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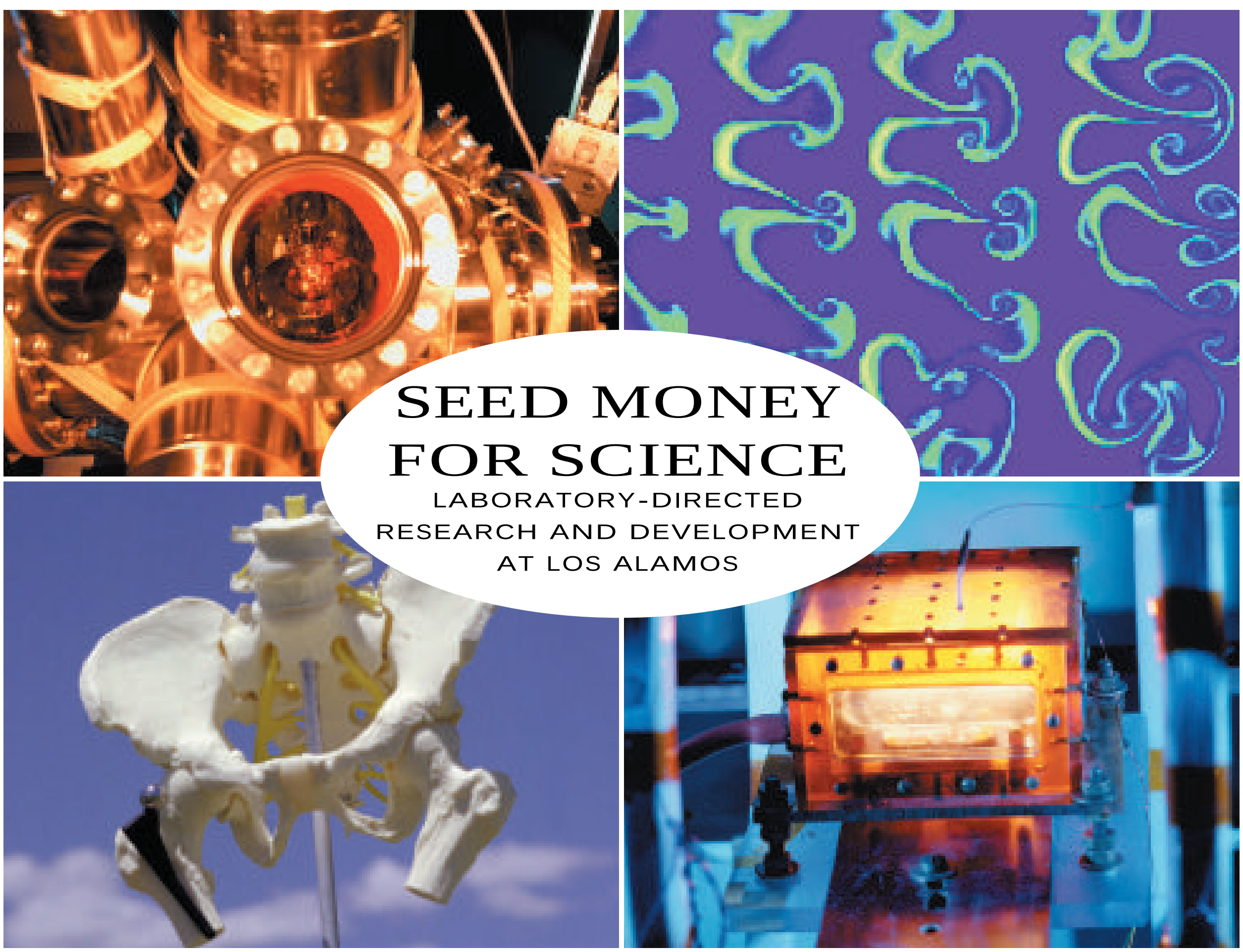
LOS ALAMOS NATIONAL LABORATORY
WHERE SCIENCE MAKES A DIFFERENCE

DATELINE LOS ALAMOS

U.S. DEPARTMENT OF ENERGY
UNIVERSITY OF CALIFORNIA



SEED MONEY FOR SCIENCE

LABORATORY-DIRECTED RESEARCH AND DEVELOPMENT AT LOS ALAMOS

DATELINE: LOS ALAMOS

Since Los Alamos National Laboratory was established in 1943 to build the world's first atomic weapons, a vigorous Laboratory-initiated research and development program has been part of its scientific agenda. The program has had several names: Weapons Supporting Research, New Research Initiatives, Institutional Supporting Research and Development. Whatever it's called, the fundamental thrust has remained the same: to focus resources on the early exploration of creative ideas in areas that address the Lab's core national security mission and support emerging new mission objectives of the Department of Energy. In 1991, the program was revised and renamed Laboratory-Directed Research and Development. This special issue of *Dateline: Los Alamos* highlights the LDRD program and some of the innovative science originating from it.

DATELINE LOS ALAMOS

A MONTHLY PUBLICATION OF THE PUBLIC AFFAIRS OFFICE OF LOS ALAMOS NATIONAL LABORATORY

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DATELINE: LOS ALAMOS

LABORATORY-DIRECTED RESEARCH AND DEVELOPMENT SPARKS EARLY EXPLORATION OF CREATIVE SCIENCE IN SUPPORT OF NATIONAL SECURITY

LDRD FUNDING IS INVALUABLE TO RESEARCHER

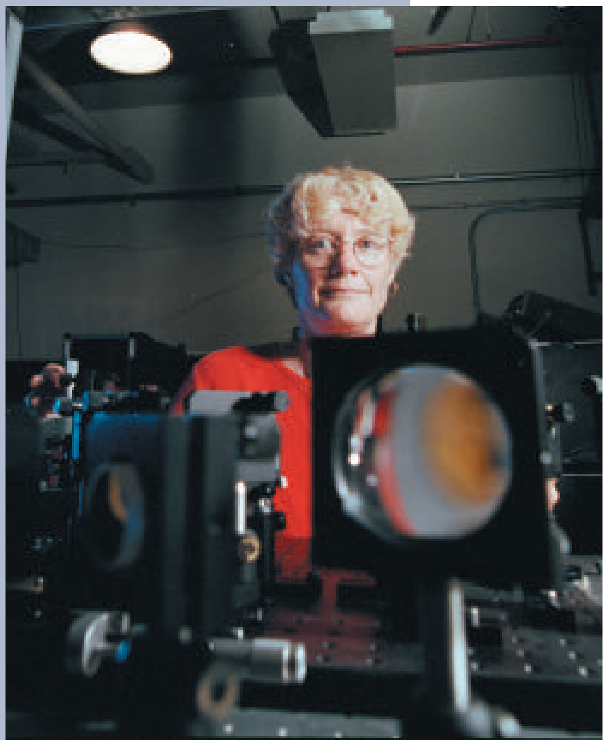
For physicist Toni Taylor, a program providing "seed money" for innovative research at Los Alamos is invaluable to the researcher, the Laboratory and the nation.

Taylor, who specializes in solid-state physics, has conducted research on several projects funded by such a program, called the Laboratory-Directed Research and Development (LDRD) Program. One of her projects is featured in this special issue of *Dateline: Los Alamos*.

One project for which Taylor and several colleagues received funding several years ago involved the development of a special laser system. The project was designed to perform fundamental scientific research, but the laser system eventually became an important component of a subcritical test conducted at the Nevada Test Site in 1998 to obtain information about the safety and reliability of U.S. nuclear weapons without underground testing.

"The basic science that LDRD funds often has valuable applications that you don't foresee, that can't be foreseen," Taylor said.

The program also is valuable because it's competitive, which keeps the technical staff challenged, encourages innovative ideas and ensures high-quality projects, she said. It also supports projects that are funded for a long enough period (usually three years) and that are interesting enough to attract top-flight postdoctoral staff, a valuable source of scientific "new blood" at the Laboratory.

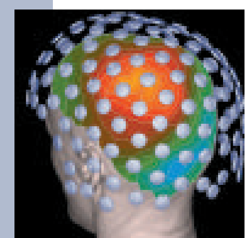


Physicist Toni Taylor in her lab.

"LDRD has provided crucial funding to me and other researchers," Taylor said. "If you have a new idea, it's one of the only ways to get resources to see if it will amount to anything. It contributes to the technical base of Los Alamos. Without it, we'd just be another laboratory without the reputation that we have now."

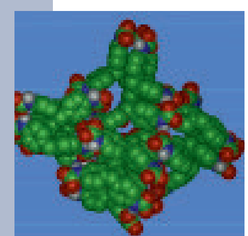
DATELINE: LOS ALAMOS

LDRD AT LOS ALAMOS



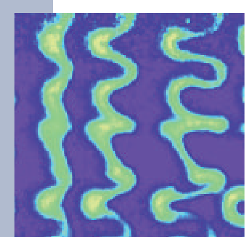
The Los Alamos program, and similar programs at Lawrence Livermore and Sandia national laboratories, operates under appropriate Department of Energy orders to ensure that it complies with all departmental policies and requirements. Its funding limit is 6 percent of the Laboratory's total operating and capital equipment budget.

For Los Alamos, the total funding of about $70 million a year supports more than 200 projects in fields ranging from weapons diagnostics, environmental cleanup and unusual materials behavior to high-performance computing, genetic coding and fundamental particle physics.



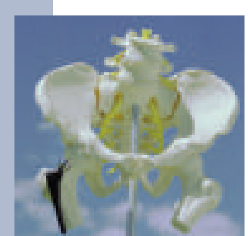
Over the years, LDRD projects at Los Alamos have allowed the Laboratory to stretch its core competencies to fulfill its national security mission and to provide a rapid response to emerging scientific ideas and opportunities.

The projects have played a vital role in strengthening the Laboratory's scientific reputation by building mutually beneficial ties with other research institutions and industry and attracting top-flight scientists to the staff. They also have made significant contributions to the world's science and engineering knowledge base.



Although the program receives only 6 percent or less of Los Alamos' annual budget, in the past 10 years LDRD projects have accounted for about 30 percent of the Laboratory's publications, 40 percent of its patents and 60 percent of its R&D 100 awards (presented by *R&D Magazine* to the nation's top 100 technological achievements each year).

PROGRAM COMPONENTS



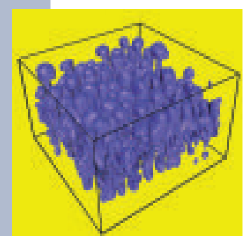
LDRD projects tend to be relatively small. They may involve advanced studies of new hypotheses, innovative approaches to solving technical or scientific problems, "proof of principle" demonstrations of new ideas or conceptual technical analyses of experimental facilities or devices. The program at Los Alamos is divided into two components: Directed Research and Exploratory Research.

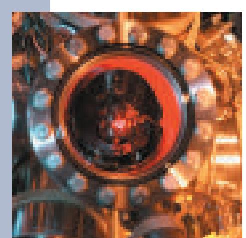
Directed Research, which typically receives about two-thirds of the funding allocation, provides funds to make strategic investments in R&D projects that are largely guided by the Laboratory's Strategic Plan. The projects are usually multidisciplinary and involve researchers from several organizations.

Recently funded DR projects include research into the effects of aging on polymeric materials (Page 15), the performance of nuclear weapons with aged or remanufactured components (Page 10), the safety and security of urban areas possibly threatened by natural or human-made hazards (Page 25) and the behavior of natural phenomena that impact human activities, such as weather and wildfires (Page 39).

Exploratory Research provides funding for staff-initiated projects that are highly innovative and often on the cutting edge of a scientific field.

Researchers funded through this component are studying ozone depletion in the atmosphere (Page 42), the feasibility of using carbon-based prosthetic devices (Page 37), the identification and characterization of certain human DNA repair mechanisms (Page 33), the development of instruments to peer deeper into the microscopic world (Page 9) and many other areas.





PROGRAM IMPACT

Research funded by LDRD has resulted in breakthroughs in sophisticated methods to study the effects of aging on nuclear weapons components, the development of the high-performance parallel interface (HIPPI) that allows high-speed computers to communicate with each other, the remote detection of nuclear activities barred by international treaty and understanding of the physical phenomena surrounding potential black holes.

"The lifeblood of scientific research institutions is the ability to tap the creativity of individual scientists," said Bill Press, deputy Laboratory director for Science, Technology and Programs, who has oversight of the LDRD program.

"At Los Alamos, LDRD provides an essential mechanism for scientists and engineers to offer their best ideas that can advance the science and technology underpinning our missions.

"As a consequence, LDRD-supported projects are providing fundamentally new insights into issues that are highly relevant to our ongoing mission, while helping us retain our highest-caliber scientific staff and attract vital new talent to replenish the work force. LDRD is essential to the future vitality of Los Alamos."

For more information on the Los Alamos LDRD program, visit the web site at http://ldrd-web.lanl.gov:8090/ on the World Wide Web.

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DATELINE: LOS ALAMOS

WEAPONS AND THE STOCKPILE

STEWARDSHIP AND MANAGEMENT

A major focus of Los Alamos' national security mission of reducing the global nuclear danger is Science-Based Stockpile Stewardship — making sure the nuclear stockpile is safe, secure and reliable. Scientists are investigating ways to determine what happens to a nuclear weapon throughout its lifetime without underground testing. LDRD projects add significantly to this understanding, from research into how weapons parts age and decay, to simulations of the behavior of a weapon, to creating a software tool to tackle the huge amounts of information acquired throughout the years.

ACTINIDE RESEARCH

Unlocking the deeply complicated mysteries of radioactive elements as they decay and interrelate with other materials will bring scientists to the edge of solving the most profound problems of the nuclear age.

The radioactive elements known as actinides both serve and plague humanity. Plutonium, the most famous member of the family — uranium, thorium, neptunium and americium are some cousins — is both hero and villain.

It is the heart and soul of a nuclear weapon, and provides a valuable energy source for electrical-power generation and deep-space travel. At the same time, it causes the balance of international power to tip precariously on a manmade element that has not reached its 60th birthday, and it has produced immensely difficult waste problems.

"We are working in one of the last frontiers of chemistry," says Carol Burns, an inorganic chemist and a leader of one of science's most unusual teams.

The Actinide Molecular Science Project pulls together a band of tightly focused scientists examining these puzzling actinides at the molecular level.

In a painstaking effort, researching chemical behavior at the level of an individual atom may one day provide a roadmap to solutions to nuclear stockpile management, materials storage and the awesome burden of cleaning up the actinide legacy of the atomic age.

"Our knowledge of actinides is just not adequate," says Burns. "To process actinides, we must know how they are going to behave in varying environments."

As with other Los Alamos projects, the strength of a multidisciplinary approach is key. "We have theoretical chemists, electrochemists, structural chemists and spectroscopists working together," explains Burns. The team is able to validate computational models of the actinides with hands-on bench science. And the results form a solid base of understanding that will solve some of the nation's most intricate waste problems.

Researching how actinides attach to surfaces, for example, could be the key to decontaminating and decommissioning buildings, such as the former production buildings at the Rocky Flats Plant near Denver.

"Our work here will hopefully provide them with the chemical know-how to take plutonium and other actinides from a multitude of waste types and process them into a manageable package," Burns says.

Another long-standing legacy waste issue bubbles in the tank farm at the Hanford Reservation in Washington state, where, for years, solutions used in plutonium processing were put in tanks. The contents of these vessels now are being characterized to enable scientists to determine what elements are in the soupy concoctions and how best to deal with them and treat them.

"This is a formidable technical challenge," Burns says. "Our work on actinides at the molecular level will bring us a far greater understanding of these individual elements and how they react to different conditions. This is key to being able to treat them and clean them up."

For years, the tanks continued to be filled without a clear picture of the contents of the witches' brew. "We must know each actinide that is in the tank, and the other materials present in this goop, so that we can prove we can treat the contents," Burns explains.

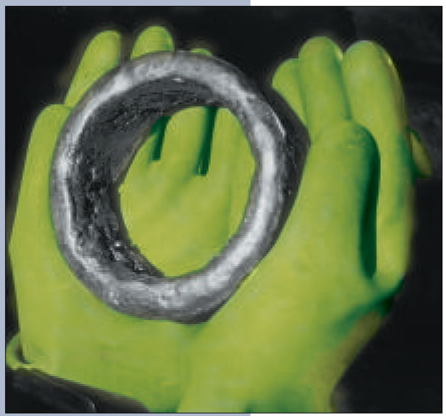
"In these mixtures, it also is important to know how each individual actinide behaves before you decide how to deal with them," she says. "People don't understand how different these are from element to element."

Back home at Los Alamos, this chemistry research will help solve another problem. Technical Area 55's Plutonium Facility has the goal of zero waste.

"How do you scrub the last picocurie of plutonium or americium out of the wastewater?" asks Burns. "To be successful, we need to know far more regarding these elements and how they react, so that we can figure out how best to process them."

Further advancements in actinide molecular science also could play key roles in better characterizing the waste headed to the Waste Isolation Pilot Plant near Carlsbad, N.M., or waste that might be stored at the Yucca Mountain Site in Nevada.

A ring of plutonium metal held inside a glovebox.



The project also could provide key data for tackling the problem of migrating radionuclides at the Nevada Test Site, where for decades America's nuclear stockpile was subjected to the nuclear tests now confined to the virtual reality of a supercomputer's microprocessors.

Actinide research is increasingly becoming the rare bird of chemistry. Because of the environmental, safety and health issues enveloping a laboratory that houses plutonium research, there are few outposts in which the actinide explorer can pitch a scientific tent. And most are within the Department of Energy, the keeper of the nation's nuclear genie.

And colleges and universities offering study in actinide chemistry are a dying breed, again for reasons of difficulty when it comes to meeting tight federal regulations to keep these radioactive elements safe and secure. "There are precious few places to be an actinide chemist," says Burns.

So for members of Los Alamos' Actinide Molecular Science Project, research at the molecular level eventually will solve monstrous problems.

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ELECTRONS IN HIGH-MAGNETIC FIELDS

Often scientists are blessed with discovery by being in the right place at the right time. Sometimes, however, it's more a matter of simply being in the right place. A project studying electrons in high-magnetic fields is just such a case.

At first blush, this research project looks like the kind of condensed matter physics investigation that could be run at any major scientific laboratory, yet in reality this research could only be done at Los Alamos. The project not only calls upon the multiple scientific disciplines available at Los Alamos and its expertise in working with plutonium and related transuranic compounds, but also on the Lab's unique High Magnetic Field Laboratory. The combination of these talents and facilities is instrumental to the project's goal of advancing a frontier of condensed matter physics.

The project involves research into the electronic structure and dynamics of plutonium metals, in the form of crystals, while they are under the influence of 60-tesla magnetic fields. The research includes work measuring the dynamic as well as static properties of atomic energy states in the correlated electronic structure of plutonium itself.

In other words, the researchers not only studied the mysteries of how electrons in plutonium move, but how their movement is connected or correlated with the movement of other electrons. This study of correlations was particularly significant since plutonium is one of the 5f metals — metals where the movement of one electron affects another electron in a sort of correlated electron dance. In most other metals electrons are free to move in a background field and do not “see” other individual electrons.

The most significant development in the project so far has been the first successful measurement of heat capacity in the pulsed magnetic field of the High Magnetic Field Laboratory. Heat capacity — the amount of heat required to raise a system one degree in temperature — had never before been measured in a high magnetic field.

This research work not only provides a better general understanding of condensed matter physics affecting 5f metals, but can also be applied directly in the analysis of nuclear materials as part of the Laboratory's role in Science-Based Stockpile Stewardship.

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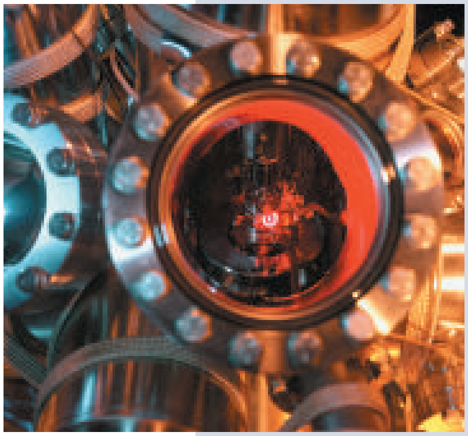
FEMTOSECOND SCANNING TUNNELING MICROSCOPY

In the past few decades dozens of novel experimental techniques have allowed researchers to examine the exquisite details of the universe. Recently, researchers at Los Alamos developed an instrument that sees further into the depths of the microscopic world than ever before.

Researchers have combined a conventional scanning tunneling microscope with a gallium-arsenide tip and a pulsed laser. The result is an ultrafast microscope that views events at the atomic level lasting mere trillionths of a second.



Scientists equipped a conventional scanning tunneling microscope with a unique gallium-arsenide tip and combined it with a pulsed laser. They use this ultrafast scanning tunneling microscope to view atomic-level resolution — as low as 10 nanometers (billionths of a meter) — at atomic-level time scales — events lasting a mere 1.5 picoseconds (trillionths of a second). This unique ability allows researchers to track, both spatially and temporally, atomic phenomena such as single-electron transfer, soliton conduction in molecular wires and chemical reactions on surfaces.

The instrument will no doubt have an impact in the many fields of physics, biology, materials science and chemistry.

DATELINE: LOS ALAMOS

The femtosecond scanning tunneling microscope will allow researchers to probe the dynamics of complex materials systems at an atomic level, enabling a better understanding of fundamental processes in strategic materials. For example, this instrument could provide information on how materials are changing over time in the heart of an aging nuclear weapon.

However, the most compelling technological applications most likely will be in the development of next-generation electronic devices that embody submicron spatial features and subpicosecond switching times. These devices might include submicron electrical contacts or optical switches for integrated circuits. The ultrafast scanning tunneling microscope also could provide critical subatomic views for nanotechnology device designers.

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MULTISCALE SCIENCE FOR STOCKPILE STEWARDSHIP

The end of the Cold War and the subsequent U.S. ban on nuclear testing pose a daunting challenge to weapons scientists, who must now predict the behavior of the aging and remanufactured weapons in our nuclear arsenal without the benefit of observation.

Two Laboratory theoretical physicists are involved in a project applying the techniques of multiscale science to improve the predictive capabilities of computer models used in simulating the performance of nuclear weapons.

Multiscale problems involve the interaction of physical processes that occur over widely different scales of length and time. For example, the effect of structure (microcracks and pores) on small scales can be related in a statistical way to the behavior of a solid on a larger scale.

Len Margolin and David Sharp propose to develop and apply the methods of multiscale science to the problems of fluid and material mixing, and to materials characterization, allowing them to improve the models necessary to simulate the behavior of a nuclear weapon. These new models will then be implemented in existing weapons-simulation codes to run on supercomputers as part of the Science-Based Stockpile Stewardship mission.

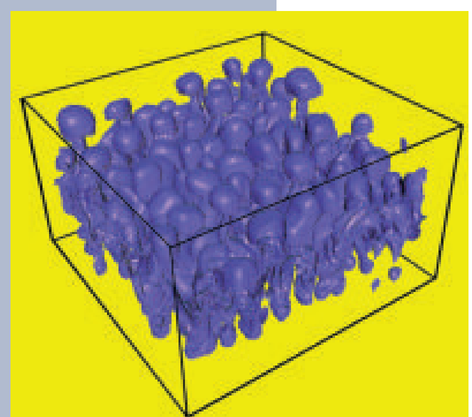
"As we move away from testing, we will have to rely more on improved predictive capabilities to assess how an aged weapon will perform," said Sharp. "In the old testing days there was always a bottom line. We now have to find a replacement for one of the pillars on which we try to build predictability.

"We used to have a high degree of confidence in our predicted results," he said, "but even then we had no certainty. We do, however, need to predict the level of uncertainty we have so we know how much faith we should have in our answers. When dealing with nuclear weapons, the difference between a 90 percent and a 99 percent degree of certainty is enormous."

The essential step in developing more predictive computer codes to simulate nuclear weapons performance rests on identifying the microscopic physical processes that underlie the macroscopic behavior in a nuclear explosion. Even when these processes are identified and understood, an additional difficulty arises.

The smallest scale and the largest scale processes cannot be simultaneously resolved due to practical limitations of present-day computer speed and memory, even if the detailed microstructure were known.

The multiscale science solution to this problem starts with models of microphysical processes, followed by a coarse-graining step to represent macrophysical influence of these processes.



↑ Simulation of gravity-driven mixing of fluids of different densities. The mixing rate is close to agreement with experimental value.

Simulation by Xiaolin Li as part of a Los Alamos/State University of New York at Stony Brook collaborative study

"Aging and remanufacture change the physical state of a weapon," said Margolin. "Our project aims to identify the factors associated with aging and remanufacture that lead to sensitivity in performance and relate these factors to weapons performance."

The project addresses critical processes involving the turbulent motion of fluids and the mixing that occur at material interfaces due to fluid instabilities. The project will develop quantitative descriptions of these key processes, which will allow researchers to model hydrodynamic and materials mixing under shock compression.

To foster meaningful interactions and to tie the research more closely to the needs of the nuclear design community, Sharp and Margolin sponsor biweekly seminars and also schedule informal, but more deeply focused, discussions on current research topics.

Multiscale science is central to such diverse fields as fluid dynamics, materials science, biology, environmental science, chemistry, geology, meteorology and high-energy physics. The researchers hope multiscale science becomes recognized as a common issue cutting across many areas of contemporary science and technology.

DATELINE: LOS ALAMOS

Margolin and Sharp's work will enhance Lab capabilities in areas such as environmental remediation, the design of novel materials, the modeling of industrial manufacturing processes such as thin films and resin transfer molding, and climate modeling. The research has the potential to provide a technical foundation for the analysis of a broad class of complex systems across the Laboratory.

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3-D SIMULATIONS OF MIXING

In the absence of nuclear testing, scientists increasingly rely on numerical simulations to determine what happens to a weapon during all phases of its lifetime. An example is understanding the changes metals go through during the casting process of complex weapons parts. This is an important component of Science-Based Stockpile Stewardship.

William Rider and Doug Kothe are developing computer simulations to precisely mimic physical phenomena. The goal is to duplicate on a computer what would happen in reality.

The results are improved three-dimensional Eulerian hydrodynamic calculations that, among other things, will help scientists better understand and predict the phenomena of mixing.

Los Alamos has a long history of calculating hydrodynamics under extreme conditions where a metal flows like a liquid. Traditionally, the calculations have used the Lagrangian method, in which the researcher's reference point moves with the fluid being modeled, but this method has limitations once the fluid begins to mix.

For example, current research to simulate the mixing processes involved in pouring and casting requires the Eulerian method where the point of reference is fixed. Eulerian computations are necessary to simulate a number of important physical phenomena ranging from the molding process for metal parts to nuclear weapons safety issues to astrophysical phenomena such as supernovae.

DATELINE: LOS ALAMOS

Additionally, Eulerian codes are useful for a wide range of other industrial processes, such as aerospace engineering, automobile design, internal combustion engines and chemical processing, to name a few.

The most direct application of the project has been Telluride, a computer tool that models in three dimensions the complex processes involved in casting.

For thousands of years metal casting techniques were based on a "pour and pray" method — a foundry term for trial and error. Because many complicated physical processes occur during the casting process, the components often contain flaws that cannot be fixed once cast, and parts must be discarded or remelted.

Unlike industrial simulation tools, the Los Alamos-developed Telluride simulation tool addresses the special needs of the alloys commonly used in Laboratory foundries: uranium and plutonium. Taking the guesswork out of the casting process will save time, money and materials.

When conducting simulations, comparisons between experiment and calculation are essential for credibility. Recent hydrodynamic instability experiments have provided an opportunity to make such "apples to apples" comparisons between experiment and simulation.

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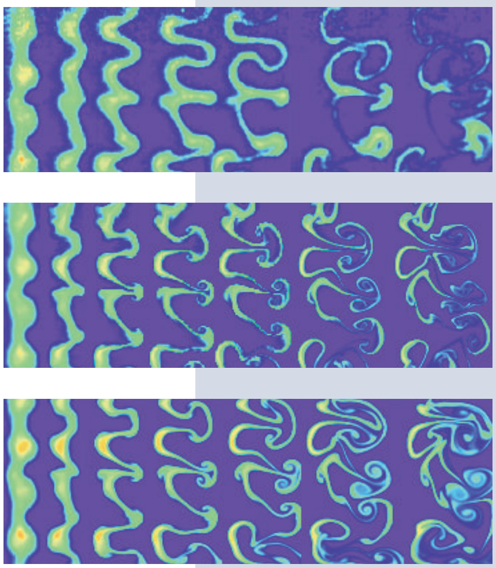

The top figure shows the evolution of a shock-wave-driven mixing instability imaged from an experiment. The center and bottom figures are simulations of the experiment. The experiment and simulations are being used to validate the ability of hydrocodes to compute the details of fluid mixing.

DATELINE: LOS ALAMOS

DATA MINING

Finding useful information or significant connections in large quantities of data is a challenge for nuclear weaponeers and financial analysts alike. The process of extracting essential information from large data sets is called "data mining," and it has grown increasingly important as science and society churn out greater collections of data.

Researchers have developed a software tool that makes it easier for data miners to tackle large collections of unstructured data, collections containing upward of trillions of bytes of information.

The software, called PADMA for PArallel Data Mining Agents, performs three main functions. It accesses data in a parallel, distributed fashion, simultaneously probing data collections in different locations. It uses "agents," or autonomous subroutines, to conduct initial filtering or analysis of the distributed data. And it also provides feedback that guides the users' overall analysis.

The agents let users scale PADMA to the needs of the problem. The larger or more diverse the data set being studied, the more agents a user can assign to the task.

Extracting information from archived nuclear weapons data is one possible application for PADMA. Such data exist at various Department of Energy sites and in scattered locations within each site.

Documents, which exist as scanned images, may present numerous typographical errors and, because they span many years and authors, inconsistent terminology usage. Ongoing Science-Based Stockpile Stewardship experiments will add to the database. A tool such as PADMA could efficiently access this hoary yet burgeoning corporate memory.

Improved data mining tools can not only support the analysis and assessment needs of Los Alamos' nonproliferation and stockpile stewardship missions, but also have broad application in the financial or medical sectors.

For example, PADMA's ability to discover patterns in data was demonstrated on laboratory test data from a Hepatitis C study and on autopsy reports. Data mining can explore medical records to help determine causes of known diseases or detect the outbreak of new or suspicious health problems.

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DATELINE: LOS ALAMOS

POLYMERIC MATERIALS AGING

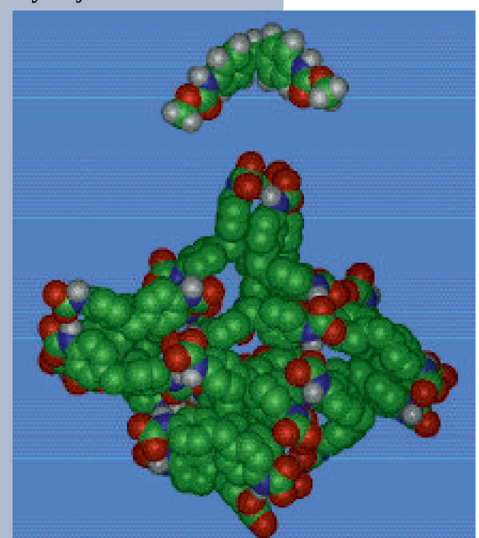
Those tires on your car or other parts that make up today's lighter vehicles. The soles of your shoes. Certain adhesives. Or that Saran Wrap™ you used to lock in the freshness of last night's dinner.

What do they all have in common? They're made in part of polymeric materials, of which there are two big classes, petroleum- and silicone-based. "They're just all over the place and used many different ways," said Ed Kober, principal investigator of a team studying polymer materials and the effects of their aging. "This leads to a very diverse project."

When car tires or shoe soles wear out, they're replaced or repaired, while the Saran Wrap™ usually gets tossed. It's a little different with nuclear weapons.

One of Los Alamos' missions is safeguarding and ensuring the reliability of the nation's nuclear weapons stockpile. Scientific research and analysis of how weapons parts age is critical to Science-Based Stockpile Stewardship.

The thrust of the polymeric materials aging project is to identify and characterize aging mechanisms in polymeric materials in Los Alamos-designed weapons and predict material properties in a weapon environment over an extended lifetime.



Atomic-level views of hard segments of Estane™. The top image shows a single unit and the bottom image shows the segments aggregated into a domain (green = carbon, gray = hydrogen, blue = nitrogen, red = oxygen). Most of the hydrogen atoms are not shown in the bottom segment.

Illustration by Thomas Sewell

"We're trying to understand these materials across the tremendous length scale ranging from angstroms to centimeters and over time scales of microseconds to years," said Kober. (An angstrom is one ten-billionth of a meter in size and not seen by the naked eye.)

In the weapons arena, polymer-based materials are used as a binder in some high-explosive compositions, according to Kober. "It's the glue that holds them all together," he said, also noting that because of the polymer material's elasticity characteristics, it can be molded into various shapes.

At about 100 degrees Celsius, it softens significantly, while at temperatures of about 80 degrees Celsius, it can be cast or shaped for use in explosives. It also can stand up to reasonable temperature variations, external pressures and vibrations. "It functions like a shock absorber," Kober said.

Research at Los Alamos has focused primarily on Estane™ 5703, a class of polymer manufactured by B.F. Goodrich. Los Alamos researchers also are studying another of class of polymers called polydimethyl siloxanes.

DATELINE: LOS ALAMOS

Estane™ 5703 is a co-polymer of polyester and polyurethane, two materials that don't particularly like each other, but are married together molecularly. The polyester is soft and rubbery while the polyurethane is much harder. The molecular mixture results in a tough elastomer with the desired properties.

Polydimethyl siloxanes have silica filler particles that act like the polyurethane in Estane™ and help give the material its strength. Kober said the polydimethyl siloxanes also pose structural problems similar to Estane™ and hence similar questions about aging effects.

In the weapons arena, polydimethyl siloxanes are used as foams and adhesives. Outside of weapons, they are found in seat cushions and silicone adhesives.

Kober and his colleagues hope the weapons science research they have undertaken will determine how aging drivers such as time and water affect the polymer material used in weapons. Water is a driver, Kober explained, because it is used in the casting machining processes.

Water molecules interact with the polymer's molecular chain, so there are trace amounts left in the polymer material. This can effect the mechanical properties of the polymer directly, and also can result in chemical reactions that degrade the material.

Laboratory researchers use experiments and modeling to test Estane™ 5703. Vibrational spectroscopy shows researchers the phase segregation between polyester and polyurethane material, for example. At the molecular level, atoms are bonded to each other and they vibrate. Vibrations can be shifted slightly by interactions with other molecules.

Using computer models, researchers can calculate vibrational shift and observe interactional shifts in the materials. "Some of the shifts we can explain; others we can't understand yet," said Kober. "Quite frankly, with this material, it's a structural problem that people have been trying to solve for more than 20 years."

Researchers also use small-angle neutron scattering experiments at Los Alamos' Neutron Science Center — a unique capability. The polymers are bombarded with neutrons that can distinguish between the hard and soft domains of the material, and this shows up in the scattering profile. There are literally tens of hundreds of urethane segments that coalesce together to make a domain.

According to Kober, scattering patterns can tell researchers the shape and size of a hard domain and how far apart they are from each other. This is important because the size and shape of the hard domain controls the strength properties of the polymer materials. Understanding how they change with age will tell researchers how the material changes over time, which is important for polymer materials inside nuclear weapons.

DATELINE: LOS ALAMOS

Los Alamos researchers also conduct accelerated aging experiments with polymer materials to subject material to elements harsher than normal. To study polydimethyl siloxanes, researchers also use electron microscopy to better observe silica particles in the siloxanes.

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REACTIONS OF ENERGETIC MATERIALS

High explosives make nuclear weapons work. Yet the chemical reactions that make explosives blow up when they are detonated — and prevent them from exploding in accidents — are among the least understood processes in any weapon component.

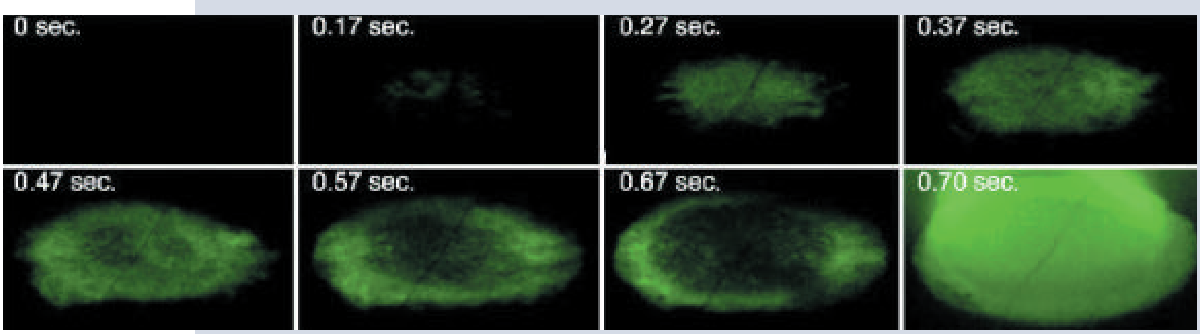
That's why a Los Alamos team is developing fundamental computer models that will predict reactions in the most common class of explosives, high-melting explosives, or HMX.

But building these models to predict how HMX ages and behaves when it reacts requires much more than advanced mathematics. Team members will dirty plenty of beakers and create a lot of small explosions.

There are four interacting focus areas to this project: measuring how the explosives decompose, assessing all the available data to define which reactions are fundamental to the behavior of HMX and therefore must be modeled, incorporating those reactions into simulation codes and developing new experiments to test these models.

In other words, the team is doing what Los Alamos does best: integrating experiments in both fundamental and complex processes with mathematical models of how the molecules in explosives behave under ideal and real-world conditions.

This figure shows the evolution of the surface temperature and second harmonic intensity indicating the occurrence of a solid-solid phase change during ignition. Selected images of the pellet surface show the evolution of the second harmonic generation intensity. The darkening near the middle of the pellet at 0.47 seconds indicates the onset of melting.



Condensed phase kinetics is widely recognized as the weakest link in our understanding of the decomposition of energetic materials. It has been recognized for 30 years that the crystalline phase changes in the condensed phase of HMX may play a role in the decomposition chemistry.

However, no *in situ* measurements of the rate of transformation have been reported for fast phase transitions of interest. In this work, a novel nonlinear optical technique was developed to study the kinetics of a solid-solid phase transition that occurs in heated HMX.

This application of second harmonic generation to HMX, and other energetic materials, constitutes a fundamentally new probe in the dynamics of energetic material decomposition, ignition and combustion. For the first time, solid-solid phase transformations were shown to occur on combustion time scales.

These experiments are allowing the research team to draw a more comprehensive picture of HMX decomposition chemistry over a broad range of pressures.

The multidisciplinary team includes researchers from the Laboratory's Dynamic Experimentation, Chemical Sciences and Technology, Applied Theoretical and Computational Physics and Theoretical divisions along with collaborators from the Universities of Utah and California, Davis.

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DATELINE: LOS ALAMOS

ACCELERATOR TECHNOLOGIES

FOCUSING ON A BEAM

Without nuclear testing, researchers must develop an even greater understanding of the science of nuclear weapons performance. Los Alamos' world-famous half-mile-long linear accelerator plays a vital role in stockpile stewardship, as scientists use its beam to develop new diagnostic techniques to ensure the safety and reliability of the stockpile. LDRD funding contributes to a variety of accelerator-based-science projects. Three projects discussed here include a new capability to take high-resolution photographs of explosive detonations, better computer models of beam dynamics and a "spin filter" that lets researchers do big science without a big accelerator.

PROTON RADIOGRAPHY

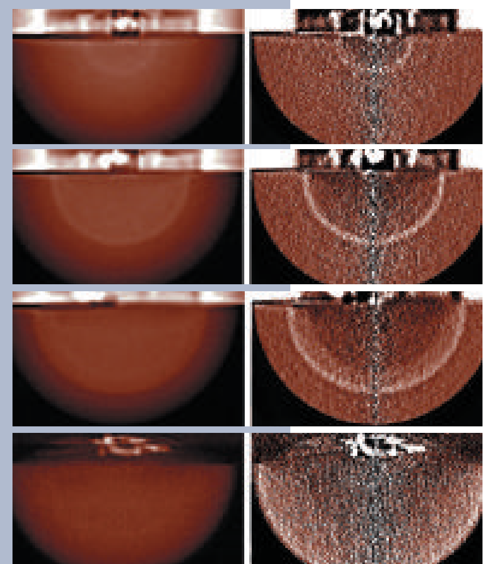
The art of taking pictures has come a long way from the days of those old box cameras that grandma and grandpa used to capture images that would last a lifetime. To wit, digital cameras are replacing analog cameras for taking still photographs, eliminating the need for negatives, film paper and messy chemicals used in the development process.

At Los Alamos, researchers are using the Laboratory's 800-million-electron-volt proton beam at the Los Alamos Neutron Science Center as a "camera" to capture images of a detonation wave from a small-scale explosion. Proton radiography is the newest tool aiding Los Alamos in its mission of Science-Based Stockpile Stewardship.

"In the era of the Comprehensive Test Ban Treaty, which heralds an end to nuclear tests, we have a real need for new radiographic tools, especially those that can be used for dynamic experiments, if we are to understand how weapons components age over time," according to Chris Morris, chief scientist for the Laboratory's proton radiography project. "The success of research in Los Alamos has led to the recent decision to use protons in a future facility for hydrodynamic testing of nuclear weapons mockups."

In 1997, Los Alamos scientists demonstrated the possibilities of proton radiography in the stockpile stewardship realm when they photographed the detonation wave from a small-scale explosion. Scientists detonated a small amount of high explosives inside a chamber specially designed to contain the explosion and let the proton beam at LANSCE enter and exit to produce a clear, high-resolution image of the explosion's shock wave.

DATELINE: LOS ALAMOS



↑ Proton radiography generates many frames of an explosion, producing a kind of motion picture. These radiographs from a high-explosives experiment at LANSCE show the propagation of shock waves (left) and the reconstructed density images (right). Current technology provides up to 7 time frames at each image pane for each explosion. This will be expanded to 24 frames in the near future. Future technology is expected to provide thousands of frames per event.

Researchers are developing a capability for multiframe flash radiography. A new three-lens proton radiography system has been designed, installed and commissioned in one of the LANSCE proton beam lines by a team from the Physics Division and LANSCE Division led by John Zumbro. The three-lens proton radiography system provides more information than normal radiography by measuring the angular spread of the protons.

A team led by Nick King has supervised the design and construction of a seven-frame detector system that has been used to make motion pictures of small exploding systems.

The experiments were designed by John Sarracino in the Applied Theoretical and Computational Physics Division and mounted by a team from the Dynamic Experimentation Division lead by Eric Ferm. “Proton radiography has been a truly interdivisional effort,” says Morris.

Conventional radiography is most often done with X-rays or neutrons. One way to study the behavior inside a weapon’s non-nuclear, high-explosive components is to detonate them (so-called dynamic experiments) and look at the resultant shock waves and material motion using radiography.

But in the recent Los Alamos experiment, researchers used protons — which have several potential advantages over X-rays — to take a picture of what happened shortly after detonation. “X-rays don’t provide a probe with the necessary quantitative precision for stockpile stewardship,” said Morris.

Unlike X-rays or neutrons, which use photons to expose film, proton radiography uses protons, which are shone on the material to be studied. As protons interact with the material from which an image is to be obtained, some of the protons are absorbed or scattered.

Protons that exit the material strike a recording medium, such as a special type of film or electronic camera, and create an image much like conventional photographic film or digital cameras. However, because protons are electrically charged, they undergo a large number of small-angle scatterings as they pass through the material. If not corrected, these scatterings would cause unacceptable blurring of the image as they pass from the object to be photographed to the recording medium.

“The big problem is how protons lose energy and diffuse in angle because of multiple scattering when they interact with the target,” Morris said. Although each of these effects started as a problem, in the end they have provided new radiographic capabilities.

DATELINE: LOS ALAMOS

To help overcome the proton scattering problem, Zumbro and Tom Mottershead developed a magnetic lens to refocus scattered protons. The system uses a series of four quadrupoles — devices that produce magnetic fields — to focus the protons onto the image plane, a process similar to a camera lens focusing light onto film. This new focusing system was the key to overcoming many of the problems that researchers believed would limit the usefulness of protons as radiographic probes.

The use of two lenses on a single axis allows the multiple scattering angle to be measured and analyzed in combination with the conventional radiography data to provide material identification. Work aimed at measuring a proton energy loss image may drastically reduce the dose needed for a given radiographic measurement. If this latter technique works, protons may provide good position resolution at low dose for dynamic biological radiography.

Los Alamos researchers will continue to use LANSCE for additional experiments to develop proton radiography, understand its potential and obtain scientific data on the behavior inside dynamic materials. Data obtained from experiments at LANSCE have shown researchers that proton radiography is a unique diagnostic tool that can be used to better understand the performance of high explosives.

A team led by Arch Theissen is leading an effort to develop a conceptual design of a new high-energy accelerator at LANSCE to extend proton radiography to the region where it is useful for full scale hydrotests of weapon systems.

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ADVANCED MODELING OF HIGH-INTENSITY ACCELERATORS

Research institutions worldwide are increasingly looking toward accelerator-based technologies to help solve a variety of problems, including producing a fresh supply of tritium for the nation's nuclear stockpile, transmuting nuclear waste materials into more stable waste forms, creating new spallation neutron sources for materials science research and producing energy.

Controlling beam loss is essential to using these high-intensity accelerator technologies, because even small losses of particles can degrade components and result in unacceptable levels of radiation. Computer modeling plays an extremely important role in better understanding beam dynamics and controlling beam loss.

Until recently, however, most computer modeling of high-intensity accelerators was done only in two-dimensional form, and simulations were limited to 10,000 to 100,000 beam particles.

Los Alamos researchers Robert Ryne, Salman Habib and Thomas Wangler have developed a new three-dimensional computer modeling capability using massively parallel computers at Los Alamos' Advanced Computing Laboratory and Lawrence Berkeley's National Energy Research Scientific Computing Center. They developed both the software needed for high-performance computing platforms and the highly advanced numerical methods and algorithms.

The need to combine single-particle magnetic optics techniques with a capability to model high-intensity beams led to the use of “split-operator” methods. This allows, for the first time, the systematic inclusion of nonlinear “space charge” effects with nonlinear effects associated with focusing magnets.

Using these techniques, the researchers developed a three-dimensional code called IMPACT (Integrated Map and Particle Accelerator Tracking) to model high-intensity linear accelerators. They also developed HALO3D, a code for studying “beam halo” phenomena, a diffuse region of charge that sometimes forms away from the beam core as accelerated particles move down the pipe, causing beam loss.

By implementing these codes on parallel computers, researchers now can simulate problems involving as many as 1 billion particles with greater accuracy and include more physics in their computations to make their simulations more realistic. Simulations with 10 million to 100 million particles now are performed — a 1,000-fold increase in capability. The new capability and methods also may have widespread applications in such areas as plasma physics, astrophysics and molecular dynamics.

The cost of building major accelerator systems in the future will range from hundreds of millions of dollars to more than $1 billion, according to the researchers. Three-dimensional simulations are essential to have confidence in the designs and to ensure the success of these projects. This modeling also makes it possible to design accelerators faster and cheaper. Large-scale, high-accuracy simulations can lead to cost savings of more than $100 million in a billion-dollar-class machine.

Ryne and his colleagues are proposing to perform halo experiments at the Low-energy Demonstrator Accelerator at Los Alamos to provide a benchmark for the three-dimensional computer codes they developed under LDRD. The experiments are designed to predict how and when beam halo will occur and how to minimize such occurrences.

The researchers also are involved in the Department of Energy's Grand Challenge for Computational Accelerator Physics, a high-profile DOE project designed to develop new beam dynamics and electromagnetics modeling software, which will be used for designing the next generation of accelerators.

Los Alamos and the Advanced Computing Laboratory are among four other universities, labs and computing centers participating in the grand challenge. "We are the premier site in the country for doing parallel beam dynamics. Our LDRD work gave us the credibility to propose and be involved in the DOE Grand Challenge," said Ryne.

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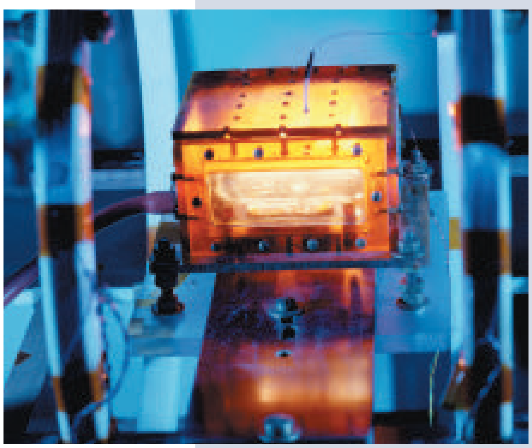
Intense laser light polarizes helium-3 gas in a glass cell. Passing unpolarized neutrons through the polarized helium-3 gas produces a polarized neutron beam.



NEW TOOL FOR NEUTRON SCIENCE

The Superconducting Supercollider is history, of course, and accelerator time at CERN, the European Center for Particle Physics, is limited. However, Los Alamos scientists using new technology are doing big science without the high energies offered by those big accelerators.

The Los Alamos Neutron Science Center (LANSCE) is the most powerful pulsed neutron spallation source in the United States, and Seppo Penttila and his collaborators are taking full advantage of its capabilities.

Penttila, a nuclear physicist, has developed an instrument that uses a dense volume of helium-3 gas to polarize, or line up, a beam of neutrons. Precisely measured neutron beam polarization allows scientists to do the kind of particle physics usually reserved for the big accelerators.

In both low- and high-energy accelerators the same nuclear properties are present. The difference is that scientists need much more accurate instruments when using lower-energy accelerators. Penttila says the helium-3 polarizer is such a tool and is valuable because it covers a large neutron energy band, making a whole wide range of new physics possible.

Applications for polarized neutrons in neutron scattering span a broad range of issues in physics, chemistry, materials science and biology.

Sometimes called a "spin filter," a helium-3 polarizer works because the helium-3 nucleus spins in the same direction or opposite direction as its neutron. When neutrons spinning in the opposite direction interact with helium-3, they are absorbed, but neutrons spinning parallel with the helium-3 are transmitted. This yields a highly polarized neutron beam.

The helium-3 polarizer is useful with all neutron sources, but is particularly effective with pulsed spallation sources like the one at LANSCE where the neutron energy can be determined very accurately. Penttila will use the polarizer to study the weak interaction between nucleons and to test the standard model of electroweak interactions, central to the present basic understanding of matter.

This could not be possible without the helium-3 polarizer tuned specially for the LANSCE source.

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DATELINE: LOS ALAMOS

THREAT REDUCTION

DISASTER, DETECTION, DECONTAMINATION

Weapons of mass destruction come in three types: nuclear, biological and chemical. Controlling the proliferation of these weapons is integral to Los Alamos' national security mission. LDRD funding has been instrumental in the development of new sensors to detect chemical and biological warfare agents as well as novel ways to decontaminate things without destroying them in the process. Using the Lab's powerful computers, researchers have developed an initiative to help emergency responders deal with large-scale disasters, whether caused by a terrorist or Mother Nature.

URBAN SECURITY INITIATIVE

Cities are enormously complex, vulnerable on many levels to terrorist attacks and natural disasters, and they are getting bigger. As their size increases, both in area and population, so do their vulnerability and their importance to the national infrastructure, making the study of cities critical to national security.

To help emergency responders deal more effectively with large-scale disasters and to help planners prepare for them, Los Alamos researchers have developed the Urban Security Initiative.

↑ Researchers are studying how the interwoven strands of a city's fibers operate in times of disaster.

The project involves a wide range of scientists — from chemists and engineers to mathematicians and physicists — plus researchers and officials from academia and government. It links many urban subsystems — including transportation, energy distribution, weather, infrastructure damage, water distribution, ecosystems, economic activities, geology and demographics — into an integrated system that takes advantage of the Laboratory's powerful computing capability.

DATELINE: LOS ALAMOS

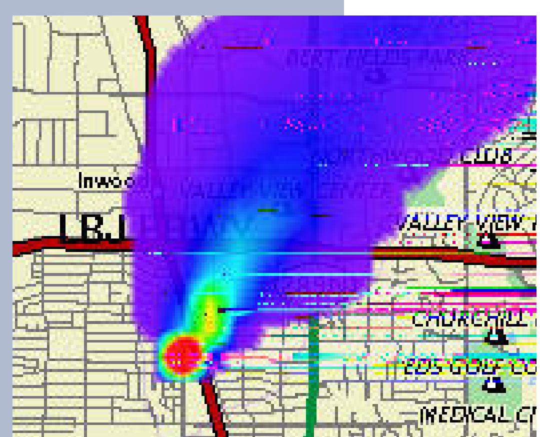
"The goal is to combine new and existing computer models, along with a World Wide Web-based communication tool, to understand how the interwoven strands of a city's fibers operate in good times and bad," said Los Alamos researcher Grant Heiken.

The system under development will allow such organizations as the Red Cross, local utilities and highway departments to interact effectively. While all have the same goal in the event of an emergency, their agendas may vary so far as to put them in each others' way at critical times.

A large-scale technical approach is the key to grasping the complex reality of a city, its infrastructures, its people and their needs in time of disaster. Computer modeling plays a vital role in such massive approaches, allowing these multilevel problems to be visualized and understood by urban planners and emergency response agencies.

To determine the effects of an earthquake, for example, researchers must understand the interwoven pieces that are under stress: the soil types through which the shock waves travel, destroying some areas and sparing others, and the damaged roadways and routes of emergency responders who must find alternate paths. Working with the Southern California Earthquake Center, researchers have linked models of seismic ground response, earthquake damage and the infrastructure of Los Angeles.

This simulation of a toxic release in the Dallas area shows the expansion of a ground-level plume.



Researchers also must analyze the electric power grid to understand the effect of outages and disruptions on communications, lights, computers and even building air-circulation systems and elevators. They must understand how the poisons in a toxic flow from a damaged chemical-storage tank leak into the groundwater, flow into nearby rivers and are taken up into the atmosphere to be redeposited elsewhere.

In the event of a terrorist attack, responders must understand the errant eddies of wind that carry biological or chemical toxins throughout the city, drifting past homes and office complexes, along traffic routes and through subway tunnels.

The initiative's researchers have modeled airborne toxic releases in an urban setting, analyzing the dispersion of a toxic plume and the exposures to traffic passing through it. A study of the Dallas area used a traffic model called TRANSIMS tied to meteorological and fluid dynamics models that showed where and how the plume would travel, and mapped how much toxin each vehicle was exposed to as it passed through the cloud.

The researchers also are examining the effects of a city on its environment over time. Focusing on the pathways of air and water pollution, the team is narrowing its analysis to the difficult nitrogen family. Nitrates have important health, local ecosystem and global climate implications, and their chemical precursors are produced by auto emissions and industrial processes.

By using combined air- and water-modeling systems, the researchers hope to understand how these chemicals are produced, dispersed into the air, fall to the ground and flow into storm drains during rainy periods, and subsequently flow into lakes, oceans, rivers and wetlands.

For the Los Angeles basin and coastal region, the researchers are trying to determine how much of the nitrate pollution comes from the atmosphere as opposed to other sources. This will have an impact on strategies for improving both air and water quality.

Understanding the urban system as a whole also can improve the long-term viability of a city, guiding its future development and expansion.

"The stability of the United States, as well as the stability of the international community, will depend to a large extent on the vitality of our cities," said geologist Greg Valentine. "Infrastructure is vulnerable, especially in certain cities that have grown so large, and have become 'metastable,' making them flash points for international problems, globally and regionally."

Another direction for the team is to encourage further studies of urban systems by other organizations and institutions, driving toward a declaration of the years 2001-2010 as "The Decade of Science in the Cities."

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BIOMIMETIC AND COLOR-CHANGING CHEMICAL SENSORS

Spotting a chemical or biological agent in the field before you've breathed it, touched it or tasted it, is one of the toughest challenges in the new realm of threat reduction. Unless those in terrorist or combat zones are outfitted 24 hours a day in biohazard suits and gas masks, there's always a chance that the first people on scene in a bad situation will be the first victims.

With a spray bottle, a crop duster or a simple weed-killer pump, a terrorist or rogue nation could infect or expose dozens or thousands of people while remaining anonymous, and critical time could pass before the deed is uncovered. With several known biological agents (toxins or pathogens), such as anthrax or cholera, days may go by before symptoms begin to appear, stealing valuable treatment time from the victims. Knowing of an exposure as it happens and understanding its nature can be the most challenging parts of the biological agent warfare puzzle.

New directions in detection equipment, however, are bringing some of nature's own tricks to the rescue — mimicking the receptors on the surface of a cell that would normally react to toxins such as cholera.

For chemical warfare agents, a badge using an array of small electrochemical sensors and a simple color-change indicator, along the lines of litmus paper, is under analysis. Inexpensive, easily read and not dependent on fragile technology, the polymer coatings of the chemical detector can be worn into the field on a uniform or as a badge.

In the biological field, chemist Basil Swanson and his team are developing sensors based on membrane architectures containing receptors that mimic cells in the body.

When cholera toxin is present, it binds to receptor molecules in the synthetic membrane, and when a tiny laser light is shone across the membrane, the receptor responds with a fluorescent color change. Two fluorescing dyes have been attached to the receptors within the membrane, providing a fail-safe system that is unaffected by temperature and other environmental variables that can throw off analyses in the field.

While cholera has been the initial target for development, Swanson says the concept could easily be applied to a variety of toxins or pathogens, providing assistance from distant battlefields to local hospitals or health clinics.

For chemical exposure situations, electrochemical sensors derived from polymer electrolyte fuel cells, as well as a multilayered sheet similar to instant colored film, are the subjects of Los Alamos chemist Tom Zawodzinski's efforts.

Called point sensors, the products Zawodzinski envisions could be worn in the field, placed on a vehicle or even hung from a tree, instantly warning solders, law-enforcement or medical personnel of the presence of chemical toxins before extensive lethal exposures have occurred.

The electrochemical cells use thin, multilayer structures that behave like batteries. Different chemistry is introduced into a series of patches to provide responses to different agents. In the presence of mustard gas, for example, an electric current flows from catalyzed electrochemical oxidation of the agent. Small electronic packages, available today in glucose test kits for example, use this current to drive a warning light or sound.

One compound used to simulate properties of mustard gases is oil of wintergreen. Zawodzinski and co-workers demonstrate the sensitivity of their sensor by showing an instant response to the breath of someone chewing wintergreen gum.

DATELINE: LOS ALAMOS

The multilayer color-change system uses enzymes separated from reactive dyes by a thin layer of another chemical, called a redox-active product. In the presence of certain chemicals, such the VX nerve agent or mustard gas, the enzymes are inhibited, reducing their normal action on the redox-active product.

The dyes beneath depend on a particular chemical recipe to retain their "normal state" coloration. When that chemistry is changed by the enzymes' contact with nerve agents, the dyes react and alert the wearer by altering their color in the presence of the new chemical profile. A green badge, for example, suddenly becomes bright red, as the enzymes crucial to maintaining the green color are damaged by the nerve agent.

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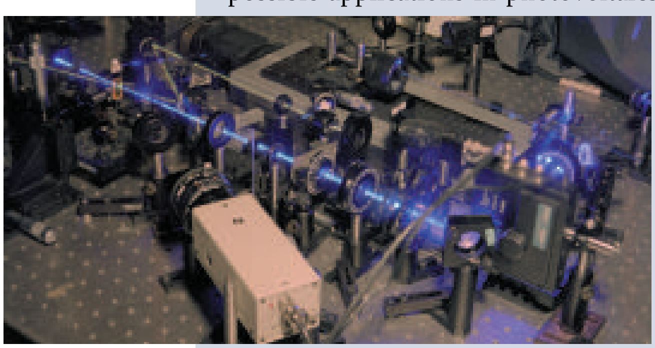
ELECTRON TRANSFER RESEARCH LEADS TO SENSOR DEVELOPMENT

One of the advantages of basic research is that while researchers are investigating processes in a particular field of study, they sometimes uncover unexpected results that have an impact on wider fields.

Los Alamos researchers Duncan McBranch, David Whitten, Victor Klimov and others know this firsthand. While studying electron transfer in conducting polymers for possible applications in photovoltaics and nonlinear optics, the researchers discovered they can create luminescent sensors capable of detecting biological and chemical agents. These sensors may have national security applications for recognizing pathogens of concern for bioterrorism, such as anthrax, and chemical agents in explosives, such as TNT.

Electron transfer in conducting polymers is a promising new field of photochemistry — the study of the effects of light on chemical

The femtosecond transient absorption spectrometer developed in this project is used to measure the earliest events in photo-induced electron transfer.
Photo by John Flower



systems. During electron transfer, when a conducting polymer — a linear compound with a repeating molecular structure — is excited by light, electrons from that polymer can undergo “forward transfer” to an electron-accepting molecule such as buckminsterfullerene (C_{60}) in less than 300 femtoseconds, or three-quadrillionths of a second.

However, the speed in which the electrons return to the polymer (called back transfer) can be up to nine orders of magnitude slower, in the range from millionths to thousandths of seconds.

McBranch and his colleagues developed new high-sensitivity instrumentation for femtosecond transient spectroscopy. They applied these techniques to determine the dynamics of the processes in the charge-transfer cycle: the initial photoexcitation events, the ultrafast forward electron transfer and the subsequent (often much slower) back transfer.

They also devised methods in which they might apply these charge transfer states in photovoltaic and nonlinear optical devices.

“We wanted to know the nature of the photoexcitations in conducting polymers and whether we could control these excitations,” said McBranch. “If you want to work with electrons in photovoltaic or photosynthetic devices, you want to control the speed, so that the electrons live long enough to perform electrical work or initiate chemical reactions.”

Together with control over the speed, the researchers developed methods of making polymer films that allow the direction of charge transfer to be controlled. For example, funneling electrons toward a surface is possible by building films by multiple deposition of individual molecular layers, each of which is tuned to have slightly different structure.

The creation of luminescent sensors for biological and chemical agent detection followed from the discovery that polymers have an amplified sensitivity to charge transfer.

“We first excite the polymer so that it emits light along the entire polymer chain,” McBranch explained. “If you put an electron-accepting molecule in the vicinity, it can react rapidly with the photoexcited polymer chain so that it can no longer emit light. In other words, a single small molecule can quench the luminescence of a very long polymer chain.”

The researchers have filed four patents on their research, including those for the chemical/biological sensor concept and instrument design, femtosecond transient spectroscopy and nonlinear optical processes that use photoinduced electron transfer.

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DATELINE: LOS ALAMOS

DECONTAMINATION OF CHEMICAL AND BIOLOGICAL WARFARE AGENTS IN THE URBAN ARENA

Chemical or biological terrorist attacks in urban areas present unique challenges for those responding. Once the first responders have pulled the terrified citizens to safety, the surroundings that are contaminated need to be flushed, scraped, sprayed or treated in some way to destroy the chemical or biological threats that remain.

In strictly military surroundings, this is less of an issue, because many military items used in the field are specially hardened and developed for battlefield conditions. But what about a release of a toxic compound or biological agent in a museum, layering the thousands of treasures there with anthrax spores or worse?

An artist's conception of a subway train being decontaminated with a jet of plasma.

Illustration by Donald Montoya

Clearly, treating the priceless items within the building without damaging them is a complex and delicate issue.

Such knotty decontamination issues have come under close scrutiny at Los Alamos with groundbreaking technology development under physical chemist William Earl and plasma chemist Gary Selwyn.

Recognizing that this combined area of chemical and biological research could be a promising and important area for new work, Earl and Selwyn proposed to study two methods for decontamination of chemical and biological warfare agents.

For both biological and chemical agents, Selwyn, along with postdoctoral researcher Hans Herrmann, explored using a jet of charged oxygen feedgas, known as a plasma, to destroy many organic compounds without damaging the surfaces on which they sit.

Selwyn designed a jet device that, driven by radio frequencies, converted helium mixed with oxygen to a flat jet, or sheet, of oxygen-containing plasma that could be simply swept across a surface.

On this project, the plasma jet's effectiveness on the insecticide malathion was tested, as a simulation of its effect on nerve agents. In the course of the research, the researchers acquired new understanding of the detailed chemistry that occurs when low-temperature plasmas interact with various surfaces and chemicals.

They also determined that a variety of products generated by the plasma, including atomic oxygen and metastable molecular oxygen — a highly activated form of ordinary oxygen — effectively destroyed a wide variety of chemical and biological agents, including surrogates of the infectious disease anthrax and mustard gas, a debilitating chemical agent.

For purely chemical attacks, Earl examined a group of alumino-silicates called zeolites, used in industry as molecular sieves and catalysts thanks to their microporous crystalline structure, which will soak up chemical toxins, and potentially reduce their toxicity over time through further chemical reactions.

The potential of zeolite catalysis is especially interesting to the researchers, as many chemical-weapons compounds contain sulfur or phosphorous, which frequently poison various catalytic systems. Both molecular modeling and experimentation demonstrated that zeolites can adsorb surrogates for the classic chemical weapons compounds. In a special case, the research team demonstrated the ability to oxidize malathion on several modified zeolites.

"Our technical findings were that both methods work, but they needed refining and fine tuning to be useful under varied field conditions," said Earl. "We used those projects as sort of an introduction to the business," he said, exploring how Los Alamos could put its considerable chemical and biological research resources to work in a new direction of importance.

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BIOSCIENCE AND BIOTECHNOLOGY

HEALTHY RESEARCH

A weapons laboratory has a special interest in health research: Working with special nuclear materials requires an understanding of their effects on the people who are exposed to them. Over its 50-plus year history, Los Alamos' expertise in the life sciences, combined with its capabilities in the design of complex instrumentation, has enabled researchers to contribute to national problems related to health care. Recently funded LDRD research has delved into DNA, the brain and hip joints.

DNA DOUBLE-STRAND BREAK REPAIR

Los Alamos research into the health effects of radiation stems from the earliest days of the Manhattan Project, when people first fashioned plutonium into the heart of a nuclear weapon. Research continued through the Cold War years, as scientists sought ways to better understand the effects of radiation on the human body and the environment as well as to monitor atmospheric radiation levels.

The Cold War is over, but its nuclear legacy remains. Los Alamos' role in safeguarding and dismantling the weapons remaining in the nuclear stockpile still requires that people work with radioactive materials. Continued research into radiation impacts, including genetics, is vital to developing ways to limit workers' exposure to hazardous materials.

Over the years, LDRD funding has opened new avenues of research into the study of genetics. One project, led by researchers David Chen and Robert Cary, has greatly enhanced the understanding of DNA repair and the proteins involved using a two-pronged approach: genetic screening and atomic force microscopy, or AFM.

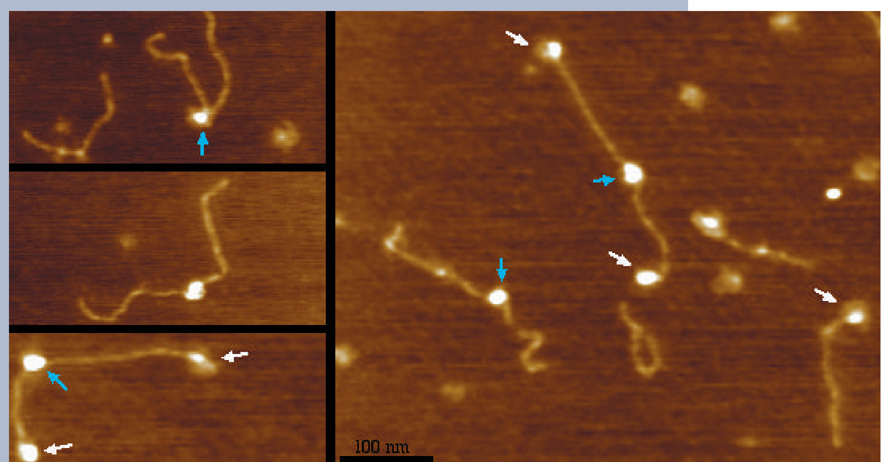
DNA is responsible for the transmission of hereditary characteristics and for building proteins in cells. Until recently, researchers knew little of the healing mechanisms involved when a double-strand of human DNA breaks in a cell. In particular, researchers did not have a good understanding of which proteins were involved in the healing process and the specific roles they played.

If left unrepaired, DNA double-strand breaks can become lethal or mutagenic in the human body, leading to cancer and other diseases.

DATELINE: LOS ALAMOS

Chen and Cary performed genetic screening experiments on protein/protein interactions, crucial to DNA repair and normal development of the immune system and maintenance of human genome integrity. They studied seven proteins, all of which they suspected play some role in the healing of broken DNA ends. Studying these interactions led to better understanding of how DNA repairs itself and which proteins are involved in such repair.

For example, through genetic screening they identified a novel protein that interacts with the complex responsible for the actual repair, called the DNA ligase IV complex. The researchers also discovered that this complex may, in turn, associate with a chromosomal structural protein, and so on down the protein interaction chain. The researchers now are studying the specific protein interaction mechanisms involved and their role in DNA repair.



Images like this obtained from atomic force microscopy led researchers to determine that a protein complex that binds to broken DNA ends (white arrows) actually holds the broken ends together (blue arrows).

AFM is an offshoot of scanning tunneling microscopy, or STM, in which the wavelike properties of electrons permit them to "tunnel" beyond the surface of a solid. In STM, the sharp tip of a tungsten needle is positioned a few angstroms — three-tenths of a billionth of a meter — from the sample surface.

A small voltage is applied between the probe tip and the surface, causing electrons to tunnel across the gap. As the probe scans over the surface, it registers variations in the tunneling current. This information is then processed to provide a topographical image of the atomic structure the surface.

AFM is similar, except that it has a spring attached to the tip that's sensitive enough to respond to inter-atomic forces. The atomic force between the spring and the sample is used as the feedback signal to control the microscope. This force is measured by the deflection of the needle tip and the subsequent amount of displacement of the reflected laser beam off the back of the tip. The reflected beam enters a photodetector, which converts the amount of displacement into an electric signal.

AFM originally was developed in the mid-1980s for studying the surface structure of a wide variety of materials, but is well-suited for obtaining three-dimensional, high-resolution topographical images of protein surfaces without staining, coating or other molecule sample processing. AFM can be used to obtain images from samples in air, aqueous environments or organic solvents.

The researchers fine-tuned the AFM technology so that it could be used with almost any DNA protein complex and characterize how the proteins affect DNA and associate with it. The researchers also used a “tapping mode” probe, which lightly taps the protein surface without damaging it and reduces the probe's oscillation amplitude. This amplitude change tracks the surface topography.

Los Alamos researchers also developed robust sample preparation techniques that allows them to look at a wide range of proteins and DNA complexes with great reproducibility.

Images obtained from AFM led the researchers to determine that a protein subunit called Ku and an enzyme called DNA-dependent protein kinase play structural roles in the DNA repair process. “People knew that Ku binds to the broken DNA ends, but until we looked at it with atomic force microscopy, they didn't know that once bound, the Ku actually holds the ends together,” said Cary.

In particular, the images obtained from AFM demonstrated that Ku has properties that allow it to bind to each of the broken DNA ends and temporarily “tether” the ends together without bonding to each other. This significant finding has led Los Alamos researchers to hypothesize that Ku is the first protein to recognize a double-strand break in a cell and call for DNA-dependent protein kinase to enter the damaged DNA region.

Chen and Cary suspect that when the kinase is activated with the broken DNA ends and the Ku holding them, it signals for ligase IV to come in and do the actual repair.

Researchers are further developing the AFM technology to obtain even better three-dimensional, high-resolution images that can be used to study large proteins, which cannot be studied by current technologies such as nuclear magnetic resonance and X-ray crystallography. Large proteins are much more complex in structure than small proteins. NMR and X-ray crystallography, which are limited to looking at smaller proteins, cannot adequately decipher such complexity.

“It's possible that the image resolution can be pushed to such a level that we can actually see the submolecular details of proteins,” said Cary. “We can use this information to help better understand how proteins function and to determine how protein/protein complexes affect each other.”

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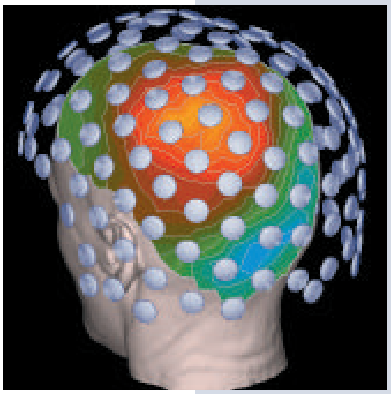
DATELINE: LOS ALAMOS

MEASURING THE IMMEASURABLE

Electromagnetic fields abound in our world. Some, like the gigantic magnetic fields that protect Earth from solar winds, are obvious and powerful. Others, like the magnetic fields found in videocassette recorders, cellular phones and electric toothbrush motors, are far smaller. Still others, like the electromagnetic fields that exist within the human body, are almost immeasurable.



A composite image generated by combining anatomical information from a magnetic resonance imaging scan, magnetic field contours measured by the SQUID sensor array, and the SQUID sensor array represented by small "discs" placed around the subject's head.

Graphic by Doug Ranken

These human biomagnetic fields, generated by electrical currents produced by neurons in the brain, are a billion times weaker than Earth's magnetic field and 10,000 times weaker than the field surrounding a household wire. The strongest neuronal currents are generated by normal brain activity when we respond to light, sound, touch, smell or other sensory input; or even the impulse to move a muscle or express a thought.

Researchers have successfully used Superconducting QUantum Interference Device (SQUID) sensors to measure a variety of extremely small magnetic fields. New concepts for applying SQUIDs, the most sensitive magnetic field detectors known, were developed at Los Alamos in the 1980s and are being applied in a number of areas today. SQUIDs detect and convert weak magnetic fields into electrical voltages that can be easily measured and recorded. This ability allows researchers to employ SQUIDs in a number of medical and scientific areas.

Biomagnetism research at Los Alamos includes work in magnetoencephalography (MEG), a method of measuring the tiny magnetic fields produced when small groups of the brain's roughly 100 billion neurons are active, and magnetocardiography, a method for measuring the magnetic fields produced by cardiac activity.

Researchers have created a scanning device and computational methods that permit more sophisticated analysis of clinical MEG data. The helmet-like device, containing 155 ultrasensitive sensors, is currently being built for use in clinical settings such as the National Foundation for Functional Brain Imaging in Albuquerque, N.M. Future work with the MEG device could help neurosurgeons pinpoint areas associated with brain injury or functional abnormalities such as epilepsy and help medical researchers study such disorders as Parkinson's disease, multiple sclerosis and schizophrenia.

Other scientific applications of SQUIDs currently focus on corrosion processes in metal containers that typically cause tiny electrical currents known as corrosion currents. These currents induce weak magnetic fields that can be detected by SQUIDs. Los Alamos scientists have developed a prototype device capable of detecting corrosion currents in nuclear waste storage containers. The technique detects the natural magnetic emanations from the corrosion process and does not require exposing the sample to radiation or other external energy sources. It also can be used to investigate corrosion and ablation in other metallic materials including aircraft, sea vessels and pipes.

In addition to corrosion current detection, SQUIDs are being used as sensitive gravity gradiometers to measure and map variations in gravitational fields. The process detects localized changes in the gravitational field caused by bodies of material that differ in density from their surroundings. The technology holds significant promise for the passive measurement of oil reserves and the location and mapping of subterranean voids.

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CARBON-BASED PROSTHETIC DEVICES

Anyone who has ever had a finger joint replaced with a prosthesis due to serious injury or disease such as rheumatoid arthritis knows about the trade-off involved: The implant may eliminate the pain, but the recipient invariably loses strength and agility in that finger. These small prostheses, typically made of silicone rubber, also pose wear problems and may require replacement.

Los Alamos researchers David Devlin, David Carroll, Robert Barbero, Tom Archuleta and others demonstrated that it is feasible to make endoprosthetic devices from carbon or carbon-reinforced composites, greatly improving joint mobility and reducing the risk of joint failure. The researchers also developed processes for increasing the strength, density and wear of carbon-based prosthetics.

Prosthetic carbon hip joints may one day replace currently used metal joints. A half-size hip joint prosthesis is shown with a full-size human pelvic structure. ↓

Carbon has been proven biocompatible with the human body and has mechanical properties similar to bone. In fact, heart valves made of isotropic pryolytic carbon have been implanted in several hundred thousand patients over the past 25 years. The researchers wanted to find out whether carbon-based finger joints could be made with adequate strength and wear resistance.

They tested two carbon fiber structures, one a three-dimensional carbon-fiber preform made of 80 percent satin fabric and 20 percent chopped fiber, the other a unidirectional carbon-fiber with 40,000 filaments and a carbon-fiber braid outer layer. The researchers found that for large joints such as hips the three-dimensional carbon structure was the best, while the unidirectional carbon-fiber structure provided superior strength for small joints.

The researchers fabricated the carbon composites via electromagnetic induction heating, a standard industrial method for heating metals for soldering, tempering and annealing, among other uses. They then demonstrated that this process, coupled with a process called chemical vapor infiltration, increased the strength and density of the carbon materials.

Induction heating allowed them to heat materials from the inside out. As the internal region of the material is heated, cool reactant carbon gases penetrate inward. Deposition and densification of the composite begins at the center and as the deposition proceeds, the coating moves outward toward the surface.

The result is a denser, stronger carbon composite in the inner region and a more porous outer region that allows for bone ingrowth. The researchers have filed a patent related to this porosity grading process capability.

In addition, the Los Alamos researchers developed a process for increasing the wear resistance on the ball of the joint by using plasma-assisted chemical vapor deposition.

Under this process, a carbon composite joint is placed in a high-vacuum chamber and methane gas is introduced, which forms a discharge around the composite. The highly accelerated carbon within the plasma is deposited on the part, forming a diamond-like carbon film, with about half the hardness of diamonds.

Devlin and his colleagues currently are testing half-size, all-carbon prosthetic hip joints for strength and fatigue. These prosthetics may one day replace hip joints currently made of various metals and alloys and eliminate the need for bone cement to anchor them. Approximately 250,000 hip replacement surgeries are performed annually in the United States.

Ascension Orthopedic Inc. of Austin, Texas, has signed a cooperative research and development agreement with Los Alamos to develop all-carbon hips.

Initial strength test results revealed that the half-size joints showed no signs of degradation or cracking when subjected to 200 pounds of pressure. Fatigue testing is now being performed, in which about 170 pounds of pressure will be applied to the joints, lessened, then applied again at least 5 million times nonstop.

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ENVIRONMENTAL SCIENCES

SOLUTIONS TO GLOBAL PROBLEMS

One aspect of Los Alamos' national security mission is to develop new technologies to solve the environmental problems related to the manufacture, storage, treatment and disposal of nuclear materials. This research has expanded to include studies of non-nuclear environmental problems on a global scale: among them energy, climate, and air and water quality. Projects supported by LDRD have had great impact in these areas.

COUPLED ENVIRONMENTAL MODELING

Anyone who has lived in the desert Southwest knows water is a precious commodity. Popular campaigns tout the benefits of conservation. "Agua Es Vida" (water is life) bumper stickers have become commonplace in many towns and cities.

"The Southwest is the fastest growing region of the United States," says researcher Larry Winter. "The whole Southwest faces a major water shortage, especially if it continues to grow as it is. We're hoping to be able to contribute to the solution."

At Los Alamos, researchers are using the Nirvana Blue supercomputer to model water resources in the Rio Grande Basin. Nirvana Blue is part of Los Alamos' Accelerated Strategic Computing Initiative and High Performance Computing Program.

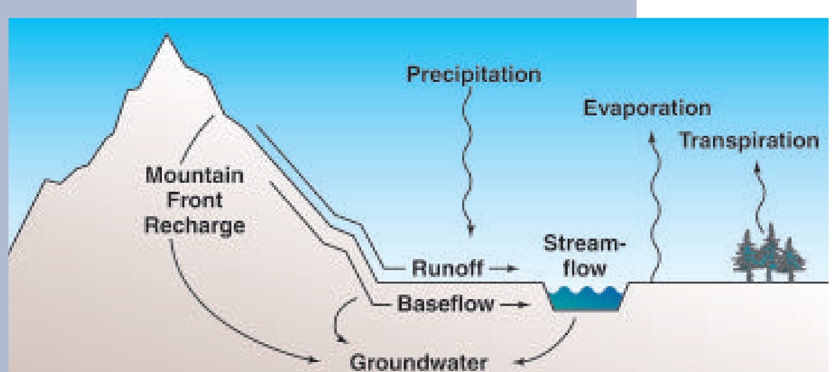
"It's not lost on us that we're able to contribute to the well-being and future of our state," said Winter.

The Rio Grande Basin's water balance depends on complex interactions among regional climate, land surface, groundwater, stream networks and multiple uses of the water.

A regional assessment of the effects of possible climate change and competing uses for water resources demand an

Researchers are using Los Alamos' Nirvana Blue supercomputer to model water resources in the Rio Grande Basin. The water balance depends on complex interactions, as illustrated by this conceptual model.

Graphic by Lori Kleifgen



understanding of the hydrologic cycle at local scales over long time periods. Modeling these systems requires coupling global-to-regional-scale atmospheric simulations with regional-to-local-scale simulations of land surface and subsurface flows.

Research so far has focused mainly on land surface and atmospheric interactions. The land surface provides water back to the atmosphere, where coupling occurs, explained Winter. Other couplings occur between land hydrology, groundwater systems and river systems.

This fall, Laboratory researchers hope to integrate river and groundwater systems into the modeling process, according to Winter.

Global climate models deal with resolutions on large grids, say, 200 kilometers, said Winter. Researchers at Los Alamos use the global climate models to develop computer models downscaled to resolutions as small as 5 kilometers — researchers eventually hope to develop climate models of 1-kilometer resolution.

"We're interested in being able to simulate thunderstorms. We want to get down to 1 kilometer because that's what it takes to model a thunderstorm," said Winter.

Global climate data includes such elements as barometric pressure, precipitation, wind and temperatures.

Los Alamos researchers recently completed their first soil moisture maps of the Upper Rio Grande Basin. Soil moisture is a key variable in determining where water is and where it should go. That's doubly important for New Mexico residents who get most of their water from groundwater, said Winter.

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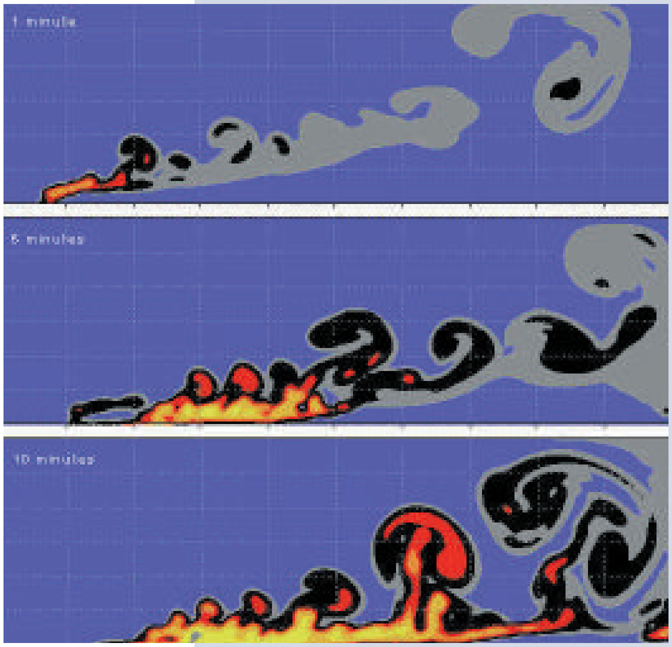
WILDFIRE MODELING

As part of the coupled environmental modeling project, researchers have developed a computer model to simulate the behavior and spread of wildfires as well as the local and regional weather conditions that drive a fire or are driven by a fire.

Fire behavior is driven by local weather conditions such as winds, temperature and moisture. Researchers use the Regional Atmospheric Modeling System — RAMS — to predict variable weather patterns. The RAMS model, originally developed at Colorado State University, uses data from all over the country to predict weather parameters.

DATELINE: LOS ALAMOS



This wildfire simulation couples a full-physics fire model with a micro-meteorological model to create the perfect tool for simulating the way a wildfire spreads and grows. In this simulation a fire fed by dry fuel and driven by wind blowing 4 meters a second consumed an area the size of a football field in less than six minutes.

RAMS then translates the information into smaller and smaller geographical areas. Weather predictions from RAMS in the vicinity of a fire are used by the high-resolution model for strong gradient applications — HIGRAD — to accurately simulate weather variables across a fire line.

HIGRAD was developed at Los Alamos in partnership with the National Center for Atmospheric Research.

HIGRAD is then coupled to a Los Alamos-developed fire behavior model — FIRETEC — that predicts the spread of a wildfire, based on the physical processes that control fire combustion, radiation and turbulent transport of hot gases.

In February 1998, Los Alamos researchers observed a controlled burn at a wildlife refuge near Cape Canaveral to gather data that led to an improvement in its Wildfire Prediction System.

Lab researchers hope that these computer models soon can help fire professionals more effectively fight fire, train firefighters and plan strategies to prevent catastrophic fire conditions.

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POLYMER FILTRATION

For nearly half a century the electroplating industry has treated its process wastewater by precipitating out the heavy metal content and burying the resulting toxic sludge. Lacking a better solution, tons of economically valuable metals have been dumped in the ground as waste. Researchers at Los Alamos have developed a commercial technology that conveniently and inexpensively extracts these metals from wastewater through a process called polymer filtration.

DATELINE: LOS ALAMOS

Polymer filtration technology couples unique water-soluble, metal-binding polymers with advanced ultrafiltration membranes to treat various metal-bearing wastewater. After the polymer binds to the metal ions, researchers filter the polymer-metal solution and then concentrate it using ultrafiltration.

At process end, clean water is discharged and the economically valuable metals are recovered as concentrate for reuse or refining so there is no secondary waste or sludge stream. The polymers never leave the filtration system and can be used repeatedly.

The polymer filtration process also has also been successfully used both for actinide removal from aqueous waste streams and the recovery of metals from acid mine drainage.

In 1995, *R&D Magazine* named the technology one of the top 100 most significant technical innovations. It has since been licensed to PolyIonix Inc. of Dayton, N.J. PolyIonix builds polymer filtration modules capable of treating from 1 to 30 gallons of electroplating wastewater per minute. As more members of the electroplating industry adopt this novel technology perhaps less of Earth's valuable metals will end up as waste.

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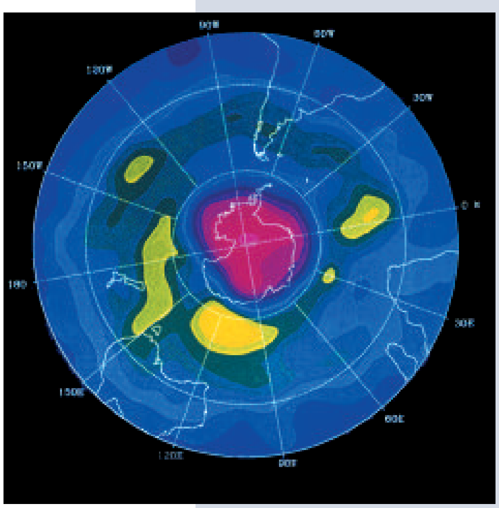
This 1995 false-color image shows the region known as the "ozone hole" over the Antarctic (the magenta-colored area). The green areas indicate medium concentrations of ozone; the orange areas indicate high concentrations.

National Oceanic and Atmospheric Administration image



WHERE HAS ALL THE OZONE GONE?

We need our ozone layer to protect us from harmful ultraviolet solar radiation, yet we continue to lose valuable ozone every day. Figuring out why is vital.

One of the most important questions in the area of ozone depletion is how ozone-eating chemicals react under upper atmospheric conditions, particularly their reaction with stratospheric aerosol particles.

The problem is the lack of a practical way to study stratospheric ice *in situ*. The stratosphere is very thin, with few particles to begin with. Even more problematic, aircraft cannot fly high enough to take a sample.

On top of that, bringing the sample back in pristine condition is practically impossible.

So Bryan Henson and Jeanne Robinson are doing the next best thing, duplicating the conditions at the top of the atmosphere in a lab. They start by growing ice samples that simulate polar stratospheric cloud particles and, using a new application of a tried-and-true laser light scattering technique called "second harmonic generation," they study the surface reactions of the ice when exposed to various gases.

Using the second harmonic technique involves looking at the laser light that has twice the frequency of the original light wave when scattered off the simulated cloud particles. Because the second harmonic light scatters from the surface of the ice sample the technique affords researchers more accuracy in making measurements.

The idea is to understand what chemical mechanisms are at work in ozone depletion using the laser technique to accurately measure concentrations of molecules on the ice surface and to explore the thermodynamics of the interaction in the most accurate temperature and pressure conditions possible.

The work challenges some of the current ideas in the mechanics of ozone depletion, which have relied on experiments that don't always try to exactly duplicate upper atmospheric conditions.

In the future, Henson, Robinson and their co-workers hope to design an experiment to determine another central question, what is the exact composition of the ice?

There are a wide variety of acids that can react with upper atmospheric ice; therefore, it's important to know the effect they may have on ozone depletion chemistry.

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DATELINE: LOS ALAMOS

ABOUT THE COVER ...

RESEARCH FUNDED BY THE LABORATORY-DIRECTED RESEARCH AND DEVELOPMENT PROGRAM HAS MADE SIGNIFICANT CONTRIBUTIONS TO THE WORLD'S SCIENCE AND ENGINEERING KNOWLEDGE BASE. Clockwise from top left: the femtosecond scanning tunneling microscope allows scientists to peer deeply into the mysteries of the universe, observing atomic phenomena such as single-electron transfer and chemical reactions on surfaces; in the absence of nuclear testing, scientists rely on simulations to duplicate on a computer what happens in reality, such as this simulation of the phenomena of fluid mixing; the helium spin filter uses a dense volume of helium-3 gas to polarize, or line up, a beam of neutrons, allowing scientists to do the kind of particle physics usually reserved for big accelerators; and carbon-based prosthetic hip joints someday may replace traditional metal and alloy joints and eliminate the need for bone cement to anchor them.

IN THIS ISSUE:

Dateline: Los Alamos is available on the World Wide Web: http://www.lanl.gov/worldview/news/dateline/.

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