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SANDIA TECHNOLOGY

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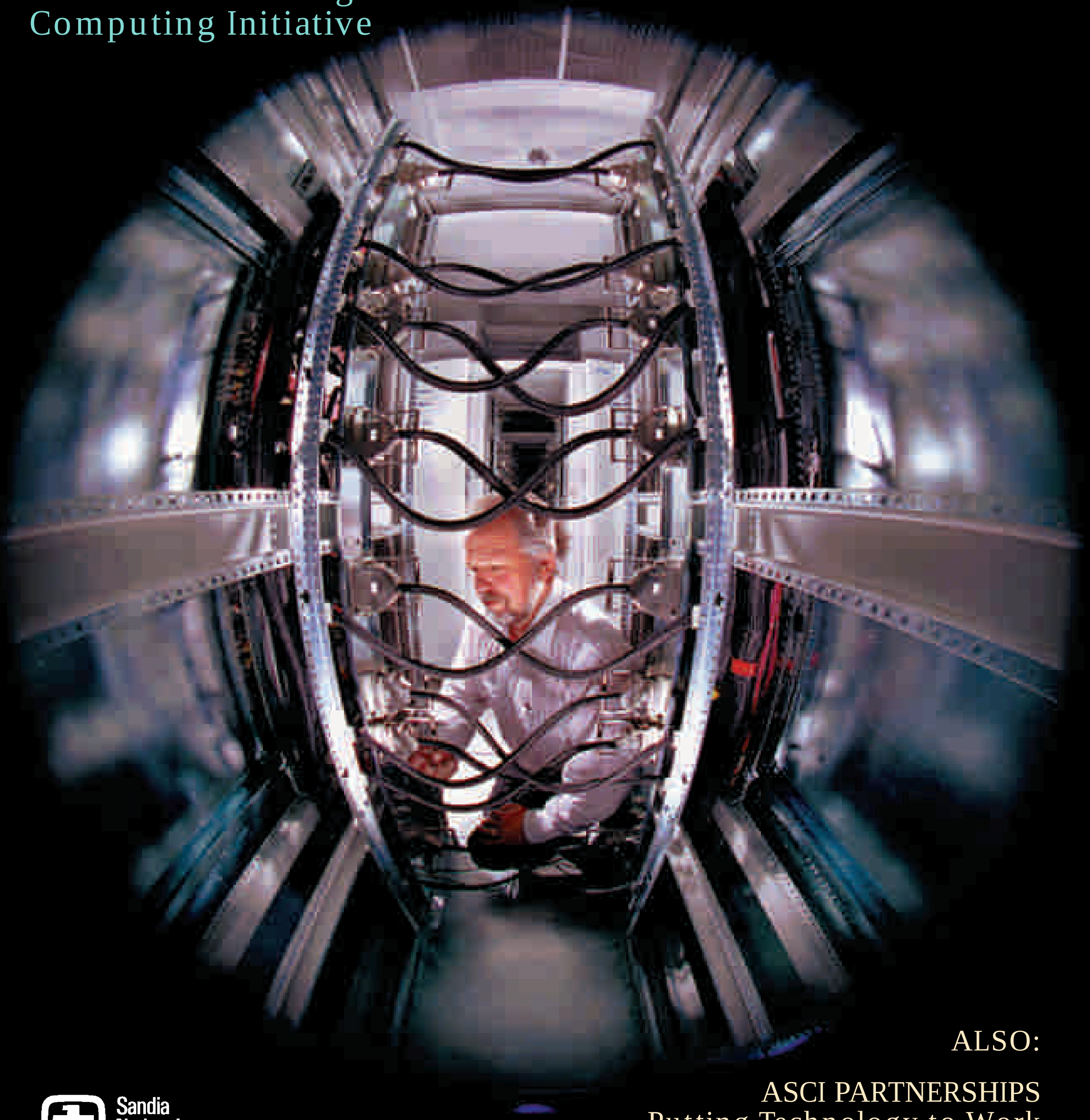
THE NEW FRONTIER
Accelerated Strategic Computing Initiative



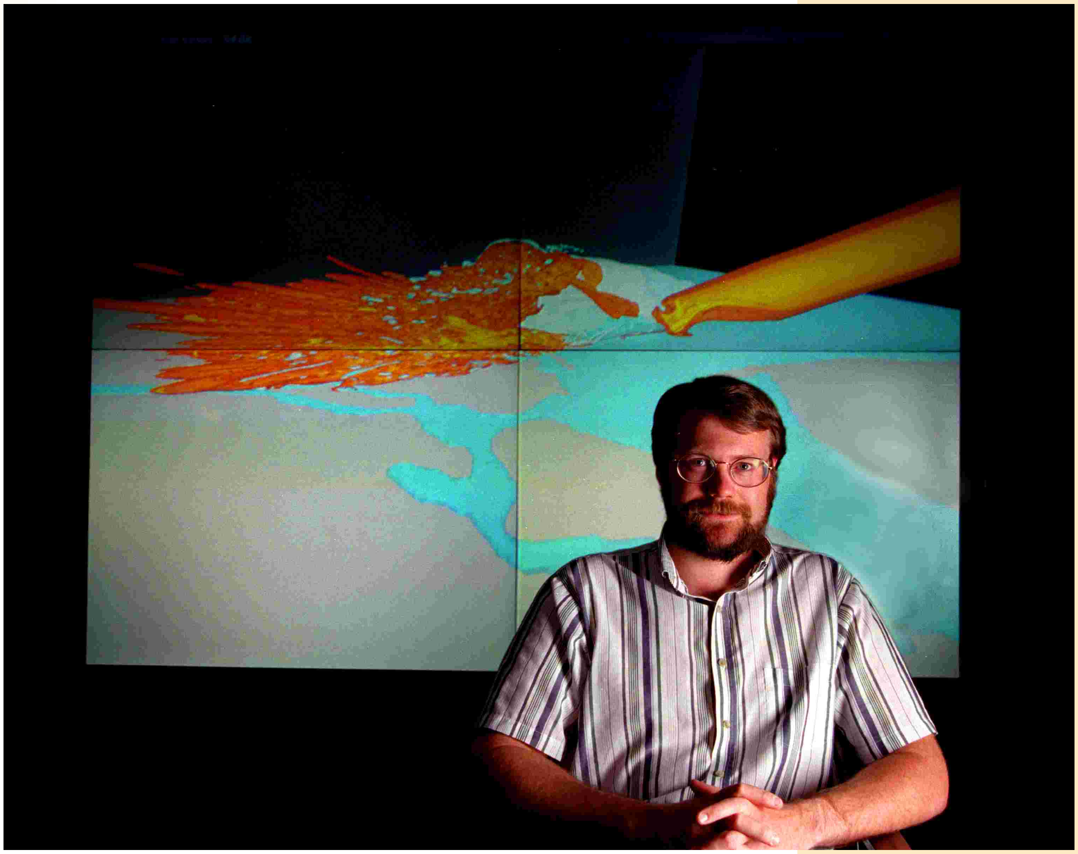
ALSO:

ASCI PARTNERSHIPS
Putting Technology to Work

Universities Team With Sandia

Sandia National Laboratories

A Department of Energy National Laboratory



Sandia scientist David Crawford sits in front of a computer-generated image that shows the impact of a computer-animated 1-km comet (or asteroid) hitting the ocean.

"It (ASCI) has pushed the computer industry to go significantly beyond where it would be otherwise. At the same time, it has not gone so fast that the industry has been unable to produce integrated systems or the software to go with them."
March 1999 Blue Ribbon Panel Report on ASCI

ON THE COVER: Archie Gibson, operations team leader for Sandia National Laboratories' Corporate Computing Facility, inspects the ASCI Red high-performance computer. The Intel computer has reached a peak speed of more then 3 teraflops, or 3-trillion floating point operations per second.

(Photo by Randy Montoya)

Sandia Technology is a quarterly journal published by Sandia National Laboratories. Sandia is a multiprogram engineering and science laboratory operated by Sandia Corporation, a Lockheed Martin company, for the Department of Energy. With main facilities in Albuquerque, New Mexico, and Livermore, California, Sandia has broad-based research and development responsibilities for nuclear weapons, arms control, energy, the environment, economic competitiveness, and other areas of importance to the needs of the nation. The Laboratories' principal mission is to support national defense policies, by ensuring that the nuclear weapon stockpile meets the highest standards of safety, reliability, security, use control, and military performance. For more information on Sandia, see our Web site at *http://www.sandia.gov.*

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FROM THE *Editor*

Dear Readers:

As computer users, we all want the latest and greatest in computing technology. The computing industry has been faithfully whetting our desires as it follows Moore's Law of doubling microchip data capacity every 18 months. Speed and memory continue to leap forward allowing for more detailed graphics, faster Web surfing, and greater storage capacity. And so it goes.

But that's not good enough for the Department of Energy and its desire to continue to ensure the safety, security, and reliability of the nuclear weapon stockpile without having to explode any more nuclear bombs. While still working with technology that adheres to Moore's Law, the DOE's defense laboratories are stretching it to the limit to create machines that seek new frontiers in computing. Developing the high-resolution, three-dimensional physics and engineering modeling needed to evaluate the aging nuclear stockpile without actual testing is no small task. And it has taken a concerted effort by many of the nation's top scientists to bring it about.

The Accelerated Strategic Computing Initiative (ASCI), the focus of this issue of *Sandia Technology*, is the outcome of that quest. Its goal is to develop computers that have peak capacities of 100 trillion operations per second by 2004. Sandia, Los Alamos, and Lawrence Livermore national laboratories are working with each other and with industry in new ways to achieve that goal. And ultimately, the American public will be the beneficiary. Not only will the program help ensure our safety and security, the multimillion-dollar technology now in our nation's top-secret laboratories eventually will be in our desktop computers. And that's really something to whet our collective computing appetites over.

Chris Miller
Editor

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by Gil Weigand, Deputy Assistant Secretary, Defense Strategic Computing & Simulation, U.S. Department of Energy

Accelerated Strategic Computing Initiative

THE NEW FRONTIER

or How to Wow a Technophile

After the Nuclear Test Ban Treaty was implemented in 1996, the question became how could researchers ascertain the effects of aging on a 40-year-old bomb?

And could Sandia, charged with U.S. nuclear stockpile stewardship, confidently certify the safety and reliability of every component in every weapon every year?

Accelerated Strategic Computing Initiative

The New Machines

One person.
One pocket calculator.
If this tireless individual does one calculation per second — with no lunch breaks and no running home at five o'clock — then he or she could accomplish in a mere 100,000 years what the latest ASCI super-computer does in — are you ready — one second.

In an age of daily technological firsts, when Regular Joes expect to be technologically dazzled, the Department of Energy's Accelerated Strategic Computing Initiative (ASCI) is a tough act to follow. But with a goal of reaching a computing speed of 100 teraflops by 2004, the nation's top computational scientists view this ASCI goal as a tough challenge. ASCI is a 10-year science-based program for developing high-resolution modeling to support certification of the nuclear stockpile annually.

Engineers from the Stone Age to the Atomic Age have relied primarily on trial and error: Make it, break it, make it again better. In the Atomic Age, the break it translated to actual bomb detonation. These tests — that is, underground nuclear detonations — demonstrated with certainty how stored weapons would react to specific situations, such as aging components, natural disasters, and terrorist attacks. Tests kept experts apprised of evolving safety concerns.

However, the Comprehensive Test Ban Treaty of 1996 ended nuclear testing by all nations who signed the agreement. (The initial treaty signers included the United States, Britain, China, France, and Russia. By August 1999, 152 nations had signed the agreement, and 43 nations had ratified it. The U.S. Congress had not yet ratified the agreement.) The treaty drove the need to create a new way to certify the U.S. nuclear stockpile as safe, secure, and reliable.

Today, ASCI-developed modeling and simulation are offering an alternative to testing. Ever-increasing computing speeds are necessary to fully simulate the complex 3-D physics of nuclear weapon-performance and analyze accident environments, such simulating an airplane crash involving a nuclear weapon and a subsequent fuel fire.

With DOE oversight, Sandia National Laboratories is working with Los Alamos and Lawrence Livermore national laboratories to ensure the ASCI program goals are met. Although ASCI is just three years old, the prognosis is good. Having attained computer speeds of more than 3 teraflops, the program already is providing enough information to support certification of the nuclear stockpile. A teraflops refers to a Trillion FLoating OPerations per Second.

The April, 1999 issue of the ASCI newsletter reported that the independent Blue Ribbon Panel of experts chaired by Dr. Venkatesh

Sandian Michael Hannah inspects cable in one of the eight disconnect cabinets that are part of the teraflops supercomputer developed by Sandia and Intel corp. The cabinets are separate repositories for classified and unclassified information.

Narayanamurti, dean of engineering at Harvard University, has concluded that ASCI hardware "is clearly a world-class effort."

"It has pushed the computer industry to go significantly beyond where it would be otherwise," states the March 1999 Blue Ribbon Panel Report on ASCI. "At the same time, it has not gone so fast that the industry has been unable to produce integrated systems or the software to go with them."

Sandia uses computer simulation to predict weapon behavior during an accident.

Testing versus Simulation

ASCI hardware and software have produced reliable 3-D models that put into action relevant spatial dimensionality and detail, and physical principles to simulate catastrophic events. Although non-nuclear components can still be tested, computer simulations —which are really tests conducted in simplified virtual reality — provide a large amount of data for Sandia's annual recertification of weapons.

High-performance computing is paramount to analyzing intricate designs, said Dona Crawford, director of Sandia's Advanced Product Realization Program. "We run hundreds or thousands of jobs. We can run a calculation a hundred different ways to get a better understanding, for the same money and same time needed for an actual test that provides only one finding (rather than hundreds)," she said. "ASCI is key to Sandia's weapons mission."

In comparing confidence in actual tests to confidence in simulations, Crawford said that scientists are able to see how a component or system will work in a single, specific set of conditions from an actual test. Although they cannot have the same confidence in a computer simulation, each simulation examines a nuclear event from thousands of vantage points, whereas an actual test provides much more limited information – sometimes just "go-no go" information. In addition, simulations can be performed for a wide variety of "test" conditions. One major ASCI milestone is the ability to certify the neutron generator for the W76 warhead in a hostile environment. Before ASCI, this could be done only with actual underground tests, Crawford said.

Although researchers cannot have the same confidence in a computer simulation, each simulation examines a nuclear event from thousands of vantage points, whereas an actual test examines it from just one.

In a statement to Congress, Sandia Director C. Paul Robinson said, "I believe this will be the first time a major component of U.S. nuclear weapons will be introduced into the active stockpile without being qualified through nuclear tests."

The New Engineering Tool

Until recently, ensuring a weapon was safe, secure, and reliable when redesigned or updated with new parts required exploding that weapon. A rudimentary simulation on a single computer supported the test, but limits on speed and memory of computer hardware restricted the quality of the simulation.

"We had reached a wall with traditional supercomputing," said Bill Camp, principal architect for ASCI hardware at Sandia and director of Sandia's Computation, Computers, and Math Center. "One big, fast processor was the old method, but we started to hit the speed-of-light limit. We hit a wall."

Today, however, high-performance, massively parallel computers allow researchers to simulate the complex 3-D physics involved in nuclear-weapons performance and to accurately predict the degradation of nuclear weapons components as they age in the stockpile.

"Driving parallel computing speed is a major contribution of ASCI to mainstream America. The things we do today (at the labs on high-performance computers) will be on your desktop in five to 10 years," Crawford said. "Another contribution is the development of a new generation of science and engineering applications, algorithms and related technologies, and the basic approach of replacing test with simulation."

She cautioned that although computing is a powerful tool, it must be used with prudence. Simulation is not a universal substitute for conducting actual tests. Engineers must still sometimes use their traditional trial-and-error technique: Make it, break it, make it again better.

the Clockworks of Massively Parallel Computing

Before these breakthroughs, most computer scientists believed using even thousands of parallel processors could increase computing speed only by 50 to 100 times the rate of a single processor.

In the mid-1980s, Sandia, with Los Alamos, Oak Ridge, and Lawrence Livermore national laboratories plus the California Institute of Technology (CalTech), began replacing single computers with many computers linked by software. Sandia computer scientists developed complex software for the new processing technique, a challenge many thought impossible. The software was designed to let multiple processors solve different parts of a single problem simultaneously. This software distributed computations across multiple processors. The processors then communicated with one another, integrated their findings, and quickly produced a single answer to the problem. This became known as *massively parallel computing* and offered tremendous speed and memory advantages.

Inventors had no precedent to guide the way. CalTech researchers suggested the idea of massively parallel computing, and they and Sandia developed methods to make it work, said Bill Camp, principal architect for ASCI hardware at Sandia and director of Sandia's Computation, Computers, and Math Center.

"It was considered so tough that no one (else) took it on," Camp said.

In 1988, Sandia won the Karp Challenge Prize for demonstrating unprecedented speedups using processors that worked together — as compared to processors for prior technology which ran separately. The same year, Sandia won the Gordon Bell Prize for achieving a thousandfold speedup in parallel processing.

Before these breakthroughs, most computer scientists believed using even thousands of parallel processors could increase computing speed only by 50 to 100 times the rate of a single processor.

ASCI Red, Breaking the Teraflops Barrier

The Intel teraflops computer, called ASCI Red, became operational in 1997. At 1.8 teraflops (or 1.8 trillion floating point operations per second), it was more than five times faster than the previous world-record holder. Someone with a pocket calculator would need 57,000 years to solve a problem ASCI Red could compute in one second. It used more than 9,000 Pentium Pro processors and had nearly 6-billion bytes of memory.

The $55 million computer enabled engineers to conduct detailed 3-D simulations of stresses on aging weapons.

Sandia Director C. Paul Robinson called it "a very important step in shifting from a test-centered program to a computational-centered program" for ensuring nuclear stockpile safety.

When ASCI Red surpassed 1 teraflops, then Intel Executive Vice President and CEO Craig R. Barret called it the "computing equivalent to breaking the sound barrier."

In addition to applications in stockpile security, the Red machine—said President Clinton's then Science Advisor Jack Gibbons—was capable of applying complex physical principles to simulations that supported medical, pharmaceutical, meteorological, and transportation (auto and aircraft) studies.

Over the past year, Los Alamos National Laboratory has brought the 3-teraflops ASCI Blue Mountain computer on line. At Lawrence Livermore, the 3.9-teraflops ASCI Blue Pacific computer also came on line. Meanwhile, Sandia has upgraded ASCI Red with new processors to exceed 3 teraflops.

The three laboratories are working together to create a seamless collaborative environment in which scientists at each site will work remotely on all three computers over a secure network.

Cplant Puts Off-the-Shelf Units to Work

Sandia computer scientists, over the past two years, have built on their expertise in parallel computing. A major development has been the computer cluster system, known as Cplant for computational plant.

A computational utility, Cplant was created for adaptation to change; it can grow and be pruned and, therefore, be readily available for modeling and simulation. Every year a new phase or branch will be added to the "plant" to increase its capability with the latest, cost-effective hardware components. Older and perhaps obsolete hardware can be pruned every three years.

A large-scale massively parallel computer, Cplant architecture is derived from the ASCI Red architecture, which is a proven technology. However, Cplant differs from ASCI Red in that Cplant is a large system constructed from off-the-shelf computers.

Off-the-shelf Cplant modules act as microprocessor nodes. A new technology, Cplant is not as singularly powerful as the teraflops machines, but users can independently run complex software programs on individual nodes or assemblies of nodes, and users can do so simultaneously. In 1999, Cplant represents a combined capability of 1.024 teraflops at Sandia N.M., and 0.256 teraflops at Sandia, Calif.

DisCom2

The DisCom2 program combines distance computing (which supports high-end computing from a remote site) and distributed computing (which develops an integrated computing environment).

Created for adaptation to change, Cplant can grow and be pruned. Every year a new phase or branch will be added to the "plant" to increase its capability with the latest, cost-effective hardware components.

Eventually, ASCI computers that are geographically separated at the three DOE defense laboratories will be linked, along with Cplant, into a computational grid that operates across distances. The computer nodes will be the power plants in this grid.

Cplant serves as a proving ground for integrating these distributed computing resources. Cplant integrates commercially available modules and nodes into a large-scale system to create a flexible and cost-effective computing fabric. Distance computing will enable remote and independent use of the major ASCI supercomputers and Cplant.

Individual computers are stacked on top of each other to create the Computional plant, or Cplant.

The future: Web Technology

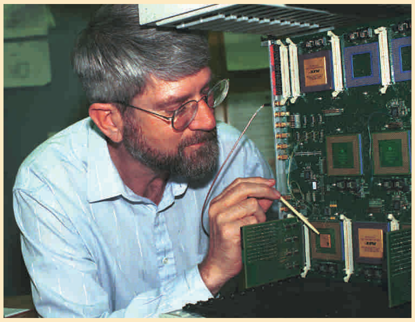
High-performance computing using a single powerful computer was once the leading edge of the computing industry, said Art Hale, Sandia deputy director for Computer Sciences. "The Web has turned that whole model on its head," he said. "The computer industry, with venture funding and Internet/Web resources, is making dramatic advances in computing technology."

Indeed, the Worldwide Web has set a precedent for distance computing. Anyone anywhere can now tap into computer resources and capabilities anywhere in the world.

"We can learn a lot by observing what works on the Web," Hale said, adding that Cplant technology could be put on the Web as a computational utility for modeling and simulation. "You could run your own simulation on the Internet using Cplant technology. Cplant itself is being put on the Sandia Intranet (internal Web)."

Web-like technology for high-performance technical and scientific computing represents a direction of Sandia computing research and development. Sandia scientists envision huge numbers of individual work-stations that are cost-effectively networked to one another, to information sources, and to high-performance capabilities. Users will interact with these resources in a "webtop" fashion.

NEWS Notes



Lyndon Pierson points to the unclassified encryptor chip – the world's fastest encrypytion device – that his Sandia research team designed.

SANDIA RESEARCHERS DEVELOP WORLD'S FASTEST ENCRYPTOR

The world's fastest encryption device, developed at the Department of Energy's Sandia National Laboratories, should soon be protecting data being transmitted from supercomputers, workstations, telephones, and video terminals. It encrypts data at more than 6.7-billion bits per second, 10 times faster than any other known encryptor.

Designer Lyndon Pierson says the device "has both the security and bandwidth necessary for the protection of all types of digitized information — voice, audio, video, cell phone conversations, radio and television transmissions, banking and credit card information, and general purpose computer data — at speeds previously unimagined."

The device consists of 16 sets of 16,000 transistors on an integrated circuit chip the size of a dime. Data, broken down into single bits of information in 64-bit units, are pipelined through the transistors, where a computationally intense algorithm scrambles the information so that it becomes incomprehensible to anyone who does not have the cryptographic key.

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lgpiers@sandia.gov

In Massively Parallel Computing

Sandia Software Expertise Key to Success

The challenge to massively parallel computing has been getting all the independent processors — and the current model has between 9,000 and 10,000 of them — to work together seamlessly.

Here are two examples of the direction that Sandia software development is taking to support high-performance computing:

• Parallel Material Contact Software

Special software is enabling researchers to run models of complex systems quickly, accurately, and efficiently on hundreds of thousands of parallel processors. The ability to distribute a problem to many processors on a parallel computer is called scalability. The software has been used to simulate the crushing of metal structures, such as thin-walled cans. As the can crumples, the buckling and consequent material contacts are detected and contact forces are properly treated. The codes that make up the software are enabling researchers to conduct simulations with unprecedented resolution to solve problems in nuclear stockpile stewardship, reservoir modeling, and structural dynamics. For U.S. industry, such capabilities will greatly increase the power and fidelity of virtual safety testing of vehicles.

• Dynamically Adaptive Software Environment

Sandia researcher Robert Clay is designing a software architecture — called the Dynamically Adaptive Software Environment or DASE — that will allow Cplant (see ASCI Hardware & Software, the Clockworks of Massively Parallel Computing, page 5) users to call up an operating system, tools, and other applications as needed. One environment will resemble that used for massively parallel computing. Another would be useful for engineering design and visualization, such as the Product Realization Environment, or PRE, where objects carry out transactions for the user.

Once developed, DASE will help Sandia revolutionize engineering and further advance modeling and simulation.

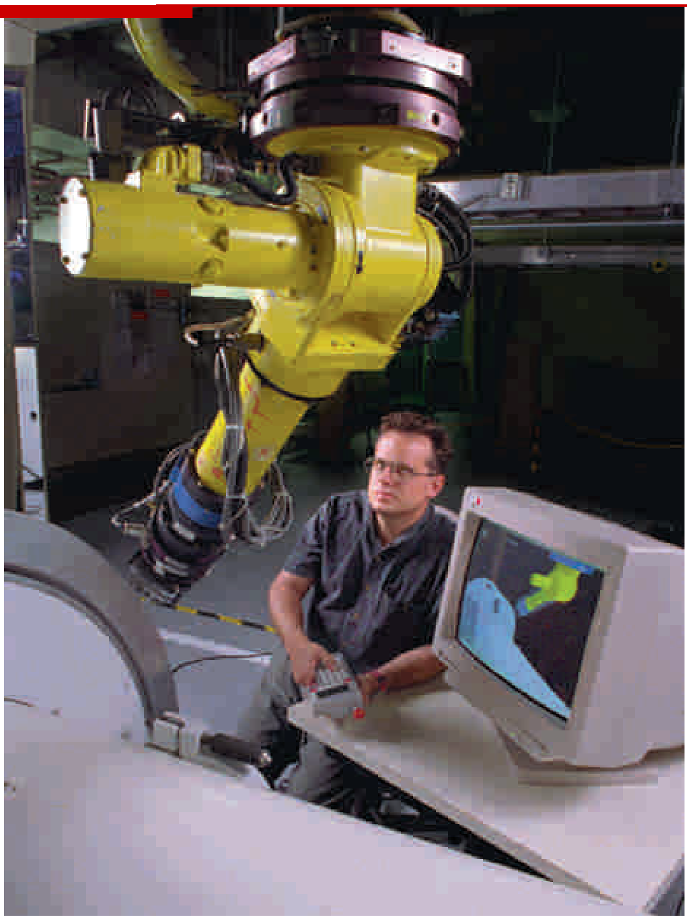
"It's a new way of looking at these resources," Clay said.

ASCI Partnerships & Large Applications
Putting Technology To WORK

The mission of weapons stockpile stewardship has driven Sandia advances in modeling and simulation. Research supporting this stewardship spans a broad area of complex physics with wide applicability both inside and outside the weapons complex, said Paul Hommert, director of Engineering Sciences Center.

Traditionally, engineers could not simulate in 3-D. "We had to make engineering judgments to go from 2-D to 3-D. Today, we go directly to 3-D," Hommert said.

"Through the kind of simulations that ASCI is enabling, we can more effectively embed a scientific understanding of how materials, components, and systems respond to various forces. We did this before, but what we produced involved significant approximations," Hommert added, comparing past technology to current simulation technology. "Now we can see how it reacts in very great detail, how each component responds. It's a huge enabler for science. It can bring science directly into the engineering decision." And this is just the beginning; computing power is expected to grow by another two orders of magnitude in the next decade.



Sandian Michael McDonald models the movements of a robotic system for remediating nuclear and hazardous waste. Modeling and simulation capabilities, designed to support nuclear stockpile stewardship, are revolutionizing manufacturing processes.

ASCI advances in modeling and simulation at Sandia have been driven by two factors: aging of the nuclear stockpile and the need to annually recertify the stockpile as safe, and to do so without actual testing. Today many of the resulting software codes are beginning to be applied outside the weapons complex. Since 1997, Sandia computer scientists have run simulations that demonstrate the broad potential for applications in other government agencies as well as in academia and industry. Utilizing ASCI technology in non-ASCI situations helps validate the usage of ASCI technology, and provides a good independent assessment of its effectiveness.

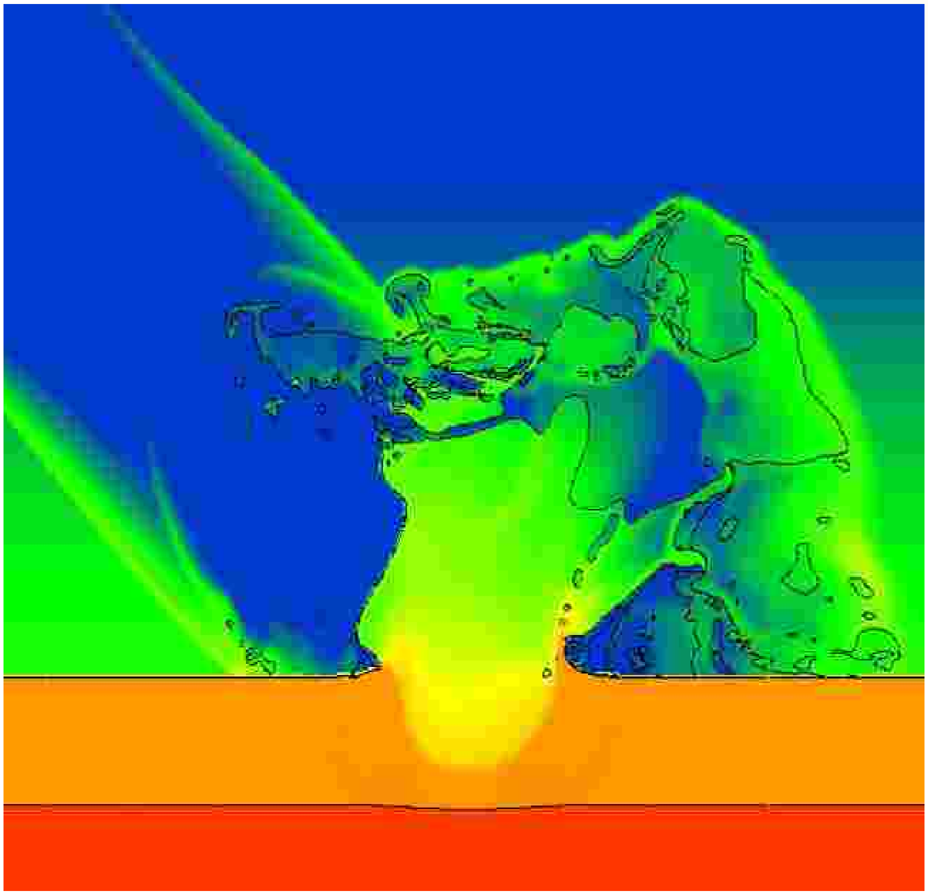
Bill Camp cites a Sandia simulation demonstrating the catastrophic effects of a comet one-half mile in diameter hitting the Atlantic Ocean at a 45-degree angle. This represented the first high-resolution, 3-D simulation of a comet hitting Earth and the first to show the progressive physical changes of air, water, and rock occurring simultaneously and interacting upon one another. These simulations are teaching us how such collisions have helped shape geology and even climate. Currently, scientists are investigating whether such collisions can explain sudden species elemination and even the onset of ice ages.

Working with the oil and gas industry, Sandia has used high-performance computing hardware and software also to solve problems such as how ocean currents affect offshore drilling. Modeling has been key to preventing serious environmental problems that can result if a fuel line breaks. Sandia has also developed advanced technologies to evaluate geologic profiles to locate gas and oil deposits that may be obscured by underwater land formations. The result is the ability to locate resources faster and more economically. These tools have been licensed to industry and are being used today.

Sandia is also working with DOE, NASA, and the National Oceanic and Atmospheric Administration to help develop models for climate studies.

A Sandia-developed virtual reality program allows law enforcement officers to practice freeing a hostage and disarming the captors in virtual reality.

But the best is yet to come, Hommert said. "In the past to bring science and technology to bear on a problem, you had only a few experts who could do it," he said. "Now in 10 years, we'll put the power of simulation into the broader base of engineering practice, into the hands of designers to solve problems in a virtual environment and do things never imagined before."



An early demonstration of Sandia's capabilities in using the teraflops computer was to simulate the effect of a comet hitting the Atlantic ocean. Above: Splashdown and the beginning of tidal wave formation.

Medical researchers are beginning to use simulation to develop more effective drugs and prosthetic devices as well as to track blood disorders and identify environmental carcinogens.

But the best is yet to come, Hommert said. "In the past, to bring science and technology to bear on a problem, you had only a few experts who could do it," he said. "Now in 10 years, we'll put the power of simulation into the broader base of engineering practice, into the hands of designers to solve problems in a virtual environment and do things never imagined before."

Here are some more recent Sandia projects and partnerships that show the expanding diversity of applications for ASCI technology:

• *Working with industry, Sandia has used high-performance computing codes, developed for stockpile stewardship, to define and make computational simulations of manufacturing processes.* The simulations create ever-finer detail, allowing designers to realize more exact duplications of an ideal design. Many early causes of failure have been eliminated, and designers can see how a modification will affect the entire manufacturing process or device. Also, simulation has led to developing manufacturing and performance improvements that have reduced the need to build costly, time-consuming prototypes.

Simulation capabilities that spin off from ASCI research make manufacturing processes occur faster and more cost-effectively. For instance, brazing two pieces of metal once required 100 hours to do calculations that can now be completed in less than one hour.

In learning how weapons react during accidents, Sandia is developing 3-D computer codes that simulate crash-and-burn scenarios. Although these codes are being developed for stockpile stewardship, they will also be valuable to industry, such as in exploring the dynamics of an automobile or plane crash, or in learning how fire spreads through a building. ASCI simulations could be used to help the building, automotive, and aircraft industries design safer products.

A fire code called FUEGO is being developed to predict the effect of fire on objects. "ASCI is developing this numerical simulation of fire because accidents involving fire pose one of the greatest threats to the safety and security of a nuclear weapon," said Sandia manager Carl Peterson. "Although the fire code is intended to support Sandia's nuclear stockpile stewardship mission, we believe FUEGO could be useful in dealing with a much broader set of fire threats that apply to personal, commercial, residential, and military safety issues."

The Nuclear Test Ban Treaty, still allowes tests for non-nuclear components. Above: a fire test subjects nuclear material shipping casks to a jet fuel fire.

solutions to tire and weapons mechanics problems that were previously intractable.

The partnership with Sandia has "greatly enhanced the chances of success by making it a win-win situation for both the lab and the company," said Goodyear Vice President of Corporate Research Nissim Calderon (recently retired). "Say Goodyear has a two-component project, A and B, while Sandia has another project characterized by A and C. Why not do A together and share the risk, share the effort, share the cost?"

• *Sandia advances in data-sorting are benefitting the business and communication sectors.* Compaq Computer Corp., the world's largest personal-computer supplier, and Sandia have teamed up to triple the speed of data-sorting techniques.

"Our joint work ... was driven by Sandia's need to process and visualize simulation data from other large, massively parallel computers, while Compaq's interest was the commercially important sorting application," said George Davidson, Sandia project manager.

Improved sorting capabilities should increase as large-scale data storage increases. By the year 2000, data storage is expected to reach 6.5 terabytes (up from 272 gigabytes in 1977) and by 2002 grow to a $113-billion market (up from $15 billion in 1977), according to the consulting firm the Palo Alto Management Group.

Ford is looking into applying the technology from Sandia crash codes in its automotive safety codes.

"It would allow us to complete simulations in a lot less time than alternative codes," said Alex Akkerman, Ford technical specialist in high-performance computing.

A consortium of manufacturers uses another Sandia code created to support the weapons mission by solving neutron-generator problems. The Coating and Related Manufacturing Processes Consortium (CRMPC) includes Avery Dennison Corp, Eastman Kodak, Imation Corp, 3M Co., Polaroid Corp., PPG Industries, Inc., Procter & Gamble, and Xerox Corp.

Sandia partners in developing simulations for manufacturing include the microelectronics industry, as well as Goodyear Tire and Rubber Co.

Hal Morgan, manager of Sandia's Engineering and Manufacturing Mechanics Department, said that for both Sandia and Goodyear, the research has resulted in reduced time and cost by applying simulation-based

"Say Goodyear has a two-component project, A and B, while Sandia has another project characterized by A and C. Why not do A together and share the risk, share the effort, share the cost?"

"Compaq, along with key partners like Sandia, is demonstrating that clustered Windows NT systems can deliver the performance, reliability, and cost-effectiveness required by high-end applications in technical and commercial markets. This ... demonstration is striking evidence of how far and how fast we've progressed," said Compaq Senior Vice President John Rose.

"Compaq, along with key partners like Sandia, is demonstrating that clustered Windows NT systems can deliver performance, reliability, and cost effectiveness required by high-end applications in technical and commercial markets."

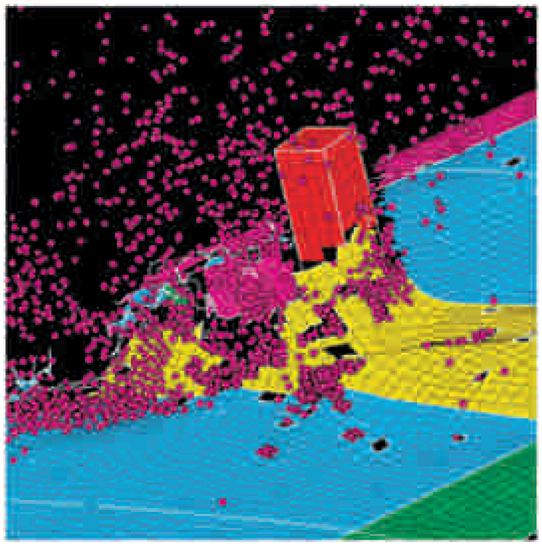
- *On-board diagnosis of automotive emissions represents another coup for ASCI technology.* Through a co-operative research and development agreement (CRADA), Sandia is working with members of an automotive consortium called USCAR and which includes Ford Motor Co., General Motors, and Daimler Chrysler Corp. New and pending regulations from the U.S. Environmental Protection Agency make the program of great importance to the industrial partners. USCAR estimates that the development of a successful on-board diagnosis system could gain a market share for the U.S. automotive industry of 10 percent in 10 years, producing an additional 250,000 jobs.

Sandia's contribution includes signal processing and data analysis, reliability modeling and risk analysis, life testing, failure analysis and risk reduction, test design, and software and human-factors engineering, and reliability studies.

Goodyear Tire and Rubber Co. has teamed up with Sandia to apply ASCI modeling technology to automobile tire design.

- *For the Federal Aviation Administration, Sandia analyses for aging aircraft are preventing disasters.* Delta Airlines is using a Sandia-developed laminate patch for sections of weakened aluminum on commercial jetliners, thus extending their useful lifespan. To ensure the airworthiness of the new patch, Sandia "tested" the laminate in simulations of the most stressful flight conditions. The simulations demonstrated that the bonded patch, which replaces riveted metal patches, would work. Computer models were also developed for enhanced study of future patch designs.

In addition, a variety of nondestructive inspection techniques were certified using computer modeling and simulation. Those techniques include ultrasonic, eddy current, and X-ray inspection to detect crack growth, disbonding, and delamination of patches. Sandia developed inspection procedures,



Modeling an aircraft wing hitting an object requires millions of elements, the interaction of which depends not only on one another, but also on potentially millions of variables. The teraflops computer made modeling this complex interaction possible.

which have been integrated into industry-approved maintenance practices.

• *Sandia scientists are working with physicians to develop 3-D computer imaging techniques that may in the future refine brain surgery techniques.* Magnetic resonance imaging (MRI) scans allow medical professionals to view specific features.

In an effort to provide surgeons with immediate data, Sandia is extracting and distilling data from MRI and processing them so they can be viewed using a conventional computer workstation.

Another innovation is the superimposition of 3-D computer models with video footage of the surgery as it takes place. The combined media may eventually help guide surgeons as they work.

• *New York's Metropolitan Museum of Art partnered with Sandia in 1997 to use computer modeling in producing a coating that increases the longevity of art and architecture,* as well as other structures by a factor of 10. Acid rain is making its mark on the national capital and elsewhere. Marble statues and the Pentagon building are just two examples of acid-rain victims. Sandia modeling has eliminated inefficient molecular arrangements in the laboratory tests, thus, greatly speeding up the research and reducing costs. These studies have used simulations of individual molecules as they bonded to the surface of, for example, a statue. The studies allow researchers to predict how protective selected coatings may be.

NEWS *Notes*

SANDIA DISCOVERY ABOUT PROTEINS MAY HELP CLEAN UP POLLUTANTS, FIND CURES FOR DISEASES

A discovery linking the shape of a unit called the heme in a protein to protein function may prove useful in a range of scientific advances, including finding cures for diseases and cleaning up pollutants, says discoverer John Shelnutt, a physicist at Sandia National Laboratories. The first time such a correlation has been made, the discovery is being heralded by the biochemical and biophysical communities as one of the most intriguing new findings about proteins in recent years.

Proteins strings of amino acids are found in all living cells and are where the work of a cell occurs. The heme, which consists of a ring of carbons and nitrogens, is the portion of a hemoprotein that clasps the protein's iron atom in place. A single protein may contain as few as one heme or as many as 10.

Before, people always thought the heme's primary function was to simply hold the iron in the protein so that the iron could carry out some biochemical reaction, Shelnutt says. They weren't aware that the heme acted as part of the protein machine and changed shape or even had shape.

Shelnutt's discovery was made possible by a new computer program that uses a mathematical procedure for characterizing the structure of hemes in terms of normal coordinates.

So far Shelnutt has used the program to study more than 400 existing protein crystal structures. And while he has identified some 70 different heme shape variations (called distortions), he has determined that only six are important for hemes in proteins including saddling, ruffling, doming.

Shelnutt believes that his discovery might lead to changes in the way diseases are treated in the future or for other scientific advances. In collaboration with a French scientist, he is already using his knowledge to develop new anti-inflammatory drugs.

Another possibility is to understand how hemes from another protein Shelnutt is working with convert sulfites or nitrites, (common pollutants), into hydrogen sulfide or ammonia. Then, analogous arrangements of hemes could be chemically engineered, produced in batches, and released to clean up waste sites.

The revelation that heme shape is correlated to a protein's function is so new that we don t yet know where this knowledge can take us, Shelnutt says. We have a new key to better understand life and now we have to figure out what to do with it.

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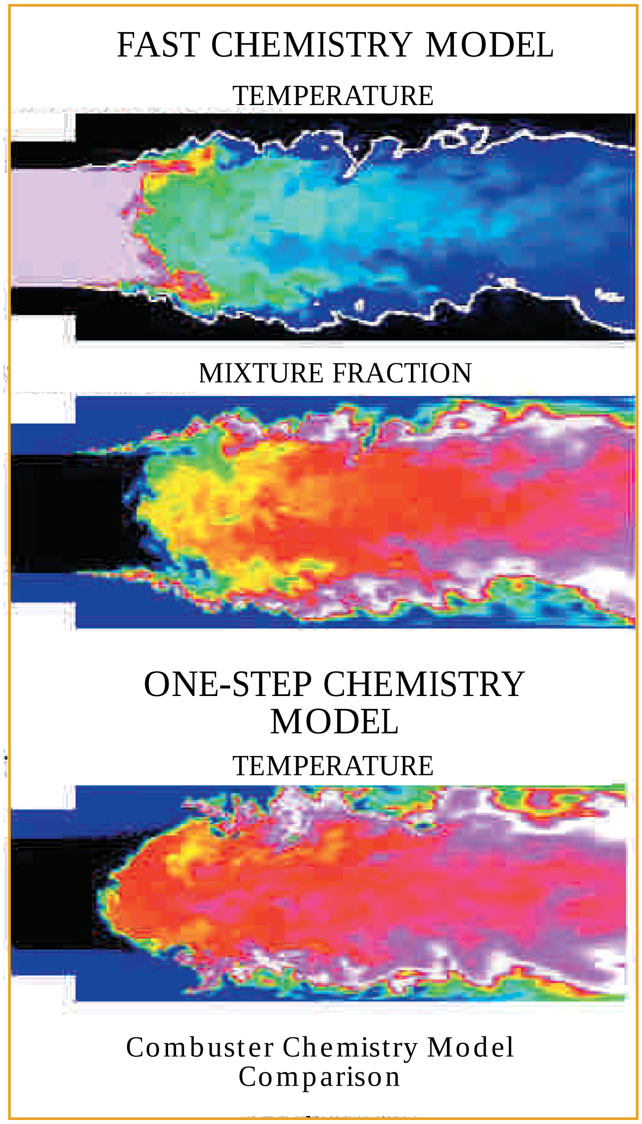
Five Universities Team with Sandia in Tri-Lab Plan to Gain PRECISE SIMULATION RESEARCH

Computer simulations of nuclear flashes in space, accidental fires, and rocket explosions are among those being developed by five U.S. universities in a unique alliance with the three Department of Energy Defense Program laboratiories – Sandia , Lawrence Livermore , and Los Alamos national laboratories.

The alliance is a key element in ensuring the goals of the Accelerated Strategic Computing Initiative (ASCI) are met.

"We're finding many pleasant surprises that are very interesting to us. As the universities conduct their research, they have things pop up unexpectedly that could be useful tools for us," said Charles Hartwig, who represents Sandia in ASCI's Academic Strategic Alliances Program (ASAP), a tri-lab effort with the DOE.

"Among those surprises these are turbulence modeling in aircraft-engine simulations, and the chemistry of radiation in soot from fires", said Hartwig, senior manager in Sandia's Materials and Engineering Sciences program.



Computer simulations depicting flame development

Sandia is working with these universities in the following research areas:

1) California Institute of Technology: performance and failures of engineered components that incorporate high explosives; and mechanism failures as well as material performance under high dynamic mechanical loads.

2) Stanford University: fluid mechanics in fires and chemistry dealing with combustion, performance modeling of the turbomachinery, and combustor in gas turbine eingines used for aircraft.

3) University of Chicago: the spread of fires, heat transfers, and computational tools; extra-terrestial nuclear flashes, including supernovae.

4) University of Illinois at Urbana-Champaign: propellant fires, how propellants respond in different situations, and real-time data extraction tools; and the performance and potential failures of solid propellant rockets.

5) University of Utah: the physics in turbulence, magnetohydrodynamics (MHD) solvers, and numerical capabilities to solve differential equations; the ignition, spread, and consequences of accidental fires.

The universities are focusing on visualization and data rendering, algorithms, and computational architecture for a five-year program. The DOE provided each university with $3 million for the first year and will fund each university $3.5 to $5 million annually for the remainder of the program.

The Academic Alliance was formed primarily to—

1) Train students in computational multidiscipline methodology

2) Apply the use of high-performance computing to solve complex problems, thereby providing independent assessment of a computational approach to problem solving

3) Provide a formal mechanism for university and lab interactions.

"There is great connectivity between the labs and the universities. We were concerned about how quickly they

While the alliance is proving to be a success, it is posing challenges and ensuring national security is never compromised.

would come up to speed, but we've been pleased with their performance," Hartwig said. "It has been great to see each university work together as a single team without any turf (battles). For example, we've got mathematicians, chemical engineers, and computational scientists all working together on the milestones."

While the alliance is proving to be a success, it is posing challenges in ensuring national security is never compromised.

"We've had to address in real-time the legal and national security issues, while enabling the universities to respond," said Hartwig. "It has created difficulties. Universities want to do the right thing, but they understand our role. However, they ask whether their full set of faculty can participate in the program."

Hartwig noted that up to 50 percent of the university graduate students and faculty within the alliance are foreign nationals.

Foreign nationals cannot compute on the ASCI Red machine. U.S. citizens at each of the ASCI alliance centers working on unclassified computing problems have access to the machine. Hartwig said the security issue centers on export-control restrictions for foreign nationals. Policy is being developed to deal with resident aliens' use of the machine, he said.

NEWS *Notes*

Sandia National Laboratories and the University of Montana are trying to determine whether foraging bees can detect buried landmines. In the foreground are two unused antitank mines.

RESEARCHERS TRAINING BEES TO FIND BURIED LANDMINES

Bees dutifully going about their daily business gathering nectar and pollen and taking it back to the hive may one day help protect the lives and limbs of people if a landmine-detection demonstration at Sandia National Laboratories is successful. Sandia chemists are working with entomologists at the University of Montana to see if foraging bees can reliably and inexpensively detect buried mines and safely return hundreds of thousands of acres of uncharted land back to productive use. The work is funded by the Defense Advanced Research Projects Agency's (DARPA) Controlled Biological Systems Program.

In the bee demonstration, Sandia is working with Jerry Bromenshenk at the University of Montana, Missoula, to see if bees can be trained to find residues of TNT, the primary ingredient of most landmines, and bring the evidence home.

The project builds on three decades of explosives-detection work at Sandia and 25 years of biosystems research at the University of Montana.

Bromenshenk and his colleagues have shown that as bees forage for nectar and pollen, they attract particles of dust, soil, and pollen to their fuzzy, statically charged bodies and bring samples back to the hive. All landmines leak small amounts of explosives into nearby soil or water.

We are conducting new studies to see if plants rooted in TNT-tainted soil will uptake the residues into their roots, stems, and flowers, and even incorporate them into their pollens, says Sandian Susan Bender. If plants that readily accumulated the TNT could be identified, a suspected minefield could be seeded with those plants (by air) to maximize the bees' chances of finding the mines. One goal of ongoing tests at Montana is to determine which explosives bees can smell and then train them to seek those chemicals.

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Don Cook, former director of Pulsed Power Sciences at Sandia National Laboratores, with the Z machine.

ASCI's Pulsed-Power Studies Help Validate Computer Models

One important outgrowth of the Accelerated Strategic Computing Initiative (ASCI) is validation experiments (that is, tests that can determine if simulations are accurate) that use pulsed-power machines. For example, the Z-machine and Saturn are powerful X-ray generators that are used to learn the effects of high-level radiation on materials. To support weapon-safety certification, Sandia uses findings from pulsed-power machines to develop ASCI modeling and simulation codes.

"Testing on the Z machine provides us with a valuable tool in figuring out what materials will survive high-radiation exposures," said Sandia researcher Christine Coverdale.

This knowledge is being applied to upgrading components and subsystems in aging weapons. Tests on pulsed power machines allow better understanding of failure mechanisms and thresholds. Thus, researchers can choose materials that are more reliable.

"Testing on the Z machine provides us with a valuable tool in figuring out what materials will survive high-radiation exposures."

"If our findings are close to the computer modeling of the same event, it means the modeling is on track, giving us more confidence in what the model is telling us for regimes that we can't test," said Sandian Chris Deeney, a Sandia scientist.

A pulsed power accelerator, the Z machine consists of capacitors, which act like large batteries charged with electricity.

The Z machine makes frequent breakthroughs in energy generation. The most recent record was 100 kilojoules (a measure of radiated energy) of high-energy radiation,thus further enabling weapons testing that could not be conducted since the Nuclear Test Ban Treaty stopped underground nuclear tests in 1996.

Other advances using the Z machine support development of fusion (the kind of energy that the sun and other stars produce) as an energy source.

Recent experiments represent a collaboration between various Sandia organizations and others within the nuclear weapons community. Experiments are sponsored by the Defense Threat Reduction Agency for the Department of Defense.

Notes

AMERICAN AND RUSSIAN NUCLEAR LABS HELP DEVELOP ARTIFICIAL KNEE FOR LANDMINE VICTIMS

In a unique arrangement, Sandia National Laboratories and the Russian laboratory known as Chelyabinsk 70 in Snezhinsk, about 900 miles southeast of Moscow, are jointly developing technologies for foot and knee prosthestics. The labs are working with Ohio Willow Wood Company, which will define the requirements for parts and perform final laboratory and clinical testing.

The project to develop an artificial knee is supported by a $1.4 million cooperative research and development agreement (CRADA) from the Department of Energy's Initiatives for Proliferation Prevention Program.

The Russians will design a titanium housing, and Sandia robotics researchers Mark Vaughn and Dave Kozlowski will design the knee s internal workings and electronics. Sandia and the Russian nuclear lab will split their half of the funding.

"This work will have many benefits," says Sandia chemist and project leader Mort Lieberman, who will also manage the Russian connection. "Someone in this world loses a limb to a landmine explosion every 20 minutes. Our work, though only remedial, will help landmine survivors and other amputees."

The first collaboration between the two labs to develop an artificial foot has reached the stage where the devices have been experimentally affixed to willing amputees.

The new project will draw upon Sandia's electronic expertise and Russian materials knowledge to create, respectively, the brains and shape of the knee.

The work is a good fit with the capabilities of both labs, says Lieberman. It involves stress analysis, mechanical testing, reliability testing, microprocessor control, and materials analysis. A knee must be able to vary the speed of its response. Then it needs to lock so that its wearer doesn't fall when standing. The knee is not simply a hinge, says Lieberman. If it were only that, it might swing back too far or not enough, letting the foot hit the ground too soon and causing its wearer to trip.

One version of a modern mechanical polycentric knee. It weighs 1.37 pounds and is 4.12 inches high.

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IMPROVED ON-LINE MEDICAL ARCHITECTURE TO THWART HACKERS, LOWER HEALTH-CARE COST

People worry that their credit card numbers will be intercepted online to finance the purchases of strangers. Another problem is the potential for hackers to access and misuse medical or psychiatric data, whether in transit or stored online.

People with long-term diseases like diabetes, or even those only genetically predisposed to them, could face job turndowns and insurance rebuffs if information stolen from data banks were sold to corporate bidders. Patients relying upon intravenously delivered medicine, remotely controlled, could have their lives threatened by a cyber attacker altering their medicinal flow rate.

Researchers at Sandia National Laboratories have developed and applied for an intellectual property patent on a computer architecture that incorporates built-in security mechanisms to protect information sent between medical system components. Rather than relying on turn-key systems, the framework encourages hospitals and individual patients to buy and assemble off-the-shelf medical equipment the same way home stereo components are bought individually and assembled. Competition between suppliers of subcomponents should lower prices and rescue consumers from the need to buy all the features manufacturers of entire systems might incorporate.

Sandia researchers are interested in the storage and transmission of medical information because they believe that the capability to use the Internet will substantially aid the potentially large numbers of civilian casualties that could be expected from a natural disaster or terrorist event.

Equipment complying with the Sandia architecture will be used at New Orleans Alton Ochsner Medical Foundation in the care of patients suffering from hypertension. The formal clinical tests, conducted over the next eight months, will be used in part to evaluate the cost-effectiveness and diagnostic feasibility of telemedicine in this arena.

The research team at Ochsner Clinic is currently using a commercial, turn-key telemedicine system manufactured by TelAssist Corporation, Ridgefield, N.J., for its hypertension study. Sandia, in an effort to test the effectiveness of the plug-and-play approach to telemedicine, is renovating that commercial system for use on Sandia's secure telemedicine device architecture. The new system will be tested jointly by Sandia and Ochsner Clinic in a controlled clinical study that assesses the cost-effectiveness and diagnostic feasibility of the approach.

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INSIGHTS

by Gil Weigand, Deputy Assistant Secretary, Defense Strategic Computing & Simulation, U.S. Department of Energy

The creation of advanced simulation technologies is well under way, with 3 teraflops supercomputers already on line

Gil Weigand, Deputy Assistant Secretary, Defense Strategic Computing & Simulation, U.S. Department of Energy

ASCI program is creating leading-edge computational modeling and simulation capabilities

The aging of our nuclear weapons stockpile, resulting from the end of the Cold War and halt in design and production of new weapons, has brought exciting challenges to the Department of Energy's Office of Defense Programs. Our task, as directed by the president, is to maintain a safe, secure, and reliable nuclear weapons stockpile without further underground nuclear testing.

We are meeting those challenges through science-based stockpile stewardship, using computer simulations combined with experimental data from the subcritical experiments at the Nevada Test Site, the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory, the Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos National Laboratory, the Z-Machine at Sandia and other non-nuclear tests, surveillance activities and experiments, combined with archived data from U.S. nuclear tests, to assess and certify the stockpile.

The scientists and engineers at the defense laboratories and plants are vital to the success of stockpile stewardship. Their ability to certify the stockpile in new ways, using new tools approaches, will determine whether or not we will ultimately succeed.

I have been involved with high-performance computing and advanced simulation since my early career at Sandia National Laboratories. My advocacy of the role I felt computers could ultimately play, first at the Department of Defense and now at the Department of Energy, helped lead to development of the Accelerated Strategic Computing Initiative (ASCI).

On schedule for the goal of 100-trillion operations per second (100 teraflops) by 2004, the ASCI program is creating leading-edge computational modeling and simulation capabilities critically needed to: promptly shift from nuclear test-based methods to computation-based methods, integrate stockpile stewardship elements and provide an integrated nuclear explosion testbed, and extend modeling and simulation technologies to virtual prototyping and aging.

The creation of advanced simulation technologies is well under way, with 3 teraflops supercomputers already on line at Sandia, Los Alamos and Lawrence Livermore national laboratories. Working with the U.S. computer industry, these supercomputers were built far ahead of commercial development time frames.

These supercomputers are being used to run codes that, when fully developed, will be able to simulate nuclear weapon performance at levels of detail previously unattainable, even with nuclear testing, and with comparable confidence. Data visualization corridors at Sandia, Los Alamos, and Lawrence Livermore national laboratories are already capable of visualizing and exploring data and simulations with incredible detail and speed, putting the tools necessary to meet stockpile stewardship goals into the hands of scientists and engineers today.

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