LOS ALAMOS NATIONAL LABORATORY
WHERE SCIENCE MAKES A DIFFERENCE

DATELINE LOS ALAMOS

U.S. DEPARTMENT OF ENERGY
UNIVERSITY OF CALIFORNIA

CASTING CALL FOR MODELS

NEW COMPUTER SIMULATION TOOL WILL HELP FOUNDRIES CAST BETTER METAL-ALLOY PARTS

The Chinese discovered the art of casting copper, bronze and iron thousands of years ago. Today, scientists at Los Alamos use alloys unimaginable by the ancient metal workers. They also have developed a simulation tool to help foundry workers better understand their casting processes. Such simulation tools, especially those capable of running on a supercomputer, were nonexistent a decade ago.

This new computer simulation tool will not only improve the casting process of alloys used in weapons parts, it will be invaluable to private industries that cast complicated metal parts, such as engine blocks.

→ Los Alamos researcher Doug Kothe stands in front of a plasma furnace with a cast sphere of depleted uranium and its mold. Kothe is helping develop a computer tool that models and simulates the casting process of alloys used in weapons parts. The Telluride simulation tool also will benefit private industries that cast complex metal parts, such as engine blocks.

Researchers at Los Alamos for the first time are modeling and simulating the casting process of metal parts and components produced by Los Alamos foundries. The result is Telluride — a computer tool that models in three dimensions the complex processes involved in casting, including fluid and heat flow, phase changes, solute transports, interface dynamics and material response.

"The potential payoff is enormous," says Doug Kothe, Telluride development team leader. "The use of computer tools in the area of casting simulation is in its infancy, but the potential cost savings for the Laboratory, as well as industry, are huge."

For thousands of years metal casting techniques have been 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 the part must be discarded or remelted. Taking the guesswork out of the casting process will result in less wasted time, money and energy.

Unlike casting simulation tools currently available to industry, the Los Alamos-developed Telluride code addresses the special needs of the alloys commonly used in Los Alamos foundries: uranium and plutonium. These alloys behave much differently from alloys commonly used in industry, such as aluminum. Los Alamos' casting processes also are

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DATELINE: LOS ALAMOS

unique from those of industry; often involving confined work in gloveboxes.

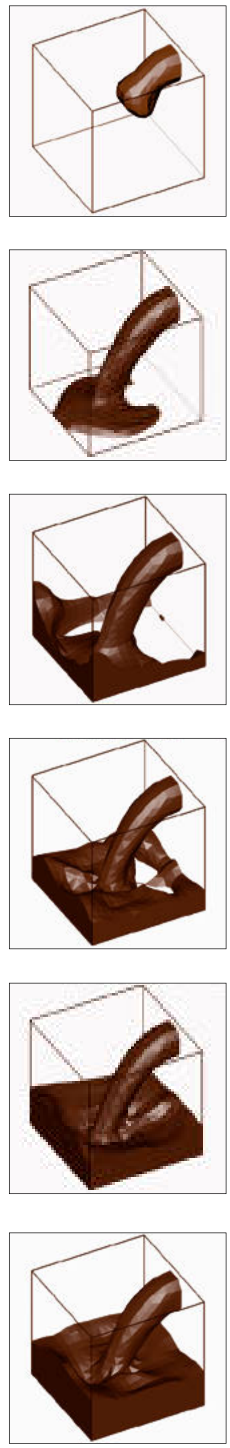
“We are ahead of currently available commercial casting simulation tools in our ability to simulate smaller and smaller length scales afforded by the Lab’s huge computing platforms,” said Kothe. “We can look at material properties as they happen in the casting process. Our goal is to be able to predict what a cast part will look like at the microstructural level.”

The microstructural properties of a cast part are responsible for its strength and resilience, and properly controlling these properties during a pour can minimize defects in the final product.

Telluride metallurgical and software engineers are using the Blue Mountain supercomputer, part of the Department of Energy’s Accelerated Strategic Computing Initiative. ASCI is a collaboration by Los Alamos, Lawrence Livermore and Sandia national laboratories to create modeling and simulation capabilities essential for maintaining the safety, reliability and performance of the U.S. nuclear stockpile in the absence of underground testing.

The software is written in Fortran 90 for high-performance computing platforms. Eventually, foundry workers hope to be able to monitor the casting process on a desktop computer and make immediate adjustments to a pour guided by Telluride simulation results. Lab foundries currently are supplying data to Kothe and his colleagues, which they expect to use to validate Telluride on actual cast pieces.

Telluride not only will help minimize “pour and pray” during the actual casting, it will be useful up front in the design process, where it can help design a better mold in a shorter time, thereby reducing mold machining expenses.



Six frames from a Telluride simulation of a side pour in a box mold.

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A uranium pour as seen through the viewport of a furnace. Mica sheet, which serves as insulation, appears in the foreground.

Telluride also could have potential in nonmetal castings, such as plastics. This area is yet untested, because Los Alamos does no plastic injection molding, but is worth exploring by industry, says Kothe. Telluride's free-surface flow problem-solving skills also may be useful predicting wildfire spread, tracking cloud movement and predicting the impact of "rock-splash" problems, such as tsunamis caused by an asteroid's impacting with Earth.

Telluride has been a multidivisional effort by members of Los Alamos' Theoretical, Materials Science and Technology, Applied Theoretical and Computational Physics, Nuclear Materials Technology, and Engineering Sciences and Applications divisions.

External collaborators came from the University of California, Irvine and Davis; Oak Ridge National Laboratory; the University of Iowa; Cambridge Power Computing Associates of Cambridge, Mass.; Blue Sky Studios of New York, N.Y.; IBM Corp.; Caterpillar Corp.; the Colorado School of Mines; the University of Munich; CSIRO, Australia; and the University of Melbourne, Australia.

The Telluride project was initiated with Laboratory-Directed Research and Development funds. Since 1996, the majority of funding has come from the DOE ASCI Program, with additional funding by a collaborative University of California/Los Alamos research program, CULAR.

Los Alamos researchers are seeking participants from private industry, especially automotive manufacturers, to test an alpha version of Telluride on their industrial casting processes. More information on Telluride is available on the World Wide Web at http://www.lanl.gov/home/Telluride.

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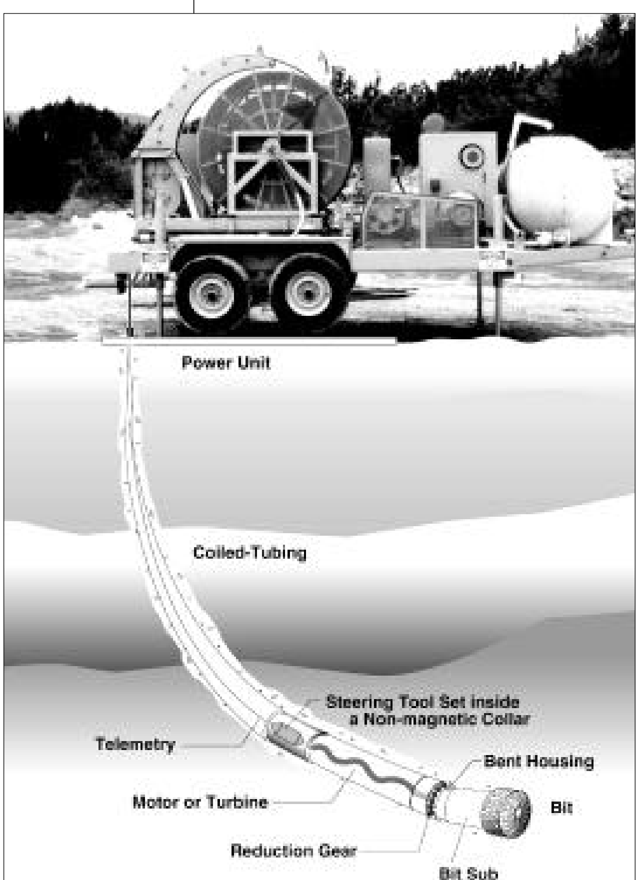
DATELINE: LOS ALAMOS

LAB TESTING NEW MICRODRILLING TECHNOLOGY

DRILL BIT ATTACHED TO THIN STEEL COIL COULD REVOLUTIONIZE UNDERGROUND OIL AND GAS EXPLORATION

Los Alamos researchers currently are testing new microdrilling technology that may revolutionize the way underground resource exploration is carried out in the 21st century, at greatly reduced cost. The technology may even one day be used on space missions for boring "microholes" in planetary bodies or used as drain holes or root systems.



This composite illustration shows the 1-inch steel coil wound on a tubing reel above ground and an artist's conception of the technology below ground.

As a complementary part of this project, the researchers, in collaboration with industry, also are developing miniature seismic instrumentation packages that can be placed inside the microholes for data gathering. Virtually any microsensor one day may be able to take advantage of the microdrilling technology.

The technology consists of a standard mining drill bit and oil field drillout turbine attached to a steel coil that's 1 inch in diameter. Conventional production well drills used today by oil and gas and other companies can be anywhere from 6 inches to more than a foot in diameter.

The steel coil is wrapped around a tubing reel that resembles a water hose holder. The reel can hold thousands of feet of coil and is part of a drilling system that

DATELINE: LOS ALAMOS

ultimately will occupy a space roughly one-twentieth that of a typical rig. The new rig costs about 90 percent less than a conventional rig.

The coil is placed through an injector wellhead, then begins drilling holes less than 2 inches in diameter. The steel coil is flexible

Microdrilling realizes additional savings because it requires only about a barrel of fluid per 1,000 feet of drilling for lubricating the bit and motor and removing dirt, whereas conventional drilling requires about 40 barrels of fluid per 1,000 feet.

“In addition to the greatly reduced cost, one of the other benefits of microdrilling is that it can be used to extend existing production wells,” said Los Alamos researcher Jim Albright.

Several major oil companies are contributing financial or technical support for technology development. The Department of Energy also is providing financial support for development of a microhole drilling infrastructure.

As electronic circuitry continues to shrink in size, microdrilling may one day become the preferred tool for placing other sensors deep underground to perform an array of data-gathering activities, including monitoring soil contamination and underground nuclear testing.

The microdrilling technology currently is undergoing the first phase of testing at Fenton Hill, a site located about 40 miles northwest of Los Alamos and managed by the Laboratory for research. Thus far, the results are encouraging.

“We need to make sure that the technology can be used across different types of sedimentary rock and that the drilled holes remain stable and don’t cave in. After all, the holes being drilled are less than 2 inches wide,” said Albright. The microdrill currently is boring through volcanic rock, or tuff, on Fenton Hill.

Los Alamos researchers hope to be able to drill down to a target depth of 6,000 feet within the next three to five years.

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DATELINE: LOS ALAMOS

WORLD'S MOST POWERFUL PULSED MAGNET DEDICATED

MAGNET'S PEAK STRENGTH IS MORE THAN A MILLION TIMES THAT OF EARTH'S MAGNETIC FIELD

A multiton magnet powered by a billion-watt generator and capable of creating powerful, pulsed magnetic fields for a longer time than any other in the world has been commissioned at Los Alamos.

"This magnet will revolutionize research in high-magnetic fields," said Greg Boebinger, director of the National High Magnetic Field Laboratory's Los Alamos Center. "Its unprecedented flexibility offers researchers the chance to conduct standard, sensitive measurements in extremely intense magnetic fields that can be provided only by pulsed-field magnets."

High-magnetic fields offer scientists one of the most effective and noninvasive tools to explore basic and new materials critical to modern technology. Research areas include semiconductors; high-temperature superconductors; magnetic resonance imaging; complex chemical and biological structures; and magnetic materials used in computers, VCRs and CD players.

Los Alamos' pulsed-field magnet, consisting of nine nested electromagnetic coils wrapped in steel cylinders, can reach a peak field strength of 60 tesla, more than a million times greater than Earth's magnetic field. The magnet lab staff finalized operating procedures during the summer, and the magnet has just recently opened to national users. Trial experiments already have demonstrated the magnet's research potential.

➔ Los Alamos researchers Jim Sims (left) and Mike Pacheco inspect the 60-tesla magnet, the centerpiece of the National High Magnetic Field Laboratory's pulsed-magnet center at Los Alamos.

Part of the magnet's uniqueness is that the shape of the magnetic field pulse can be tailored specifically to the needs of the experimenter. The field strength can be held constant at certain specified values, for example, or swept from zero to maximum strength, or taken through more complicated pulses, such as a stair-step pattern.

The magnet's ability to hold a constant magnetic-field strength has enabled researchers to make first-ever measurements of the heat capacity of materials in a pulsed-magnet system.

Heat capacity tells researchers about basic material properties, such as identifying phase transitions (because a material sheds or absorbs heat when going through a phase transition), the density of electronic states or stiffness of a crystallographic lattice. If the magnetic field is not steady, it will induce currents in a metallic material that will generate internal heat and corrupt the heat capacity measurement.

Developing the 60-tesla magnet was a challenge for engineers. The magnetic forces are so strong they want to rip apart the magnet, which is why the electromagnetic coils must be wrapped in steel blankets. The outer coil is large enough for a person or two to fit inside; the central core, where the samples are placed for study, is but a few inches across.

The magnet is cooled with liquid nitrogen to survive the tremendous heat generated when the massive generator — large enough to power the state of New Mexico — shoots its electric charge into the magnet. As the electricity circulates through the coils, it creates magnetic-field lines concentrated at the center of the magnet.

When the generator unleashes its charge, "the magnet makes a screech that bears an uncanny resemblance to an angry Godzilla from the movies," Boebinger said. No loose metal can be left in the vicinity of the magnet when it is operating, lest it get yanked violently into the magnet.

The National High Magnetic Field Laboratory, funded by the National Science Foundation, includes three separate campuses: at Los Alamos, the University of Florida and Florida State University. Under the NHMFL consortium, Los Alamos offers researchers pulsed-field magnets, and the facilities at the Florida universities offer sustained magnetic fields, magnetic imaging and ultra-low temperature capabilities.

Magnets at the NHMFL will continue to intensify, since design of a 100-tesla magnet is now under way as a joint effort between the Department of Energy and the NSF.

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DATELINE: LOS ALAMOS

MORE WATER ON THE MOON

NEW ANALYSIS OF LUNAR PROSPECTOR DATA

Lunar Prospector has revealed water on the moon in amounts 10 times greater than originally estimated in March. The additional analysis also shows the water is likely confined to localized areas near the poles, rather than spread out evenly across the polar regions, as was assumed in making the earlier estimates.

Current estimates say there may be as much as three billion metric tons of water ice at each of the poles, with 15 percent more at the north pole than at the south pole. Refined calculations of lunar water amounts and unique lunar compositional maps were published in the September issue of the journal *Science*.

"In making our initial estimates, we assumed the water was spread over the 'footprint' of the instrument," said Los Alamos scientist Bill Feldman, which is how much surface area the instrument can detect at any moment, a square approximately 120 miles on a side at Lunar Prospector's current altitude. "As we've gotten more data, we've found that it's not spread out as we first assumed, but concentrated."

When they presented their initial results in March, scientists said the water was likely in the form of a fine frost spread through the lunar soil. Further data analysis now allows the possibility of deposits of solid ice. Water amounts, inferred from measurements of hydrogen in the lunar soil, are of great interest because of their potential impact on plans for colonization.

Scientists assume comets carry the water ice to the moon. The comets basically vaporize on impact, and the water molecules migrate to the permanently shaded regions at the poles. These regions are so cold that once a water molecule enters them it gets stuck.

Lunar Prospector, part of NASA's Discovery Program of low-cost, fast-track space missions, was launched in January. Los Alamos scientists built three of its five onboard instruments.

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DATELINE: LOS ALAMOS

CENTER FOR SPACE SCIENCE AND EXPLORATION FORMED

NEW CENTER WILL PROMOTE INTERDISCIPLINARY RESEARCH AND ENHANCE NATION'S SPACE PROGRAM

The Laboratory has formed a new center that will bring a wider variety of Los Alamos capabilities to bear on national space programs

➔ David McComas heads the new Center for Space Science and Exploration.

"Los Alamos has earned a reputation as a leader in space research, both for the instruments and missions it's flown and its analysis of data," said David McComas, who heads the center. "But the Lab has expertise and unique technical capabilities in other areas that can be equally successful in supporting the nation's space exploration initiatives and space science research efforts."

Los Alamos currently receives about $9 million in annual funding from NASA for space research projects. In addition, the new center will direct the investment of $5 million in internal Laboratory funding over the next five years to promote innovative ideas and technology development.

The new Center for Space Science and Exploration evolves from an existing program office that oversees NASA-funded research projects.

In addition to keeping Los Alamos' ongoing space science research strong, the new center aims to strengthen Los Alamos efforts in the areas of planetary science and resources use; biological effects of space travel and how to look for signs of life on other planets; nuclear power and propulsion systems; and new types of alloys and other materials and structures for use in space.

These areas tie into existing expertise at Los Alamos, such as geology and environmental characterization; DNA analytical methods; advanced reactor technology and nuclear propulsion; and material sciences and engineering.

Los Alamos also has more than 50 user facilities, ranging from advanced material fabrication and characterization to supercritical fluids to powerful computers. These facilities are available to outside researchers through collaborative arrangements.

DATELINE: LOS ALAMOS

Los Alamos' expertise in building instruments for space missions began with its programmatic assignment to provide instruments for orbital monitoring for clandestine nuclear weapon detonations. This work started with the Vela program in the early 1960s and continues today on a variety of satellites. These instruments have yielded a wealth of data for scientific study, including the discovery of celestial gamma-ray bursters and the existence of heavy ions in the solar wind.

Los Alamos' astrophysics work continues to evolve and today includes significant roles in the High-Energy Transient Explorer-2; Russia's Spectrum-X-Gamma mission; Milagro, an observatory for tracking high-energy cosmic rays; theoretical studies of neutron stars and supernovae; and operation of automated telescopes for transient observations at Fenton Hill, a site near the Laboratory.

Los Alamos' space research program also has grown to form a lengthy list of successes, including most recently the announcement of quantitative measurements of the amount of frozen water at the moon's poles. (See article on Page 9 of this issue.) Los Alamos scientists designed and built three of the instruments on NASA's Lunar Prospector, including the neutron spectrometer that yielded the key data on water amounts.

Los Alamos has a role on a variety of other NASA missions, including the Cassini mission to Saturn; the Ulysses spacecraft orbiting the sun's poles; the Advanced Composition Explorer, which is measuring the solar wind upstream of Earth; and several instruments on the POLAR Earth-orbiting mission.

Looking ahead, Los Alamos is providing vital hardware for several future NASA missions, including Deep Space Millennium 1, TWINS, IMAGE and Genesis. Los Alamos researchers also are developing prototype ice-penetrating radar technology for consideration for a future NASA mission to Europa, an ice-covered Jovian moon that might possess a watery ocean. (See article on Page 12 of this issue.)

Additional information on Los Alamos' space-related research is available on the World Wide Web at http://www.lanl.gov/csse and in the January/February/March 1998 issue of *Dateline: Los Alamos*.

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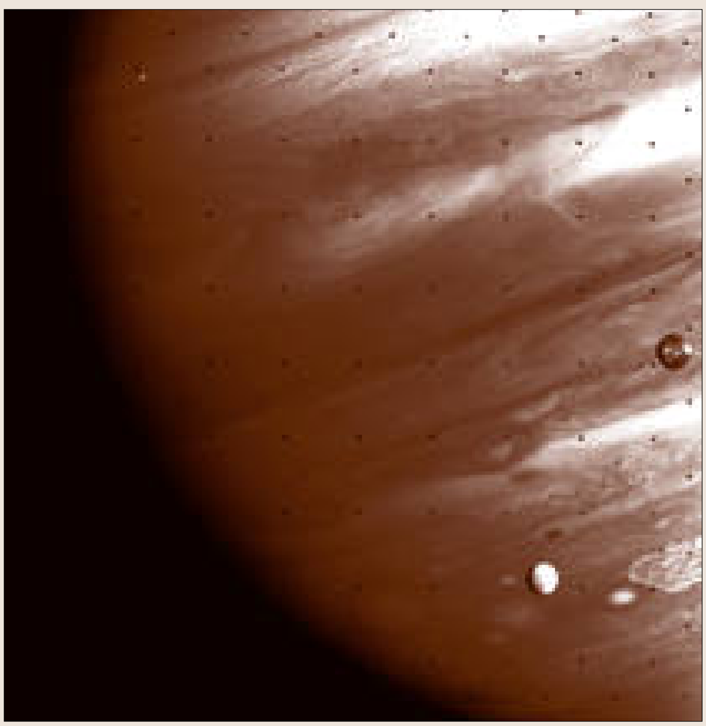
TO JUPITER'S MOON AND BACK

LAB RECEIVES NASA FUNDING FOR FEASIBILITY STUDY OF ICE-PENETRATING RADAR

Los Alamos scientists have received a $120,000 grant from NASA to determine the technical requirements of an instrument that someday may fly to Jupiter to study the icy surface of its moon, Europa.

Three Los Alamos researchers are part of a 17-member international Instrument Definition Team that is designing an Ice-Penetrating Radar, which would send millions of radar signals at different frequencies to map out the thickness of Europa's ice surface and detect, if present, a



A Voyager 1 image of Jupiter with the moons Europa and Io in the foreground.

NASA photo

subsurface Europan ocean. The IPR also would characterize Europa's ice surface.

Because ice is transparent to a large range of radar signals, the IPR will be able to record waves reflected off the top layer of ice and the ice-water interface, ultimately converting them into three-dimensional images.

Researchers think the ice crust surface could be as deep as 100 kilometers, but data received from the Galileo spacecraft indicate that the ice could be as thin as hundreds of meters. Photos transmitted by the Galileo spacecraft in 1994 presented the first evidence of the possible existence of liquid water on Europa.

The Instrument Definition Team currently is studying many things, including how to distinguish the different radar reflection signals returned by rocks, cracks in the ice, salty and nonsalty ice, and other conditions on the moon's surface. Another obstacle is making sure the IPR survives Jupiter's intense radiation that surrounds Europa.

Researchers also must determine just how much power the IPR will need to transmit and receive its radar signals and the kinds of antennas that need to be used. Testing of the IPR prototype's antennas should begin at Los Alamos later this year.

Another major factor in designing and building the prototype is the instrument's weight; researchers think the IPR should weight no more than 8 kilograms, or about 17 pounds.

The final draft design for the IPR is due to NASA next March. At that time, NASA will put out an announcement for opportunities for the Europa mission, scheduled for launch in 2004. It would take anywhere from five to seven years for the instruments to make the 400-million-mile trek to Europa.

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DATELINE: LOS ALAMOS

LIBRARY DESTROYED IN FIRE

EMPLOYEES JOIN FORCES TO HELP DIXON ELEMENTARY SCHOOL

Late one evening last September, Dixon Elementary School's library was destroyed in a fire that caused an estimated $750,000 in damage.

The loss to this small community has been felt all around Northern New Mexico, including in Los Alamos, where Laboratory employees and subcontract personnel joined together to collect books and donations to help begin the rebuilding process.

"People brought in sets of encyclopedias, for children and adults. They even donated their privately owned personal computers and printers," said Tonya Suazo, who coordinated the local donation drive. "It has just been amazing to me how Laboratory employees have come together to help Dixon Elementary School rebuild its library."

Johnson Controls Northern New Mexico, the major Los Alamos subcontractor, worked with the Lab to locate a transportable building that could be moved to the school in Rio Arriba County for use as a temporary library.

The fire destroyed or damaged thousands of library books, text books, reference books and dictionaries as well as charts, maps, globes, teaching aids, computers, software, overhead projectors, screens and desks.

"This is what the Lab is all about in terms of wanting to be a good neighbor to the communities," said Floyd Archuleta of the Community Relations Office. "This is the way we've been brought up in Northern New Mexico, to be there for our neighbors when they need help."

As of late October, employees had donated about 30 boxes of books and more than $900 in cash. Dixon residents also have collected books and are coordinating volunteer efforts for what could be a lengthy rebuilding process.

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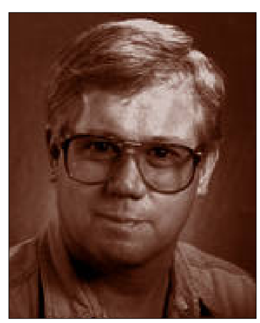
DATELINE: LOS ALAMOS

PEOPLE IN THE NEWS ...

FELLOWS PROGRAM FOSTERS MENTOR CULTURE AMONG WOMEN. Los Alamos chemist Carol Burns is one of 12 women selected nationwide for the International Women's Forum's Leadership Foundation Fellows Program. The program helps outstanding women in business, government, science, academia and other professions advance in their fields with the help of prominent women business leaders who serve as mentors. Mentors for the program have included CNN senior correspondent and anchor Judy Woodruff; Motorola (Canada) chair, president and chief executive officer Micheline Bouchard; Lockheed Martin Corp. vice president Susan Pearce; and Colgate-Palmolive executive vice president and chief of operations Lois Juliber. The program spans 32 days spread throughout the year and includes attending two IWF global conferences, studying for a week at the John F. Kennedy School of Government at Harvard University and spending 10 days with assigned mentors.

➔ Carol Burns

AWARD FROM THE INSTITUTE FOR NUCLEAR MATERIALS MANAGEMENT. Jim Tape of Los Alamos' Nonproliferation and Arms Control Program Office has received the Institute for Nuclear Materials Management's Meritorious Service Award. The INMM is an international professional organization dedicated to helping ensure that nuclear materials are properly protected, managed, handled, stored and used for purposes approved by treaty or law. The Meritorious Service Award is given to those members who have demonstrated outstanding contribution or service to nuclear materials management and the institute. Tape currently serves on the board as INMM immediate past president and is a 22-year INMM member. Tape also currently is a senior technical adviser to the U.S. delegation for the United States/Russian Federation/International Atomic Energy Agency Trilateral Initiative for the Verification of Excess Weapons-Origin Fissile Material.



🡐 Jim Tape

DATELINE: LOS ALAMOS

BRIEFLY ...

LOS ALAMOS' ELECTRONIC WEB PAGE HAS BEEN NAMED ONE OF *POPULAR SCIENCE* MAGAZINE'S "50 BEST OF THE WEB" FOR 1998. This year's award-winning sites were featured in the September issue of the magazine. The Lab's home page is five years old and was redesigned last year, along with the supporting web pages. The home page can be reached at http://www.lanl.gov. Other science-oriented web sites listed in *Popular Science's* 50 best include the MIT Media Lab, Bell Labs Innovations, IBM Research and Sandia National Laboratories. *Popular Science*, which specializes in covering cutting-edge technology, is a 1.8 million-circulation magazine published in New York City by Times Mirror Magazines. Regular features, in addition to science, include electronics, computer hardware and software, home technology and automotive.

IN THIS ISSUE:

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