CIA wanted to test the system and told us, 'We've set up four bugs in a Virginia safe house. See if you can find them.' We gathered up the equipment, flew out there, and found five out of four. They never told us if that fifth was an actual part of the test."

As time went on, Z Division evolved to respond to the growing list of countries that concerned the nation's intelligence agencies. The division teamed regional and country-specific experts with weapons scientists and engineers to make analyses based on technical knowledge about nuclear weapons development and testing, specifics about each country's nuclear capabilities, and evaluation of nontechnical issues that motivate nuclear programs. Z Division also provided technical knowledge and intelligence information needed to control U.S. exports that could support WMD proliferation.

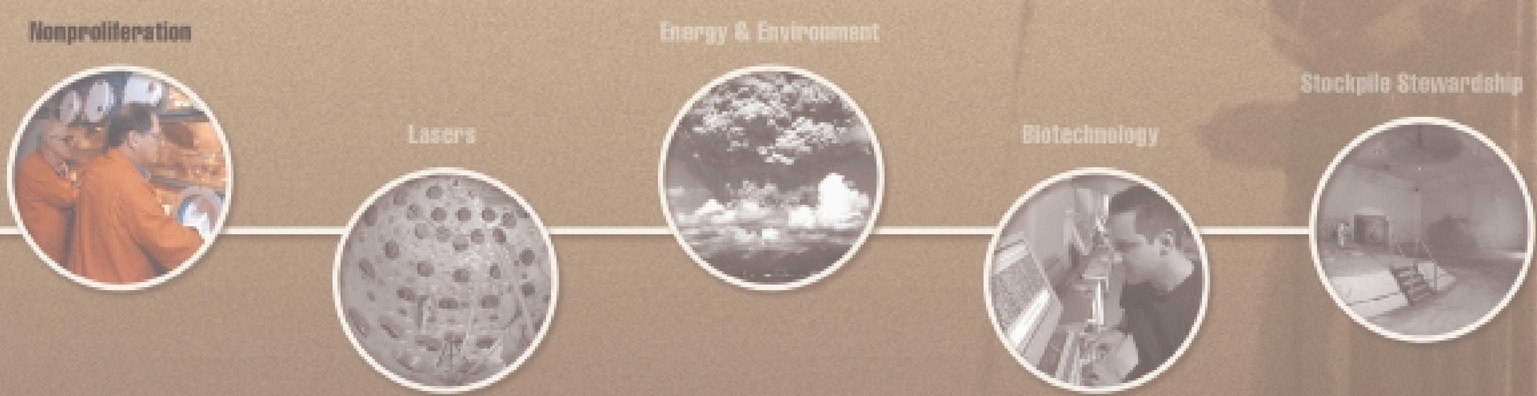
With the formation of the NAI Directorate, Z Division became the International Assessments Program and broadened its focus to include chemical and biological weapons proliferation. In addition, with the globalization of commerce and technology, Livermore's intelligence analysts recognized the need to assess the WMD capabilities of nonstate groups such as terrorists and patterns of cooperation among countries and groups of concern.

Researchers in the International Assessments Program are also addressing the national security implications of the U.S.'s rapidly growing reliance on critical networked infrastructures. The country—indeed the entire world—is becoming more dependent on computing, communication networks, and information technology. These researchers have developed a suite of sophisticated network analysis tools to assist government agencies in detecting, responding to, and preventing computer network attacks. Through this work, Livermore has become a national leader in information assurance technology.

Preventing Proliferation

The most effective way to prevent the spread of nuclear weapons is at the source, through treaties limiting or banning such weapons and, in the case of nuclear weapons, by securing weapons-usable nuclear materials. Material control is less effective in preventing the proliferation of chemical or biological weapons because the starting materials for these weapons have many legitimate uses.

The Laboratory first became involved in arms control in the 1950s. Public concern over atmospheric testing led the U.S. and the Soviet Union to establish a Conference of Experts to examine the technical issues associated with a comprehensive ban on nuclear weapons testing in all environments—the atmosphere, outer space, under water,



and under ground. Ernest O. Lawrence served as one of three U.S. representatives to this conference. Harold Brown, who became Livermore's director in 1960, was a member of the delegation's technical advisory group that developed a concept for verifying compliance with a comprehensive ban on nuclear weapons testing.

A number of Laboratory scientists participated in the technical working groups complementing the negotiations on a comprehensive test ban, examining ways to detect—and hide—explosions. Measuring seismic signals was seen as one technique for detecting underground explosions, and a worldwide network of seismic stations was built as part of this effort. (See box on p. 29.) However, Laboratory scientists were concerned that a large cavity would reduce, or muffle, the shock wave by a factor of 30 to 50, essentially decoupling the strength of the seismic signal from the size of the explosion. The possibilities for such decoupling became a key issue in the U.S. negotiating position during early comprehensive test ban discussions. The Soviets' resumption of nuclear testing in September 1961 broke the bilateral moratorium and ended the negotiations at that time.

The 1964 Salmon Event, a 5-kiloton detonation conducted 280 meters deep in a Mississippi salt dome, confirmed the theory of decoupling as a means of concealing clandestine nuclear explosions. In this photo, experimenters are lowering a canister containing the nuclear explosive for the Salmon Event.

In the ensuing decades, Laboratory personnel continued to contribute to various arms control negotiations on both strategic force levels and nuclear testing. For instance, Livermore scientists participated in the technical working groups supporting Limited Test Ban Treaty negotiations and in the Nuclear Non-Proliferation Treaty. In the fall of 1977, negotiations on a comprehensive test ban resumed after a hiatus of many years. In the 1980s, issues regarding the verification of the Threshold Test Ban Treaty were resolved with the Joint Verification Experiment (JVE), a pair of nuclear tests jointly carried out at the U.S. and Soviet test sites. (See *S&TR*, June 1998, pp. 10–16.)

Geophysicist Eileen Vergino provided technical support to the U.S. delegates in Geneva during the treaty's protracted negotiations. Vergino remembers, "JVE was a turning point in Soviet relations with the West. Many American–Russian friendships were forged, and the more open atmosphere anticipated the post–Cold War era." In 1992, U.S. nuclear testing ceased, and the Comprehensive Test Ban Treaty was signed, although it has not been ratified by the U.S. Senate.

After the Soviet Union collapsed, the Lawrence Livermore, Los Alamos, and Sandia national laboratories established Lab-to-Lab interactions with the former Soviet nuclear institutes in former closed cities. The activities gave rise to a suite of cooperative programs with former Soviet laboratories to prevent the spread of weapons expertise or materials to other nations. (See *S&TR*, September 2000, pp. 4–11.) Through the Materials Protection, Control, and Accounting program, Livermore is working with several Russian sites to improve their protection of fissile materials and with the Russian Navy to strengthen the protection of fresh and spent fuel for its nuclear-powered vessels. The Laboratory is also working with the Russian Customs Service to curtail the smuggling of nuclear proliferation items by equipping high-risk border crossings with radiation detection equipment and training front-line customs officials in using the equipment.

In 2001, lengthy negotiations by Livermore scientists culminated in a formal agreement between a Russian weapons assembly facility and a medical equipment manufacturer to establish a commercial manufacturing facility at Sarov. This agreement was part of the Nuclear Cities Initiative, which seeks to create self-sustaining commercial enterprises for the closed cities, thereby helping to accelerate the downsizing of the Russian weapons complex and preventing displaced weapons workers from seeking employment with potential proliferators.

Detecting and Reversing Proliferation

To reverse proliferation of WMD requires detecting and identifying proliferation-related activities. If such activities are detected, the next step is to evaluate options for reversing the proliferation. Livermore provides expertise in this area by developing technologies to monitor and evaluate weapons proliferation activities and to protect critical U.S. facilities and troops from attack.

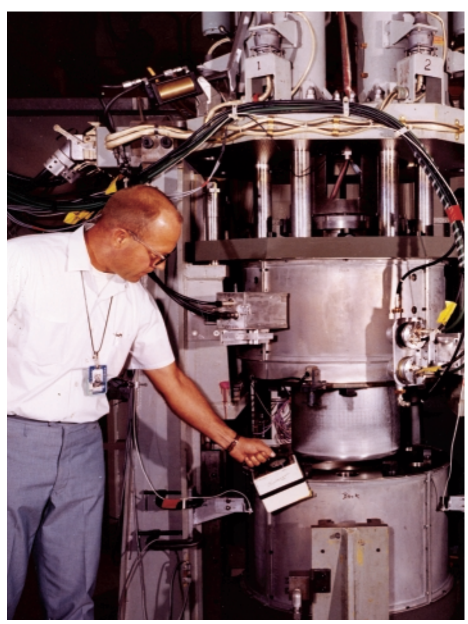
Predating this effort was work by Livermore weapons scientists who examined the consequences of various "us-versus-them" scenarios. By the mid-1960s, with the large buildup of Soviet nuclear weapons and delivery systems, the U.S. faced some serious "what-if" questions. If a nuclear exchange occurred between the U.S. and the Soviet Union, U.S. warheads would have to contend with defensive countermeasures such as a nuclear-tipped interceptor or antiballistic missile, which could deliver a blast aimed at destroying or disabling a U.S. warhead before it reentered the atmosphere. Would such a countermeasure work? Nobody knew for certain. The Super Kukla reactor at the Nevada Test Site was designed to find out. Super Kukla, an ultrahigh prompt burst reactor, produced an intense pulse of neutrons and gamma radiation to simulate the environment a U.S. ballistic missile warhead might encounter during enemy countermeasures—in essence, a nuclear blast without the blast.

This focus on nuclear effects was one mission of D Division, which was also tasked with anticipating the strategic and tactical needs of the U.S. military services. In an effort to meet these needs, the Laboratory developed an early presence in the arena of computer-driven conflict simulation. Since the mid-1970s, Livermore computer scientists have led in the development of increasingly realistic software to simulate the tactical battlefield. "At first, you had to program the orders of the opposing force into the computer ahead of time, which didn't make for a very realistic scenario," recalls Paul Chrzanowski, who joined D Division in 1977 and became its leader in 1982. "Then George Smith, a very creative guy, developed a simulation in which two opposing players observe the battle on separate computer monitors and give orders."

The Laboratory's landmark Janus program, developed in the late 1970s, was the first conflict simulation tool that was real-time player-interactive and used a graphical user interface. Livermore simulations were employed in Operation Desert Storm in the Middle East as well as in combat planning for Somalia, Bosnia, and other international trouble spots. In 1997, a team of NAI computer scientists unveiled Joint Conflict and Tactical Simulation (JCATS), the culmination of more than two decades of computer-driven mission analysis and rehearsal experience. (See *S&TR*, November 1996, pp. 4–11; June 1999, pp. 4–11; January/February 2000, pp. 4–11.)

A more recent computer-driven innovation developed for the U.S. military is the Counterproliferation Analysis and Planning System (CAPS), which is widely used by military planners to evaluate the WMD production capabilities of a country of concern and assess interdiction options. Drawing on information

Livermore provided key support in upgrades made on four nuclear refueling ships for the Russian icebreaker fleet and the Russian Navy. The upgrades improve the protection of fresh, highly enriched reactor fuel for the nuclear-powered vessels. Work such as this involves direct interactions with the Russian Ministry of Defense, an activity that would have been inconceivable during the Cold War.



The Super Kukla reactor, operated at the Nevada Test Site between 1965 and 1978, simulated the hostile environment of a nuclear exchange. Nuclear weapon components and materials were placed inside an experiment cavity, and instruments measured how well the tested samples stood up to the hostile radiation environment.

from multiple sources, CAPS can model the various processes—chemical, biological, and metallurgical—that are used to build WMD and delivery systems. CAPS identifies critical processing steps or production facilities which, if denied, would prevent that country from acquiring such weapons.

Responding to Threats

When—despite everything—bad things happen, the Laboratory has the personnel and the science and technology to help the nation respond.

(a)

(b)

(a) In the mid-1970s, the Janus code developed at the Conflict Simulation Laboratory ran an early, very simple conflict simulation. (b) Today, the Livermore-developed Joint Conflict and Technical Simulation (JCATS) models are used by the U.S. military commands and services and various U.S. security forces for training, tactical analysis, and mission planning for battlefield and urban conflict situations.

Since the early 1970s, Livermore has coordinated its responses to off-site nuclear emergencies through NEST—the Nuclear Emergency Search Team. When the Soviet satellite Cosmos 954 fell to Earth in northern Canada in 1978, Laboratory researchers tracked the reentry path, provided estimates of reentry location, and participated in a multinational effort to locate and retrieve radioactive debris. Members of NEST—health physicists, chemists, nuclear physicists, and engineers—hauled radiation detectors, liquid nitrogen, sample containers, power generators, portable computers, and even a helicopter to a desolate area populated only by caribou and Inuit hunters. The international team successfully found hundreds of very small pieces Cosmos left that survived reentry, and Livermore researchers identified the reactor fuel and estimated the fission-product inventory.

In addition to NEST, Laboratory employees also participate in the Radiological Assistance Program, which helps deal with civilian incidents involving radioactive materials; in the Accident Response Group, which responds to accidents involving a U.S. nuclear weapon; and in the Joint Technical Operations Team, a nuclear response team that assists the Department of Defense in dealing with terrorist nuclear devices.

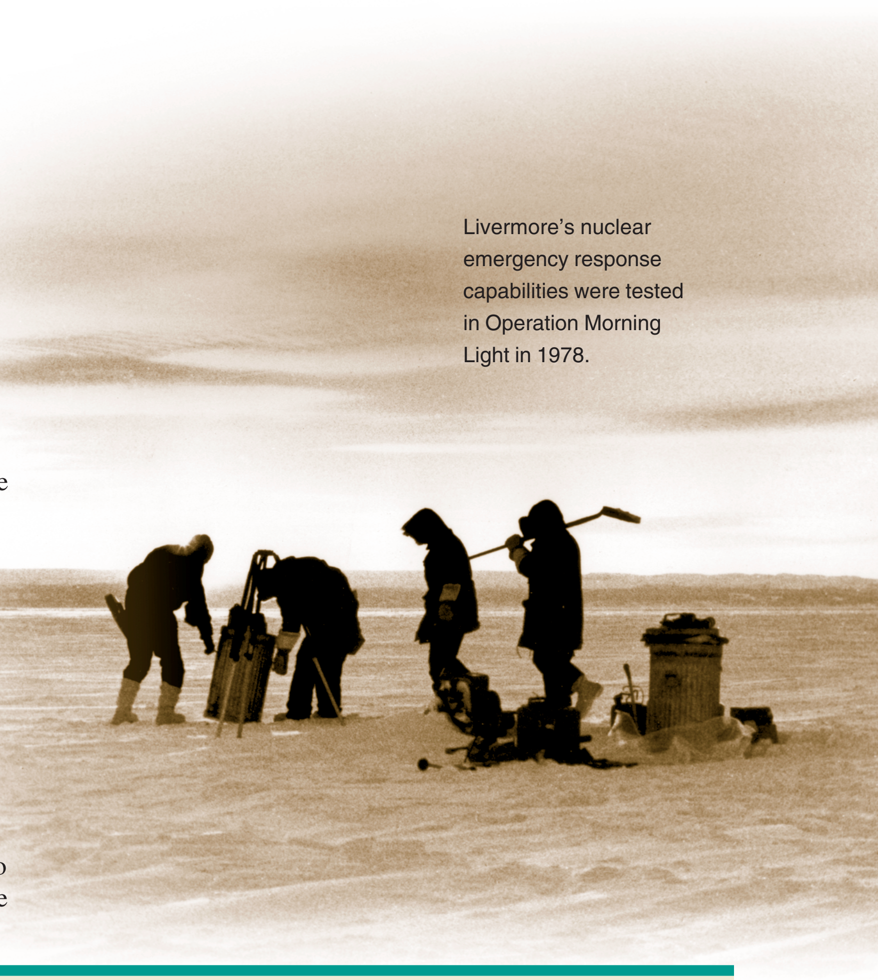
Livermore's NAI directorate is home to a number of technologies and capabilities that address the response end of the threat spectrum. In the Forensic Science Center, for example, experts in organic and inorganic chemistry and biochemistry determine the composition and often the source of minute samples of materials. (See *S&TR*, April 2002, pp. 11–18.) A major effort since the center's founding in 1991 is the development or adaptation of forensic analysis technologies for field use. In 1994, the Department of Energy asked the center to help investigate two gaseous-diffusion uranium enrichment plants that would be subject to international inspections. (See *S&TR*, August 1995, pp. 24–26.) DOE wanted to know whether an inspector could walk through a plant, surreptitiously collect samples of material, and later replicate the enrichment process. In 1998, the center used its portable thin-layer chromatography system, which can simultaneously analyze 100 samples, in the field for the first time to examine more than a thousand World War II munitions that had been unexpectedly unearthed. (See *S&TR*, December 1998, pp. 21–23.)

For almost a decade now, Laboratory researchers, working on the "when" rather than "if" premise, have been developing systems to rapidly detect and identify biological warfare agents including anthrax and plague. In 1999, Livermore scientists and engineers unveiled the Handheld Advanced Nucleic Acid Analyzer (HANAA), the first truly portable battery-powered device for identifying bioagents in the field. HANAA can analyze samples in less than 30 minutes, compared to the hours or days that regular laboratory tests typically require. (See *S&TR*, January/February 2002, pp. 24–26.) Another device, the Autonomous Pathogen Detection System (APDS), is being designed to continuously monitor the air for pathogens as a sort of biological smoke alarm for airports, stadiums, or conference halls.

Ron Koopman, an associate program leader with the Chemical and Biological National Security Program, notes that the availability of HANAA and APDS owe much to forward-thinking efforts begun in the previous decade. "A number of people recognized the vulnerability of the country to bioterrorism a long time ago," he says. "Back then, although bioterrorism seemed far away and was something we hoped would never happen, the Laboratory and members of the defense community decided to invest in the research. Thanks to that investment, we now have something to put in the hands of people to protect us all, something that can help during the current crisis and in the long run."

Laboratory scientists also worked with their counterparts at Los Alamos to develop the Biological Aerosol Sentry and Information System. This system, which reduces the time for detecting a bioagent release from days or weeks to less than a day, was deployed as part of the security strategy for the 2002 Winter Olympics in Salt Lake City.

Biodetectors require unique DNA sequences or antibodies to identify and characterize pathogens. Researchers at Livermore



Livermore's nuclear emergency response capabilities were tested in Operation Morning Light in 1978.

Detecting Clandestine Nuclear Tests and Verifying Treaties: Two Sides of the Same Coin

Lawrence Livermore scientists have long played an important role in providing monitoring technology that supports test ban treaty verification and site inspection. On September 19, 1957, the Laboratory detonated the first contained underground nuclear explosion, Rainier, in a tunnel at the Nevada Test Site. The Rainier Event was announced in advance so that seismic stations throughout the U.S. and Canada could attempt to record a signal. Information from this event ultimately led to an array of seismic detectors for monitoring nuclear test activities worldwide, as part of the Limited Test Ban Treaty.

Nearly 35 years later, when the world received news of the Indian and Pakistani clandestine underground nuclear tests, Livermore researchers used the tests to validate modern seismic methods they had developed to monitor the Comprehensive Test Ban Treaty. (See *S&TR*, September 1998, pp. 4–11.) Using data recorded worldwide by a host of seismic monitoring stations, the team successfully differentiated the nuclear blasts from typical regional earthquakes, characterized the yields of the tests, and noted inconsistencies between the announced test yields and the seismic data. The seismic signals from the nuclear tests provided important new data for calibrating seismic stations in important regions of the world.

Livermore researchers have also developed on-site inspection procedures and technologies for collecting samples of soil, gases, and water to look for radioactive materials and for identifying underground explosion cavities or rubble. In the early 1990s, a team led by geophysicist Charles Carrigan theorized that highly sensitive instruments might be able to detect small amounts of rare, radioactive gases generated in underground nuclear detonations. In 1993, a chemical explosion called the Non-Proliferation Experiment was conducted at the Nevada Test Site to simulate a 1-kiloton underground nuclear detonation. Results from the experiment and computer simulations imply that sampling soil gases for rare, explosion-produced radioactive tracer gases at the surface near a suspected underground test could help detect nearby underground nuclear explosions that do not fracture the surface, even several months after the test. (See *S&TR*, January/February 1997, pp. 24–26.)

and elsewhere are developing a comprehensive array of such signatures. One effort focuses on analyzing the genome of the various strains of the bacterium that causes plague. Laboratory researchers are searching for the DNA sequences that are unique to all strains of the pathogen but are not found in any of its close relatives. (See *S&TR*, March 2002, pp. 4–9.)

In a project for the U.S. Army in 1998, Livermore's Jeff Haas examined more than 1,200 mortars in two days using the Forensic Science Center's thin-layer chromatography screening system.

Facing the Threat, Knowing the Enemy

"Over the years, researchers at the Laboratory have had the foresight to analyze and prepare for many versions of the 'catastrophic maybe,'" says NAI Associate Director Wayne Shotts. For most of the Laboratory's existence, the consuming national security threat to the U.S. was the nuclear arsenal of the Soviet Union. The energies, talent, and resources of the national security laboratories were dedicated to checkmating the Soviet threat. "That world," notes Shotts, "no longer exists." Today, the most serious threat arises from the proliferation of nuclear, chemical, and biological weapons, and the very real threat of terrorism using those weapons. In a development that defines the national focus on this growing threat, NAI has broken ground for a new building—the International Security Research Facility. According to Bruce Tarter, who recently stepped down as Lawrence Livermore's director, this building will serve as the Laboratory's "command post for connectivity to Washington" and its efforts to fight WMD proliferation and terrorism.

Through NAI, the Laboratory applies its nuclear weapons expertise, developed through its historical weapons program and continuing stockpile responsibilities, to the challenge of nuclear nonproliferation. In addition, NAI draws on the Laboratory's chemical and biological expertise to help stop the spread of chemical and biological weapons. From one end of the threat spectrum to the other—prevention, detection and reversal, response, and avoiding surprise—Livermore stands ready to help the nation face the threat and know the adversary.

—Ann Parker

Key Words: biodetection, biological and chemical weapons, conflict simulation, Comprehensive Test Ban Treaty, forensic analysis, nonproliferation, seismic monitoring, treaty verification, weapons of mass destruction (WMD).

For more information about the Nonproliferation, Arms Control, and International Security Directorate, see:

www.llnl.gov/nai/nai.shtml

For further information about the Laboratory's 50th anniversary celebrations, see:

www.llnl.gov/50th_anniv/

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

Self Adjusting Inclinometer
Steven L. Hunter
U.S. Patent 6,349,477 B1
February 26, 2002
An inclinometer using synchronous demodulation for high resolution and electronic offset adjustment provides a wide dynamic range without any moving components. A device encompassing a tiltmeter and accompanying electronic circuitry provides quasi-leveled tilt sensors that detect highly resolved tilt change without signal saturation.

Opto-Acoustic Recanilization Delivery System
Steven R. Visuri, Luiz B. Da Silva, Peter M. Celliers, Richard A. London, William Benett, Kathryn Broughton, Victor Esch
U.S. Patent 6,368,318 B1
April 9, 2002
Fiber-delivered laser pulses emulsify a thrombus by mechanical stresses that include a combination of pressure, tension, and shear stress. Laser radiation is delivered to the locality of a thrombus, and the radiation is absorbed by blood, blood clots, or other materials present. The combination of a leading pressure wave and subsequent vapor bubble causes efficient emulsification of the thrombus. Operating the laser in a low-average-power mode alleviates potential thermal complications. The laser is operated in a high-repetition-rate mode to take advantage of ultrasound frequency effects of thrombus dissolution as well as to decrease the total procedure time. The device includes optical fibers surrounding a lumen intended for flow of a cooling agent. The fibers may be arranged concentrically around the lumen to deliver radiation and heat over as large an area as possible. An alternative design approach incorporates the optical fibers into the wall of the guiding catheter and uses the catheter lumen as the cooling channel. An eccentric tip enables rotation of the device to address all parts of the vasculature. The eccentricity can be provided via a variety of means, including spring dip, balloon, and protrusion.

Plasma-Assisted Catalytic Storage Reduction System
Bernardino M. Penetrante, George E. Vogtlin, Bernard T. Merritt, Raymond M. Brusasco
U.S. Patent 6,374,595 B1
April 23, 2002
A two-stage method for reducing oxides of nitrogen (NO_x) in an oxygen-rich engine exhaust comprises a plasma oxidative stage and a storage reduction stage. The first stage employs a nonthermal plasma treatment of NO_x gases in an oxygen-rich exhaust and is intended to convert nitrogen oxide (NO) to nitrogen dioxide (NO_2) in the presence of oxygen (O_2) and hydrocarbons. The second stage employs a lean NO_x trap to convert such NO_2 to environmentally benign gases that include nitrogen (N_2), carbon dioxide (CO_2), and water (H_2O). By preconverting NO to NO_2 in the first stage with a plasma, the efficiency of the second stage for NO_x reduction is enhanced. For example, an internal combustion engine exhaust is connected by a pipe to a first chamber in which a nonthermal plasma converts NO to NO_2 in the presence of O_2 and hydrocarbons such as propene. A flow of such hydrocarbons (C_xH_y) is input usually from a second pipe into at least a portion of the first chamber. The NO_2 from the plasma treatment proceeds to a storage reduction catalyst (lean NO_x trap) that converts NO_2 to N_2, CO_2, and H_2O and includes a nitrate-forming catalytic site. The hydrocarbons and NO_x are simultaneously reduced while passing through the lean NO_x trap catalyst. The method allows for enhanced NO_x reduction in vehicular engine exhausts, particularly those having relatively high sulfur contents.

System and Method for Characterizing Voiced Excitations of Speech and Acoustic Signals, Removing Acoustic Noise from Speech, and Synthesizing Speech
Greg C. Burnett, John F. Holzrichter, Lawrence C. Ng
U.S. Patent 6,377,919 B1
April 23, 2002
Low-power electromagnetic waves are used to detect motions of vocal tract tissues of the human speech system before, during, and after voiced speech. A voiced excitation function is derived. The excitation function provides speech production information to enhance speech characterization and to enable noise removal from human speech.

Low Resistance Barrier Layer for Isolating, Adhering, and Passivating Copper Metal in Semiconductor Fabrication
Timothy P. Weihs, Troy W. Barbee, Jr.
U.S. Patent 6,380,627 B1
April 30, 2002
Cubic or metastable cubic refractory metal carbides act as barrier layers to isolate, adhere, and passivate copper in semiconductor fabrication. One or more barrier layers of the metal carbide are deposited in conjunction with copper metallizations to form a multilayer characterized by a cubic crystal structure with a strong (100) texture. Suitable barrier layer materials include refractory transition metal carbides such as vanadium carbide, niobium carbide, tantalum carbide, chromium carbide, tungsten carbide, and molybdenum carbide.

Rotational Rate Sensor
Steven L. Hunter
U.S. Patent 6,382,025 B1
May 7, 2002
A rate sensor for angular/rotational acceleration includes a housing that defines a fluid cavity that is essentially completely filled with an electrolyte fluid. Within the housing, such as a toroid, ions in the fluid are swept during the movement from an excitation electrode toward one of two output electrodes to provide a signal for directional rotation. One or more ground electrodes within the housing serve to neutralize ions, thus preventing any effect at the other output electrode.

Water Treatment Process and System for Metals Removal Using *Saccharomyces Cerevisiae*
Paula A. W. Krauter, Gordon W. Krauter
U.S. Patent 6,383,388 B1
May 7, 2002
A process and a system for removing metals from groundwater or soil by bioreducing or bioaccumulating the metals with metal-tolerant microorganisms *Saccharomyces cerevisiae*. *S. cerevisiae* are tolerant to the metals, able to bioreduce them to a less toxic state, and accumulate them. The process and the system are useful for removal or substantial reduction of levels of chromium, molybdenum, cobalt, zinc, nickel, calcium, strontium, mercury, and copper in water.

Awards

The **Technical Information Department** has received two international awards and numerous regional awards from the 2001 **Society for Technical Communication (STC)** competitions. Among the most noteworthy of the awards is the Best of Show in Art, won in the New Mexico Kachina Chapter competition by Lawrence Livermore's *2000 Annual Report*, designed by **George Kitrinos**. The publication also won a Distinguished Technical Communication Award. It was edited and produced by **Paul Chrzanowski** and **Sue Stull**.

Another award of note was won by the *Science & Technology Review* staff, who likewise received a Distinguished Technical Communication Award from the Kachina chapter. This magazine went on to win an Excellence Award in the international competition, which, in judging only the top winners from the regional competitions, pitted the best against the best. The magazine is sponsored by the **Director's Office** under the direction of **Tom Isaacs**. Its scientific editor for the year of award was **Andrew A. Quong**.

The other winner in the international competition was the *Laser Science and Technology Program Update*, which won a Merit Award in the newsletter category. It was produced by **Cyndi Brandt**, **Hao-Lin Chen**, and **Al Miguel.**

The Outlook Is for Warming, with Measurable Local Effects

Livermore scientists are examining some of the causes of global climate change and its localized effects. One team has used sophisticated climate models to separate the effects of recent major volcanic eruptions and El Niños from other causes of climate change. These scientists identified the fingerprints of explosive volcanoes and El Niño ocean warming and factored them out of mean global climate data for 1979 to 1999. The research results indicate that cooling caused by major eruptions in Mexico and the Philippines in 1982 and 1991, respectively, has masked some of the warming brought about by human activities. At the same time, another team has brought the highest resolution yet to climate modeling, revealing regional effects accurately for the first time. The team performed global and local simulations using models with resolutions of 75 and even 50 kilometers. The former state of the art used 300-kilometer-resolution models.

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Philip Duffy (925) 422-3722 (duffy2@llnl.gov).

How Metals Fail

The Laboratory's national security missions require an understanding of how metals respond to the sudden shock waves and subsequent high-strain-rate deformations caused by high explosives. However, the current ability to predict how and when metals will dynamically fail is inadequate. Computational models need to reflect in detail how cracks form, evolve, and lead to the failure of a part. Such models are required for the National Nuclear Security Administration's Advanced Simulation and Computing (ASCI) program. The results of a wide range of Livermore experiments are supporting the construction of advanced computer models of how metals crack and ultimately fail. As part of ASCI, the new models will help to assure nuclear weapon safety and reliability. The models will also advance nonnuclear military applications, such as shaped charges and armor-defeating projectiles.

Contact
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Shocked Organic Liquids May Reveal the Origins of Life

Livermore experiments examine the possibility that the building blocks of life arrived on Earth as hitchhikers aboard comets.

Also in September *in June*

- ***Researchers using the tools of Geographic Information Sciences are discovering new ways to organize, analyze, model, and visualize spatial information.***

- ***Solid-oxide fuel cells promise clean, efficient, abundant electric power.***

- ***50th Anniversary Highlight—Since the invention of the laser in 1960, Livermore scientists have been exploring its use in national security, energy, and basic science applications.***

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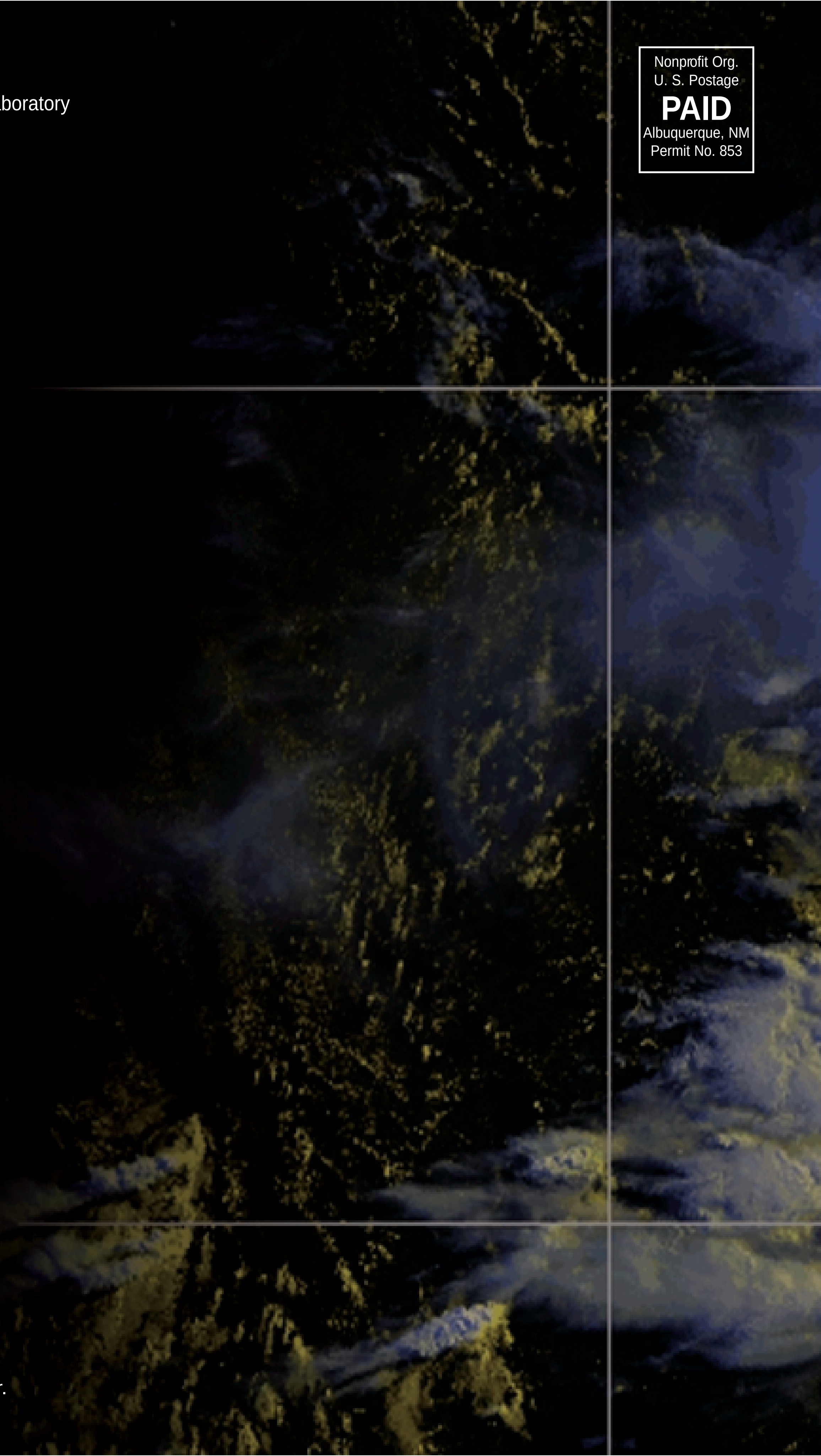

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