





## LOS ALAMOS WINS SIX R&D 100 AWARDS

DEFENSE RESEARCH BENEFITS THE PRIVATE SECTOR

os Alamos has shown its technical excellence by winning six R&D 100 awards. This year Los Alamos had its highest win-to-entry ratio, netting one award for every three of its entries.

> The six awards, which include a win shared by Los Alamos, Oak Ridge, Lawrence Livermore, and Sandia national laboratories, gives Los Alamos a total of 52 awards won during the past decade. Los Alamos has won more awards than any other national laboratory since 1988.

laboratory since 1988. The R&D 100 awards program, now in its 35th year, honors the most significant products, materials, processes, software, or systems with commercial promise. The awards program is international in its scope and technologies are nominated in open competition. The Illinois-based *R&D Magazine* uses technical criteria to pick the most important, unique, and useful entries.

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Los Alamos award winners ran the gamut — from a computer program that helps scientists predict the movement of oil and gas through underground reservoirs to an environmentally friendly method of dry-cleaning clothing with carbon dioxide.

Other winning technologies include a way to determine the size of fragments of deoxyribonucleic acid, the fundamental building block of life, and a simple test for detecting failure in concrete, a fundamental building block of another sort.

"Los Alamos' success in developing products with a high degree of commercial potential — even as it carries out its national security mission of reducing the global nuclear danger — shows that our national laboratories can benefit the private sector," said Charryl Berger, leader of Los Alamos' Civilian and Industrial Technology Program Office. "Los Alamos once again has shown its success in using scientific excellence to identify key problems facing industry and to identify scientific solutions that benefit society as a whole."

This issue of *Dateline: Los Alamos* features the Laboratory's six winning technologies. Brief descriptions of the Laboratory's other 13 entries are also included in this issue.



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#### S E Ρ Т E Μ В E R S S IJ E 9 9 7

# DATELINE: LOS ALAMOS

# THE HIGH PERFORMANCE STORAGE SYSTEM

INNOVATIVE ARCHITECTURE SPEEDS DATA PROCESSING BY REMOVING THE MIDDLEMAN

The High Performance Storage System, developed by Los Alamos researchers and their partners in government and industry, uncorks existing data-storage bottlenecks for a myriad of government and commercial applications.

Today's computer models and simulations, digitized information libraries, and high-energy physics data require a large amount of storage space. Unfortunately, system bottlenecks that interfere with users' ability to retrieve data quickly frequently develop. The primary objective of the HPSS is to move very large data sets very quickly — at least 100 times faster than what is available with today's software systems. This speed is possible because unlike traditional data-storage systems, the HPSS is distributed on a network, not on a centralized storage computer.

HPSS accomplishes those tasks using commonly available network and storage technologies and many different devices. It makes data available

HPSS increases both the performance and capacity of storage systems for large-scale computation and other applications.

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to all networked computing sites, regardless of their size or location. All computer and storage nodes may be attached directly to the network so that data is transferred by the most direct route at network speeds without interruption by a storage computer or "middleman."

HPSS inaugurates the use of "Data Movers" — specialized



software that the HPSS storage-control system uses to send large data streams, such as complex images and visualization objects, directly to the requesting computers without having to pass through the storage server itself. HPSS takes itself "out-of-the-loop" so that the only limiting factor is the maximum speed of the network.

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One of the major innovations of the High Performance Storage System is the scalable architecture that supports a very-high performance, parallel input/output function. What this means to the user is that while inputting a large amount of data, output of very large data sets can take place at the same time.

Another characteristic of HPSS is that it scales extremely well in many dimensions. This increases the data transfer rate, storage capacity, file size, the number of files, and number of simultaneous users or clients.

Another benefit of the Los Alamos software is the information protection HPSS offers both from unauthorized use and from corruption. HPSS assures that only authenticated users and clients gain access to the data permitted to them.

HPSS offers adaptability and flexibility in its hardware by making it possible to incorporate newer, faster devices and new technologies into the network. Moreover, the modularity of the system makes it easy to incorporate new pieces of software into the system as they are developed.

HPSS is already being used in very large modeling and simulation applications and in the storage of astronomy and high-energy physics data. Additionally, plans are under way to use HPSS for storage of oil exploration data, digitized film libraries, and medical records.

Another storage mechanism would link several supercomputing installations that are geographically dispersed. For example, HPSS will link the three Accelerated Strategic Computing Initiative national laboratories (Los Alamos, Sandia, and Livermore). Another will link Sandia and Oak Ridge national laboratories to the Pittsburgh Supercomputing Center.

The High Performance Storage System would tackle the storage of massive quantities of data envisioned in the National Information Infrastructure and in the Human Genome Project. Other storage and retrieval problems in animation and entertainment, airline reservations systems, and fingerprint systems would be solved with HPSS.

HPSS is a key technology that will move "ultracomputing" into the next century. It is a cooperative effort between Los Alamos, Lawrence Livermore, Oak Ridge, and Sandia national laboratories, and IBM.

> CONTACT: JOHN BLAYLOCK DATA STORAGE SYSTEMS (505) 667-8970 • E-MAIL: jwb@lanl.gov

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# CLEAN CLOTHES WITH DRYWASH<sup>TM</sup>

LIQUID CARBON DIOXIDE CLEANS CLOTHES WITHOUT HAZARDOUS, POLLUTING CHEMICALS

D ryWash<sup>™</sup> is a fast, nontoxic dry-cleaning process that uses liquid carbon dioxide as the cleaning solvent. Efficient and environmentally friendly, DryWash<sup>™</sup> removes oils, sweat, and dirt from a wide variety of fabrics, including specialty items such as fur, leather, suede, and garments with sequins.

The process — developed by Los Alamos, Global Technologies LLC, and Hughes Environmental System Inc., both of El Segundo, Calif. — can be used worldwide by neighborhood dry cleaners, hotels, military installations, corporate facilities, nursing homes, and hospitals. Future applications may include dishwashing, nuclear laundry, and decontaminating machined parts.

Because liquid carbon dioxide is an odorless, nonflammable, nonhazardous solvent, it is a desirable alternative to perchloroethylene, or PERC, the hazardous solvent currently used by most dry cleaners. The DryWash<sup>™</sup> process will help the dry-cleaning industry comply with environmental regulations by minimizing their hazardous wastes and

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emission. It cleans in half the time required for conventional dry-cleaning processes and reduces dry-cleaning costs by lowering energy consumption, cleaning time, and labor costs. And DryWash<sup>™</sup> gets clothes cleaner and brighter by reducing soil redeposition on fabrics.

The dry-cleaning industry is under severe pressure from regulators to develop an acceptable and economical alternative to PERC. Although the researchers are still optimizing the DryWash<sup>™</sup> process, research results indicate the new process could revolutionize the dry-cleaning industry worldwide.



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This food stain might send anvone scurrying to a drv cleaner. But rather than cleaning this polyester swatch in perchloroethylene (PERC), the hazardous solvent that dry cleaners typically use, the stain was removed with dense-phase carbon dioxide.

At pressures between 800 and 1,000 pounds per square inch, carbon dioxide acts like a liquid and serves as an organic, entirely recyclable solvent that extracts dirt from clothing. When the liquid carbon dioxide is allowed to return to its gaseous state, dirt just falls out. Repressurized, the carbon dioxide can be used again. The only waste generated by the process is the volume of dirt removed from the garments.

For dry cleaners to switch over to DryWash<sup>™</sup> technology, they would need to replace their standard equipment with a high-pressure apparatus to safely operate a liquid carbon dioxide cleaning process. However, a distribution network is already in place for restaurants and other businesses that require tanks of carbon dioxide to make soft drinks from a soda fountain.

Los Alamos gained expertise in the use of carbon dioxide as an alternative to chemical solvents from defense program applications. Carbon dioxide at high pressure can replace solvents used to clean plutonium weapons components.

The DryWash<sup>™</sup> project is supported by the Department of Energy's Office of Industrial Technologies and the Environmental Protection Agency's Design for the Environmental Program in the Pollution Prevention and Toxics Branch.

CONTACT: CRAIG TAYLOR, ORGANIC ANALYSIS (505) 665-3545 • E-MAIL: eggus\_taylor@lanl.gov



### SOFTWARE FOR MODELING BIG OIL RESERVOIRS

FALCON IMPROVES MODELING ACCURACY AND COST EFFICIENCY

A ll major oil and gas companies use computer simulations to predict the flow of oil and gas in underground reservoirs. Such predictions enable companies to determine the best recovery strategies; however, current production simulations are limited because they run on small, slow, single-processor computer systems.

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Worldwide, reservoirs produce 70 million barrels of crude oil per day. Of this production, 40 million barrels are from huge fields that cannot be modeled with present-day computer simulation software.

Falcon software developed by Los Alamos; Amoco of Tulsa, Okla.; Cray Research (a Silicon Graphics company) of Eagan, Minn.; and PGS Tigress Ltd. of the United Kingdom makes it possible to model large, economically important oil fields in their entirety.



This next-generation version of Falcon software lets oil and gas companies perform best- and worst-case analyses of their fields and calculate "what if" operational scenarios for reservoirs. Both features are crucial to developing thrifty recovery strategies. Oil and gas companies can use Falcon to make important resource recovery decisions. These decisions include appraising the value of oil and gas fields for leasing decisions, developing recovery procedures for current and future fields, developing short- and long-term economic strategies, and planning the development of facilities at production sites.

Although 60 percent of world's oil production is from large fields that extend over hundreds of square miles and contain thousands of wells, no simulator before Falcon could model fields of this size.

Today's commercial simulators run simulation studies on large fields by dividing the area into segments. Significant errors can arise when segment studies are used to estimate oil and gas rates and recoveries for an entire field. A 30 percent error rate in the production rate of the wells can mean the difference between a profitable and unprofitable field.

In addition, a large amount of data about the field falls through the cracks with current simulation studies because of processes that average data to approximate large areas. Given that an exploratory license for data collection can cost a company \$50 million per field, the data is too pricey to throw away. By eliminating the need for averaging data, Falcon is more cost-effective as well as more accurate.

Falcon simulates fluid flow in three dimensions and models the different fluid phases of oil, gas, and water. To simulate a reservoir, Falcon implements a mathematical model that solves the equations that govern fluid

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This Falcon simulation shows oil saturation of a 100-squaremile reservoir field after 25 years of operation. The grid used for this simulation contains 2.3 million cells.

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flow in a permeable medium — such as a petroleum reservoir. Falcon also accounts for the flow of chemical components that were originally in the reservoir or that were injected into it. In addition, a geological description that includes data such as the depth, thickness, permeability, and porosity of reservoir rock is entered into the simulation. Processing so many geological measurements results in a description with millions of discrete grid points.

Falcon achieves its high performance on large-scale computer architectures by reformulating mathematical methods to make them suitable for computers consisting of thousands of processors. This task requires a complex coordination of thousands of complicated processes that must communicate and synchronize properly to provide the correct mathematical answer.

Essentially, all the computations are divided equally among the participating computer processors. Because nearly all of the necessary computations have been reformulated for parallel processing — fewer than 1 percent are sequential — Falcon is 100 times faster than its competitors.

The most important feature contained in the Falcon code is a breakthrough linear-solver algorithm that solves fully implicit linear systems both reliably and efficiently on massively parallel computers.

The algorithm is the key to Falcon's success because in the past, linear systems, typically requiring 30 percent to more than 70 percent of the total computation time, have been difficult to solve efficiently on parallel computers.

The problem is particularly acute for fully implicit simulations, which the oil industry uses to solve the fluid-flow equations in fields containing complex physics, such as complex phase-change behavior. Falcon's linear solver enables oil and gas companies to model complex fields on the world's fastest computers.

#### CONTACTS:

WAYNE JOUBERT SCIENTIFIC COMPUTING (505) 667-7374 • E-MAIL: wdj@lanl.gov

#### ROBERT STEPHENSON

#### AMOCO

(918) 660-3081 • 4502 EAST 41ST ST., TULSA, OK 74102

#### S E Ρ Т Ε Μ В E R Τ S S IJ Ε 1 9 9 7

### **DATELINE: LOS ALAMOS**

## PLASMA SOURCE ION IMPLANTATION

INNOVATIVE TECHNOLOGY MAKES MATERIALS' SURFACES STRONGER AND LONGER LASTING

I nstead of simply coating or covering automobile, aircraft, and machine tool pieces, Los Alamos researchers have been instrumental in the development and initial commercialization of a new way to chemically change a material's surface for improved performance. Previous methods such as electroplating produce hazardous waste byproducts. The Plasma Source Ion Implantation method is safe, versatile, and potentially more economical.

The PSII process implants nitrogen or carbon ions into appropriate metallic surfaces to harden their surfaces and make them wear longer.



The technique is not a coating process, but a way to transform the component material surface into a protective "armor." In addition, the process may be used to enhance the adhesion of some more traditional coatings that are subsequently applied to the surface in a related plasma-based process.

Automobile parts, for example, are immersed in a cloud of ionized gas. Short pulses of negative high voltage are then applied to the parts. As a result, the positively charged ions are accelerated and bury themselves in the surface. The

treated part does not suffer from the problems usually associated with conventional coating techniques, such as poor adhesion, or delamination (the splitting of layers).

Electroplating has been widely used, but it produces hazardous effluents. PSII does not use hazardous or carcinogenic chemicals, nor does it require elevated target temperatures.

Traditional implantation methods require costly linear accelerators to produce the ions and complicated manipulators to rotate the object to ensure total coverage. The PSII process is a completely different approach. Instead of hurling ions at the part, the part is immersed in a plasma sea of ions. In effect, the target itself becomes the accelerator.

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A view inside the PSII process chamber. where aluminum automotive pistons are being treated to improve their wear properties. The alow is from the argon gas ionized inside the chamber by radiofrequency fields. The argon plasma is being used in a cleaning process in preparation for implantation.

This same process can be modified to specific needs using ions such as carbon, oxygen, or other ions produced from gaseous precursors. This process is environmentally friendly because it has the potential to reduce or eliminate wet-chemical processes, such as hard-chrome plating for coating manufacturing tools, that may leave toxic wastes.

The technology could extend the lifetimes of some parts as much as 10 to 50 times. The process can be used to improve the surfaces of large, complex parts weighing many tons, as well as a large number of smaller, individual components. This versatility offers the potential for economic treatment of whole new classes of components that are not suitable for surface enhancement by more conventional means. The versatility also allows more environmentally friendly surface enhancement of some components now treated by conventional means.

To date, Los Alamos researchers and their partners — Empire Hard Chrome, General Motors, North Star Research, and the University of Wisconsin — have successfully treated pistons and other automotive components and tools, such as drill bits and dies, at the world's largest PSII facility in Los Alamos.

CONTACT: CARTER MUNSON PLASMA PHYSICS (505) 667-7509 • E-MAIL: cmunson@lanl.gov



## HOME-GROWN TECHNOLOGY MEASURES UP TO A NEW CHALLENGE

TECHNIQUE RAPIDLY AND ACCURATELY SIZES DNA

A Los Alamos technology that counts and sorts cells, chromosomes, and molecules is the foundation for a new biomedical technique that rapidly and accurately measures the size of individual DNA fragments. The technique has the potential to speed up genetics research, and the diagnosis and treatment of infectious diseases.

Researchers from Los Alamos developed the technique — known as "Rapid Size Analysis of Individual DNA Fragments" — from flow cytometry technology pioneered at Los Alamos nearly a quarter century ago.

Molecular biologists routinely analyze large fragments of DNA to identify their sources, detect mutations, and provide a quality-control check for

the recombinant DNA libraries used in genetics research. The distribution of fragment sizes is characteristic of the bacteria strain or the individual and can be an indication of a genetic disease.

As scientists obtain a better understanding of the human genome, analyzing DNA will become commonplace in clinical medicine as well. Physicians will be able to treat infections faster and more accurately because determining if a patient is infected with, say, an antibiotic-resistant bacterial strain will take hours instead of days. Right now a culture must be grown before the DNA can be extracted and studied.



The new rapid-analysis method eliminates the time-consuming step of growing a bacterial population, allowing treatment specific to the infectious strain to begin much faster, thereby reducing a patient's risk and suffering.

Flow cytometers use laser beams to illuminate cells and other particles tagged with fluorescent dyes. The cells flow single file, like beads on a string, through one or more laser beams that excite the dyes bound to cells. The cells are counted, analyzed, and catalogued based on the intensity and spectral properties of their emission signals.

A conventional flow cytometer can identify and catalog hundreds of thousands of cells in a few minutes, whereas a pathologist using a microscope might analyze hundreds of cells in an hour. Flow cytometers are found in laboratories, hospitals, and universities around the world. The technology forms the basis for a \$300-million-a-year business for two U.S. companies.

Applying flow cytometry to the problem of sizing DNA fragments required several modifications to produce a system sensitive enough to measure individual DNA fragments that contain only one ten-thousandth of the DNA in mammalian cells.

First, the researchers slowed down the speed with which the fragments flowed through the laser beam by a factor of 1,000. As a result, dye

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A microscope lens behind the flow cell collects fluorescence emitted by individual stained DNA fragments as they pass through an argon-ion laser beam.

attached to the DNA fluoresces about 10,000 times, giving the researchers much more information about individual fragments. Second, the technique uses a solid-state laser about the size of a cigarette package as the excitation source. Third, a highly sensitive photon-counting detector makes the device the first all-digital flow cytometer. After the detector records a photon, it sends a signal to a personal computer that continuously records the number of photons detected and their detection times.

Together, these changes converted a conventional flow cytometer into the simplest, most sensitive analytical device yet developed for analyzing DNA.

Although capable of measuring fragments as small as 212 base pairs, the technique is best suited to analyzing fragments greater than 10,000 base pairs in length. Base pairs form the "steps" of a DNA molecule's spiral staircase. The ability to size larger fragments is significant because until now only a time-consuming technique known as "pulsed-field electrophoresis" could measure such big DNA fragments.

The Los Alamos technique has other advantages. It can size DNA fragments that exhibit either linear or circular conformation. With gel electrophoresis, the current technology, supercoiled and circular DNA must be straightened out before analysis — an extra step. Straightening the DNA is not necessary before sizing with the Los Alamos technology.

And it's fast. The technique can analyze 100 fragments per second, allowing enough data to be collected in 3 minutes to determine accurately a distribution of fragment sizes in a DNA sample. Each sample is counted, resulting in a histogram, or record of the number of fragments of each size.

#### CONTACTS:

RICHARD KELLER ADVANCED CHEMICAL DIAGNOSTICS (505) 667-3018 • E-MAIL: keller@lanl.gov

JAMES H. JETT NATIONAL FLOW CYTOMETRY RESOURCE (505) 667-3843 • E-MAIL: jett@lanl.gov



# DIAGNOSING DEGRADING CONCRETE BEFORE IT CRACKS UP

NEW TECHNIQUE IS QUICK, INEXPENSIVE, AND SAFE

EDITOR'S NOTE: This technology was featured in last month's issue of Dateline: Los Alamos.

M any of the nation's bridges, dams, runways, roads, and culverts are cracking up. In 1993, the Federal Highway Administration reported that more than 230,000 miles of U.S. roads needed immediate repair or repair within 5 years. The cost of fixing this problem is projected to be at

least \$210 billion. One of the principal culprits: alkali-silica reaction — ASR — which can prematurely degrade and weaken concrete structures. A new technique developed by Los Alamos researchers can detect ASR deterioration quickly, inexpensively, and safely.



Concrete is a mixture of cement, aggregate, and water. ASR occurs when alkali in the cement attacks silica-rich components of the aggregate. The reaction causes the concrete to fracture. Diagnosing the presence of ASR before fractures occur has always been difficult and time-consuming.

When applied to a sample concrete core, Los Alamos' ASR Detect<sup>™</sup> reveals the presence of this destructive reaction in less than 5 minutes through colorful staining that is easy to recognize and interpret. This safe, "low-tech" method uses nonradioactive agents and is perfect for on-site use, allowing many structures to be analyzed quickly.

To evaluate degrading concrete and to prescribe treatment, engineers must know what is causing the deterioration. Is it ASR or something else? (Other possible causes include freeze-thaw and formation of the mineral ettringite.) Although ASR has been known for almost 60 years,

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ASR can shorten a concrete structure's life. When applied to a sample concrete core, ASR Detect™ reveals the presence of the destructive alkali-silica reaction.

its effects can be difficult to differentiate from other effects, and the common diagnostic procedures are time-consuming, difficult to use, expensive, and produce environmentally unfriendly wastes that need special disposal.

ASR Detect<sup>™</sup>'s two reagents react with two gels associated with ASR. In ASR-containing concrete, the result is a brightly colored surface showing the presence of the targeted gels; ASR-free concrete is unaffected.

For a low cost per sample concrete core, ASR Detect<sup>TM</sup> allows a complete diagnosis without the need for special equipment or extensive training, making this method ideal for in-field analysis. The user simply applies the reagents to a fracture surface on a concrete core drilled from a suspect structure, then rinses off the excess. On ASR-contaminated concrete, the resulting stains are immediately recognizable to the naked eye.

And the stains reveal more about ASR than its presence. Their distribution shows the extent of ASR in the concrete, and their proximity to different components of the aggregate gives clues to the source of trouble. Previously, only one type of ASR gel was known, but ASR Detect<sup>TM</sup> identifies two ASR gels (one becomes yellow, the other pink). The different colors indicate the state of ASR's progression, with yellow signaling that degradation had begun and pink warning that degradation is advancing.

An important future application will be to evaluate the ASR potential of a particular concrete mix before it is used in a construction project. In other words, a concrete made from a particular cement and a particular aggregate could be tested. Or, various ASR preventatives could be tested for their effectiveness in a particular concrete mix. The use of ASR Detect<sup>TM</sup> to evaluate concrete mix designs is possible because Los Alamos' method is such a sensitive indicator of the ASR gel, even in the reaction's beginning stages.

> CONTACT: BILL CAREY GEOLOGY AND GEOCHEMISTRY (505) 667-5540 • E-MAIL: bcarey@lanl.gov

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# **DATELINE: LOS ALAMOS**

#### AUTOMATED CHEMICAL ANALYSIS SYSTEM

The Automated Chemical Analysis System processes soil samples for the detection and determination of polychlorinated biphenyl mixtures: hazardous chemicals originally used as heat-transfer fluids. These so-called



The Automated Chemical Analysis System consists of several integrated Standard Laboratory Modules. A robot arm transports a sample from module to module. The inset at right shows the Human-Computer Interface software module used to automate an entire chemical analysis.

"PCBs" are a significant contaminant at a number of government and industrial sites. Not only do PCBs have great chemical stability, they are also a potential carcinogen and the Environmental Protection Agency wishes to eliminate them from the environment. Los Alamos is leading a national laboratory effort that includes Oak Ridge, Sandia, Pacific Northwest, and Idaho Engineering to process soil samples for the

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detection and determination of PCB mixtures using the Automated Chemical Analysis System. Transported to the contaminated site in an 18-wheel semitrailer truck, the system uses standardized modules to provide consistent and reproducible analytical results. Individual modules

can be removed or added to the system. This built-in flexibility eventually will allow scientists to conduct myriad analyses for applications that range from environmental cleanup and waste management to food and pharmaceutical characterization and petrochemical processing.

> CONTACT: ROBERT HOLLEN (505) 667-3186 • E-MAIL: hollen@lanl.gov

#### AUTOMATICALLY CONTROLLED THREE-PHASE CENTRIFUGE

Approximately 100 million barrels of environmentally hazardous oil sludge must be cleaned up in the United States alone, and more than 2.5 million barrels are discarded annually. Worldwide, the figures are much higher. Much of this oil sludge comes from refineries, but a large portion is a byproduct of oil field production. Los Alamos and Centech Inc. of Casper, Wyo., have combined an



A centrifuge

site for oil

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water, and

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ingeniously designed centrifuge and an intelligent "fuzzy" controller. Computer software with fuzzy intelligence makes decisions based on a construct of rules that captures the expertise and experience of a highly skilled human operator. The fuzzy software substantially improves an already successful centrifuge technology by automating control of the centrifuge for environmental cleanup and oil recovery. The automatically controlled three-phase centrifuge will separate oil field and oil refinery wastes into salable oil, reusable water, and harmless solids. It will efficiently clean up oil spills that cause serious environmental problems and it can also be used in separation processes conducted by the steel industry.

CONTACT: WILLIAM PARKINSON (505) 667-7021 • E-MAIL: parkinson@lanl.gov

#### ERUPT: COMPREHENSIVE VOLCANO SIMULATOR



Because observing volcanic activity at close range is extremely dangerous, truly devastating volcanic events are generally recorded at a distance that obscures what is happening with the volcano itself. To raise awareness, which can save lives in an emergency, volcanologists and public officials need a way to communicate volcanic risks to the public, especially in areas close to active or potentially active volcanoes. ERUPT software meets that challenge by accurately portraying volcanic activity and its related hazards in an easily appreciated



visual format. Through a simple graphical interface, the user displays real-time animations of the flow of lava and ash clouds and, as the lava and ash are deposited in color-coded layers, builds two- and threedimensional representations of a volcano or volcanic field. Developed

by Los Alamos and marketed by RockWare Inc. of Golden, Colo., ERUPT software for personal computers is the first computer program of any kind to simulate practically any kind of volcanic activity, making it a useful teaching, research, and civil defense tool.

> CONTACT: KENNETH WOHLETZ (505) 667-9202 • E-MAIL: wohletz@lanl.gov

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An actual ERUPT simulation (bottom) of the 1975 eruption of Mt. Ngauruhoe, New Zealand The simulation shows an eruption producing billowing clouds of ash and gas that rise several miles into the sky while pyroclastic flows and surges (hot avalanches of ash and rock) race down the volcano's slopes.

#### S E Ρ Т Ε Μ В E R Т S S IJ E 1 9 9 7

# **DATELINE: LOS ALAMOS**

#### FACSIM — A FACILITY SIMULATION PROGRAM FOR NUCLEAR MATERIAL PROCESSING

The demand for nuclear energy is rising around the globe, and large new nuclear reprocessing and fuel fabrication plants are going up to help meet this demand. At the same time, the United States and Russia are producing large amounts of surplus fissile material from dismantled weapons. The International Atomic Energy Agency and its member

states are faced with the enormous challenge of ensuring that none of this fissile material is diverted for nuclear weapons. Safeguarding plutonium is a difficult task because as fissile materials move through a processing facility, they lose their identities through a series of physical and chemical changes. Traditional nuclear safeguards rely on a combination of surveillance and material accounting procedures such as measuring inputs, outputs, and inventories.



However, in the high-throughput facilities made necessary by the expanding nuclear energy market, supplementary safeguards measures based on much more detailed monitoring of the amounts and locations of material in the facility are needed to meet current IAEA standards. FacSim is a computer program that simulates the full operating cycle at facilities that process nuclear material, and it gives detailed information on the locations and amounts of fissile material at any given time. This information can be used to evaluate and improve enhanced safeguards measures such as monitoring material movements and individual process steps within the facility. In addition, it is possible to use FacSim in real time to track process operations and assure that they are consistent with the stated facility design. FacSim is currently being used to help plan and evaluate safeguards systems at several facilities around the world.

CONTACT: C. ALTON COULTER (505) 667-4964 • E-MAIL: acoulter@lanl.gov

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Representation of a FacSim calculation. Curves show plutonium inventories in the solventextraction vessels of the first of three purification cycles at a nuclear fuel reprocessing plant.

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## **DATELINE: LOS ALAMOS**

#### FASTAC — AN ULTRAVIOLET SYSTEM FOR CONTROLLING BACTERIA IN OPAQUE FLUIDS

Intense ultraviolet light is bacteria's worst nightmare. Los Alamos and Triton Thalassic Technologies Inc. of Ridgefield, Conn., have developed a UV source optimized to operate within T<sup>3</sup>I's patented flow chamber. The lamp emits light concentrated around a single wavelength and, as opaque industrial fluid or turbid water flows around the outside of the lamp, the light kills or inactivates most of the bacteria contaminating the fluid. T<sup>3</sup>I's FASTAC is the only ultraviolet



system available that can treat opaque fluids. As the first technology to offer a safe and efficient replacement for the toxic chemicals currently used to treat metal-working fluids, FASTAC will reduce health risks for millions of industrial workers.

CONTACT: JOHN COOGAN (505) 665-0186 • E-MAIL: jcoogan@lanl.gov

#### DETECTOR FOR NONINVASIVE FLUID CHARACTERIZATION

The Detector for Noninvasive Fluid Characterization is the first instrument that rapidly characterizes liquids, gases, and solids on the basis of their

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physical properties. It also identifies a large array of industrial and hazardous toxic liquids inside sealed containers, when direct access is not desirable or not possible. Portable and easy to hold with one hand, the detector is highly suited to field use in a whole range of applications. All the operator has to do is press a few keys and in less than

20 seconds, the detector gathers data, completes the analysis, and displays the name of the chemical. The detector is composed of an electronics box, which includes a computer with a large chemical database of physical properties, and a sensor head with two transducers. One transducer

Transducers are attached to a standard 4-liter glass bottle containing the chemical to be analyzed. The operator presses a few keys and in less than 20 seconds the detector gathers data, completes the analysis, and displays the name of the chemical. The inset shows a single drop of liquid being held between two miniature transducers by surface tension. The detector will sense traces of contamination in one drop.



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This quartz lamp, with its surface of intense ultraviolet light. is a bacterium's worst nightmare. Operating within FASTAC's specially designed flow chamber, the lamp emits light concentrated around a single wavelength As opaque industrial fluid or turbid water flow around the outside of the lamp, the light kills or inactivates most of the bacteria contaminating the fluid

sends sound waves into the liquid, gas, or solid to be analyzed. The physical properties of the contents determine the interference pattern, or spectrum, picked up by the other transducer. The detector determines multiple physical properties of the contents from the observed spectrum and matches these with the values in the computer library to identify the contents. The detector identifies a large number of liquids inside sealed containers; monitors mixtures, emulsions, and concentration variations; and analyzes fluid samples as small as one drop. Originally designed for chemical weapons treaty verification and nonproliferation work, the instrument has a range of civilian uses in the food and beverage, chemical and petroleum, and biomedical and healthcare industries, and in customs and drug interdiction and basic research.

> CONTACT: DIPEN SINHA (505) 667-0062 • E-MAIL: sinha@lanl.gov

#### HIGH-TEMPERATURE SUPERCONDUCTING, HIGH-GRADIENT MAGNETIC SEPARATION



This advanced separation system removes pollutants from solids, liquids, and gases. When combined with high-temperature superconducting technology, magnetic separation becomes a versatile means of decontamination and resource recovery. Because it is a physical separation process, no chemical changes occur, which means the High-Temperature Superconducting High-Gradient Magnetic Separation system introduces no pollution of its own. The HTS separator can be moved from



site to site to extract actinides such as plutonium, thorium, uranium, and americium out of soil. Developed by researchers at Los Alamos, Eriez Magnetic of Erie, Pa., and American Superconductor Corp. of Westborough, Mass., it can also be used to recover valuable compounds from medical waste water and contaminants from industrial waste water. In addition, its

use in water treatment and purification could greatly improve effluent treatment and water quality.

CONTACT: F. COYNE PRENGER (505) 665-0951 • E-MAIL: prenger@lanl.gov

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A simplified schematic of high-gradient magnetic separation. The inset (below) shows a concentrated slurry contaminated with copper oxide (dark solution) and the purified water (clear solution) that results from magnetic separations

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# **DATELINE: LOS ALAMOS**

#### QUANTUM CRYPTOGRAPHIC KEY GENERATOR

No one likes someone else reading his or her e-mail. Unfortunately, keeping communications secure in cyberspace is sometimes harder than

trying to have a private phone conversation on a party line. The primary application of the quantum cryptographic key generator is to provide secure communications over fiber-optic cables in metropolitan areas where the two communicating parties are separated by up to 100 kilometers. The key transmissions are sent one photon at a time, so they cannot be tapped because a photon is an indivisible elementary particle. The key generator



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Quantum cryptography allows "Alice" and "Bob" to exchange messages in secrecy by using a cryptographic key that is generated and shared using the quantummechanical properties of single photons. Key generation is controlled by ordinary personal computers, which also display the encrypted messages that are sent and received

can be used to provide secure communications between banks, between off-site stock-trading centers and central stock exchanges, between corporate offices, and between offices of federal agencies such as the FBI or the National Security Agency. The same system also can be used to detect anyone who attempts to "eavesdrop." The key generator produces software keys required to encode and decode messages and distributes the keys over the same fiber-optic cables used to transmit the messages. Because the key generator produces keys required for encryption just before the encrypted message is sent, they cannot be stolen beforehand.

> CONTACT: RICHARD HUGHES (505) 667-3876 • E-MAIL: rxh@lanl.gov

#### LOKI: PARALLEL SUPERCOMPUTING WITH COMMODITY COMPONENTS

Loki is a general-purpose supercomputer built by combining a large number of off-the-shelf components. Developed by Los Alamos, the California Institute of Technology, and the Goddard Space Flight Center of Greenbelt, Md., Loki provides a highly reliable and flexible computing resource ideally suited to a wide variety of large computational



Loki's novel commodity parallel processor design provides a highly reliable and flexible supercomputing resource ideally suited to a wide variety of large computational problems. Here, a scientist performs astrophysics research at the console in front of Loki.

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problems. By using Loki methods, software, and development tools, any research, engineering, or business organization can develop its own commodity parallel processor design to provide a local supercomputing capability. The Loki design provides general-purpose supercomputing capability in the range of \$55,000, which is less than one-third the price of its nearest competitor.

CONTACT: MICHAEL WARREN (505) 665-5023 • E-MAIL: mswarren@lanl.gov

#### MDH-1000: A HYDROGEN PURIFICATION SYSTEM



Ultrapure hydrogen is used to purify the silicon that goes into microelectronic devices. Ultrapure hydrogen also is used to produce high-purity iron and steel, which have the superior magnetic properties needed for high-efficiency electric motors, alternators,

and generators. The MDH-1000 system developed by Los Alamos researchers not only provides hydrogen with a purity greater than 99.9999 percent for these applications, but it also can recover the hydrogen used in them or in other industrial processes. The heart of the purification system is a metal membrane that separates hydrogen from other gases, with minimal auxiliary equipment, at flow rates 10 times greater than that of any other hydrogen filter. The materials in the membrane are sturdy and inexpensive and the whole MDH-1000 unit has several safety features that help reduce the hazards of working with hydrogen. Semiconductor manufacturers can save about \$160 million a year by using the membrane technology employed by the MDH-1000 to produce ultrapure hydrogen for purifying the silicon used in microelectronic devices. In the future, ultrapure hydrogen will be needed for proton-exchange membrane fuel cells to generate electricity at central and remote power plants. The membrane technology was conceived, developed, and patented by Los Alamos. Generex Inc. of Tryon, N.C., licensed the technology and developed the commercial product. To date, Generex has sold the MDH-1000 to companies in Sweden, Italy, and Korea.

> CONTACT: ROBERT DYE (505) 667-3404 • E-MAIL: rcdye@lanl.gov

metal membrane that separates ultrapure hydrogen from other gases, the heating unit for the metal membrane, and the purge system that protects the membrane from damage should its temperature drop below that required for proper operation. The unit on the right provides the control logic and electrical power for the purification system and indicates the temperature of the membrane.

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the left

The cabinet on

contains the composite



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# **DATELINE: LOS ALAMOS**

#### NANOPOROUS POLYMERS: "MAGIC MATERIALS" FOR WATER PURIFICATION

A completely new class of polymer, nanoporous polymeric materials reduce common organic contamination in water to parts-per-trillion levels. Unlike conventional technologies such as activated carbon and zeolites, these new polymers work effectively in both air and water. In fact, the binding between organic contaminants and the polymer is 100,000 times greater than the binding between

organic contaminants and activated carbon. A simple alcohol rinse releases the collected contamination from the polymer, enabling workers to use the material again and again. The technology preserves municipal water supplies by removing hazardous organic compounds from drinking water or under-

The Remote Container-Sampling Device and its attachments. The RCSD can pierce, vent, sample, and neutralize the contents of containers believed to hold unstable and hazardous materials.

ground water. It also has potential applications in cleaning up toxic organics at nuclear waste sites; oil or organic chemical spills, such as tanker spills in oceans; and organic explosives, such as TNT, at Department of Energy and Department of Defense sites.

CONTACT: DEQUAN LI (505) 665-1158 • E-MAIL: dequan@lanl.gov

#### RCSD: REMOTE CONTAINER-SAMPLING DEVICE

Hazardous materials response and environmental cleanup crews work day to day with potentially hazardous containers. These teams must

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characterize the materials inside such drums before they can properly dispose of them. In some cases, merely piercing a container will cause it to explode and release dangerous fumes or contaminants into the environment. The explosion could be severe enough to harm workers in the immediate area. The Remote Container-Sampling Device can pierce, vent, sample, and neutralize the contents of containers believed to hold unstable and hazardous materials. Portable and remotely operated, the RCSD reduces the possibility of spontaneous



A large

transparent film on an aluminum support is covered with organiccontaminated water droplets. Removing the water droplets reveals corresponding colored dots which indicate that the organic contaminants have been efficiently transported into the nanoporous polymer. The inset shows the polymer in its pure form (left), and the polymer having absorbed two different chemicals (middle and right). A rinse with a solvent such as ethanol returns the polymer to its original state (pure form).

ignition through the use of a self-contained, breathing-apparatus air cylinder that provides a compressed-air power source. Potential users of this device include hazardous materials teams, fire and police departments, hazardous device squads, and environmental cleanup crews.

CONTACT: DAVID VOLZ (505) 665-7357 • E-MAIL: dvolz@lanl.gov

#### ROAM: REAL-TIME OPTIMALLY ADAPTING MESHES

The military and industry spend hundreds of millions of dollars each year collecting, processing, and validating data to simulate terrain for applications such as flight simulation, virtual reality, and sensor testing and evaluation. The challenge faced by all real-time terrain-rendering software is to produce realistic and consistent scenes in milliseconds. ROAM is the first real-time terrain-generating software to operate by a strict error-minimization discipline: consequently it achieves precise displays with highly efficient use of graphical resources. ROAM operates

in two stages: a preprocessing stage and a real-time stage. The preprocessing software constructs meshes of triangles that approximate the desired terrain at progressively coarser levels of detail. The real-time terrain server starts at the coarsest level of detail, where the preprocessor stops, and works in the opposite direction; it locally subdivides the meshes to produce a sequence of nonuniform but continuous terrain meshes. Consequently, ROAM rapidly generates



high-quality visualizations. ROAM also addresses vital concerns for how simulated entities interact with terrain. ROAM's resource allocations are guided to enable objects to move naturally over terrain while maintaining accurate fields of view. ROAM was originally designed for the Navy and the Air Force to support flight simulations for integrated tests of aircraft avionics. The computer codes that underlie ROAM are flexible and have wide applicability beyond terrain rendering. In the near future, ROAM may play a role in developing a new category of interactive, multiplayer, virtual reality simulations for the entertainment, business, and medical markets, as well as finding further uses in military and scientific applications.

> CONTACT: MURRAY WOLINSKY (505) 665-0952 • E-MAIL: murray@lanl.gov

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This is a single frame taken from a realtime terrain simulation produced using the ROAM terrain server. The area shown is part of the Sandia Mountains near Albuquerque, N.M.



# BRIEFLY ...

LABORATORY FORMS NEW OFFICE TO ENHANCE COLLABORATIONS. Two Los Alamos programs, the office of Energy Technology and the Industrial Partnership Office, have merged into a single program called the Civilian and Industrial Technology Program Office. The merger will enhance the Laboratory's role in civilian federal programs such as fossil fuel and energy efficiency technologies and will work to form synergistic partnerships with industry sectors closely aligned with those civilian programs. Additionally, the office will seek to form strategic partnerships with industry that provide value to the Laboratory in terms of innovation and the ability of the partnership to enhance the Lab's ability to meet its core mission. The new office will more closely scrutinize Los Alamos' areas of science and technology that will benefit from the industrial collaboration and analyze the long-term benefits. "We'll be looking for programs and partnerships, in either industry or government, where the results of the work will help strengthen and revitalize the Laboratory's role in non-defense federal and civilian programs," said Charryl Berger, director of the new office. "We will focus on innovation and creativity rather than the amount of money the collaboration might bring in."

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