January/February 2005

Science & Technology Review

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Supercomputer Simulations Advance Science

Also in this issue:

- Jobs for Russian Weapons Workers
- New Facility for Today's and Tomorrow's Supercomputers
- Extracting Marketable Minerals from Geothermal Fluids

About the Cover

Livermore scientists use powerful machines and codes for computer simulations that have changed the way science is done at the Laboratory. As the article beginning on p. 4 describes, computer simulations have become powerful tools for understanding and predicting the physical universe, from the interactions of individual atoms to the details of climate change. For example, Laboratory physicists have predicted a new melt curve of hydrogen, resulting in the possible existence of a novel superfluid. The cover illustrates the transition of hydrogen from a molecular solid (top) to a quantum liquid (bottom), with a "metallic sea" added in the background.

Cover design: Amy Henke

About the Review

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

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Science & Technology REVIEW

January/February 2005

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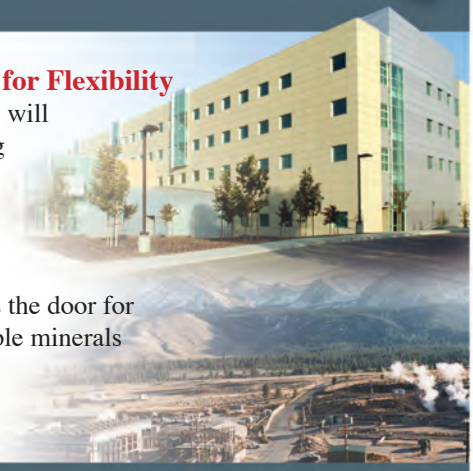

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Record-breaking supercomputing performance

On November 4, 2004, Department of Energy (DOE) Secretary Spencer Abraham announced that a supercomputer developed for the nation's Stockpile Stewardship Program (SSP) has attained a record-breaking performance of 70.72 trillion operations per second (teraops) on the industry standard LINPACK benchmark. Although the supercomputer is running at one-quarter its final size for DOE, the BlueGene/L beta system is already asserting U.S. leadership in supercomputing. The product of a multiyear research and development partnership between DOE's National Nuclear Security Administration and IBM, BlueGene/L will support the SSP's mission to ensure the safety, security, and reliability of the nation's nuclear weapons stockpile without underground nuclear testing.

Secretary Abraham, who has since stepped down, said, "The delivery of the first quarter of the Blue/GeneL system to Lawrence Livermore this month shows how a partnership between government and industry can effectively advance national agendas in science, technology, security, and industrial competitiveness. High-performance computing is the backbone of the nation's science and technology enterprise, which is why the department has made supercomputing a top priority investment. Breakthroughs in applied scientific research are possible with the tremendous processing capabilities provided by extremely scalable computer systems such as BlueGene/L."

The final BlueGene/L system will exceed the performance of the Japanese Earth Simulator by a factor of about nine while requiring one-seventh as much electrical power and one-fourteenth the floor space.

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Genome reveals role in mediating global warming

The DOE Joint Genome Institute (JGI) has generated the first genetic instruction manual for a diatom. The diatom belongs to a family of microscopic ocean algae that are among Earth's most prolific carbon dioxide assimilators. This work, published in the October 1, 2004, issue of *Science,* has yielded insight on how the creature *Thalassiosira pseudonana* absorbs the major greenhouse gas carbon dioxide in amounts comparable to all the world's tropical rain forests combined. Don Rokhsar, one of the coauthors and head of computational genomics at JGI, says, "Now that we have a glimpse at the inner workings of diatoms, we're better positioned to understand the role they and other phytoplankton play in mediating global warming."

Virginia Armbrust, a University of Washington associate professor of oceanography and the paper's lead author, says that the growth of single-cell diatoms accounts for as much as 40 percent of the 50 to 55 billion tons of organic carbon produced each year in the sea. The diatoms are just 3 or 4 micrometers wide and are encased by a frustule, a rigid cell wall delicately marked with pores in patterns distinctive enough for scientists to tell the species apart. "We discovered they have a urea cycle, something no one ever suspected," says Ambrust. A urea cycle is a nitrogen waste pathway that has been found in animals but has never before been seen in a diatom. Nitrogen is crucial for diatom growth and is often in short supply in seawater.

Forty-six researchers from 26 institutions are working on the project, including four from Livermore.

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Agreement to develop an artificial retinal device

A consortium of DOE national laboratories, including Livermore, and universities has signed an agreement with Second Sight Medical Products, Inc., to jointly develop technology that could restore sight to those who have lost their vision later in life. The Cooperative Research and Development Agreement allows Second Sight of Sylmar, California, to obtain a limited exclusive license for inventions developed during the DOE Retinal Prosthesis Project.

Attached to and functioning as part of the eye's retina, the retinal prosthesis device promises hope for those with age-related macular degeneration, retinitis pigmentosa, or related diseases where photoreceptors are damaged but the optic nerve and its connections to the brain are still intact. Engineers from Livermore's Center for Micro and Nanotechnology are developing a flexible silicone-based microelectrode array. The implantable retinal prosthesis is based on a system that converts a video camera signal into a simulation pattern. This pattern can then be applied directly to the intraocular retinal surface. (See *S&TR,* November 2003, pp. 11–13.)

Although the device will not restore full vision, it is expected to provide enough optical resolution for patients to read and recognize fine shapes. The Laboratory's pioneering use of polydimethlsiloxane (PDMS) allows the microelectrode array to conform to the curved shape of the retina. Courtney Davidson, Livermore's principal investigator, says, "PDMS is biocompatible, which makes it a good candidate material for long-term implants."

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Commentary by Dona Crawford

A Passion for Computation Benefits Every Discipline

IT'S no secret that computers are in Lawrence Livermore's blood. That passion for computation was one of the principal factors that brought me to Livermore three years ago to become associate director of Computation. Livermore's research is invariably accomplished with the aid of computers, which include the most powerful supercomputers available. Our reliance on computers to simulate the physical world started at the Laboratory's founding in 1952, and computational excellence is a major reason for our continued success as one of the world's preeminent scientific research institutions.

Supercomputer simulations allow us to understand the intricacies of physical phenomena that occur at vanishingly short time scales and at extreme pressures and temperatures. Sometimes, an experiment cannot be conducted because it is too costly, too difficult to perform or diagnose, or involves toxic materials. The computer, in effect, serves as a virtual laboratory, one whose experimental results point to scientific "truth" as effectively as other means. Physical experiments and computational simulations often complement one another, in that physical experiments validate computational simulations, and simulations aid in the design of laboratory experiments.

During the 1970s and 1980s, as computer processing power continued to increase, Livermore researchers anticipated the intrinsic role of sophisticated, three-dimensional simulations. Indeed, Livermore first coined the phrase, "Simulation is a peer to theory and experiment." However, we have not yet fully arrived. The Department of Energy's (DOE's) Stockpile Stewardship Program is leading the way because, as a matter of national policy, the U.S. does not conduct underground nuclear weapons testing to learn about the performance of nuclear warheads in our stockpile. Rather, researchers use the world's most powerful supercomputers to help characterize nuclear reactions and the aging of materials. Working on stockpile stewardship pushes us to develop new computer codes, better simulation methods, and improved visualization technologies. It also sets the requirements for new generations of machines. The resulting capabilities, in turn, are applicable to other disciplines.

As the article on p. 4 describes, many Livermore research areas, such as chemistry, materials science, climate change, and physics, also have been among the leaders in taking advantage of supercomputers to advance their fields. Other disciplines, such as the biological sciences, do not yet leverage supercomputers to such an extent. However, DOE's Human Genome Project demonstrated the power of computers in biological research. Follow-on efforts, including those describing the shape and function of proteins, can only be performed with the help of powerful simulation tools.

The competition to produce or acquire the fastest or most capable supercomputer keeps everyone sharp and raises the bar for the entire high-performance computing community. Although we avidly participate in that competition, it is important not to lose sight of why we find these computers essential. We acquire the world's most powerful machines to strengthen national security and to advance our understanding of the physical world.

To continue to provide robust computational resources to our scientists and engineers, we look for emerging technologies that can offer increased power at lower cost. The new supercomputer Purple is a very robust, massively parallel system that will have a peak performance of 100 trillion operations per second (teraops). Purple was built by IBM and will be in operation at Livermore later this year. In 2004, we installed Thunder, a cluster of standard desktop microprocessors running the Linux operating system and capable of 23 teraops. Use of Thunder can be somewhat risky for some projects, but it offers enormous potential for reducing costs and compute time.

Another computer from IBM, BlueGene/L, will eventually be capable of 360 teraops. We call its design "disruptive" because it uses 131,072 commercial microprocessors to achieve unprecedented computing power. Clever packaging allows the machine to use less floor space and consume less energy than previous computers.

BlueGene/L still will not be powerful enough to simulate all the complexities of matter at extreme pressures and temperatures, so we look to acquire a petaops (1 quadrillion operations per second or 1,000 teraops) supercomputer by 2010. The JASONs, a prestigious advisory committee to DOE, validated our need for such a machine.

Will Livermore and DOE scientists be satisfied with the astonishing capability of the petaops? Not likely. Solving grand challenge scientific problems will continue to require ever faster and more capable supercomputers. We look forward to continuing to meet that need.

■ Dona Crawford is associate director of Computation.

Experiment and Theory

Supercomputer simulations have become essential to making discoveries and advancing science.

EVEN before Lawrence Livermore opened in September 1952, cofounders E. O. Lawrence and Edward Teller recognized the need for a computer and placed an order for one of the first production Univacs. Equipped with 5,600 vacuum tubes, the Univac had impressive calculational power for its time, although much less than that contained in today's $5 calculator. Computing machines quickly demonstrated to the Livermore staff the ability not only to perform complicated calculations but also to simulate physical processes.

A computer's predictive capabilities were vividly demonstrated in 1957, when the Laboratory received an urgent call from the Pentagon. Livermore had the only U.S. computer able to compute the orbit of Russia's Sputnik I. Researchers accurately predicted the satellite's plunge into the atmosphere in early December of that year. In time, they showed how computer simulations could lend insight into a broad range of physical problems.

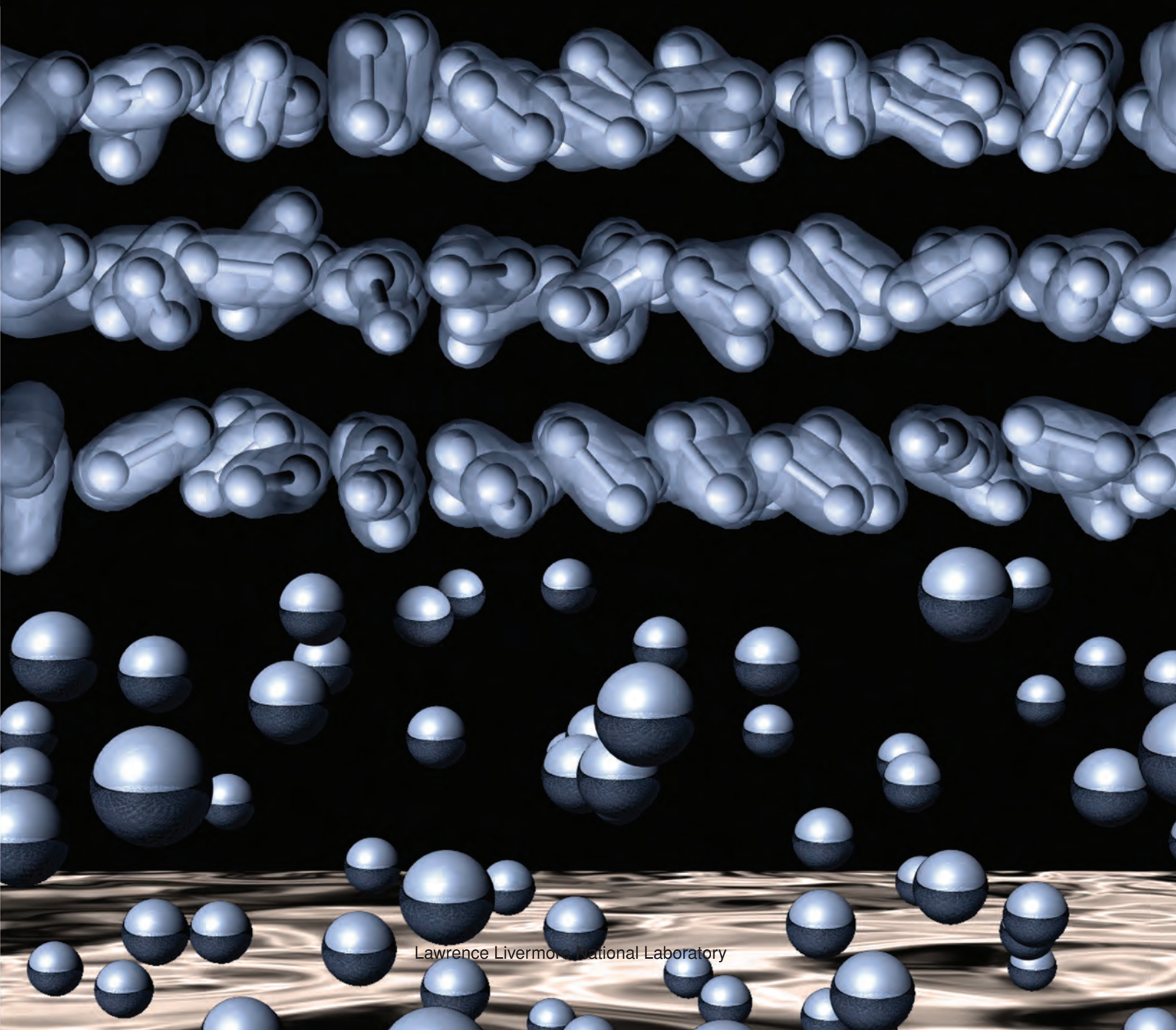
"No institution in the world has more consistently invested in new generations of supercomputers than Livermore," says physicist Tomás Díaz de la Rubia, associate director of Chemistry and Materials Science. During the past five decades, supercomputers have advanced every discipline and have helped to attract some of the brightest minds to the Laboratory. Díaz de la Rubia, for example, was drawn to Livermore in 1989 because of the opportunity to work on the world's most powerful computer (at the time, made by Cray Computer) and with some of the nation's top simulation experts.

Researchers haven't been shy about tapping the increased power of a new machine. "Every new machine has brought new insight," says physicist Francois Gygi of Livermore's Center for Applied Scientific Computing.

"Simulation has changed the way science is done at Livermore," says computer scientist Mark Seager, head of Platforms in the Integrated Computing and Communications (ICC) Department, part of the Computation Directorate. "Today, experiment and simulation are more tightly coupled than ever. At the same time, theory and computation are more tightly coupled than ever."

Laboratory scientists have predicted a new melt curve of hydrogen, resulting in the possible existence of a novel superfluid—a quantum fluid at about 400 gigapascals. This figure illustrates the transition of hydrogen from a molecular solid (top) to a quantum liquid (bottom), which was simulated using Livermore's GP ab initio molecular dynamics code. A "metallic sea" is shown in the background.

Have a New Partner: Simulation



Simulations mimic the physical world down to the interactions of individual atoms. These simulations, conducted on some of the world's most powerful supercomputers, test theories, reveal new physics, guide the setup of new experiments, and help scientists understand past experiments. Many times, the simulations conduct electronic "experiments," replicating scaled models of experiments that would be too difficult or expensive to perform or would raise environmental or safety issues.

ASC Leads the Way

For the past decade, the driving force behind increasingly realistic simulations has been stockpile stewardship, which is the Department of Energy's (DOE's) National Nuclear Security Administration (NNSA) program to ensure the safety and reliability of the nation's weapons stockpile. A major element of stockpile stewardship is the Advanced Simulation and Computing (ASC) Program, which had an initial 10-year goal to obtain machines that could run simulations at 100 trillion operations per second (teraops). To meet this requirement, ASC spearheaded a transition during the mid-1990s to scalable parallel supercomputers composed of thousands of microprocessors that solve a problem by dividing it into many parts.

Since 1996, proprietary scalable parallel supercomputers running vendor-supplied system software have been used to simulate the physics of nuclear and chemical reactions. ASC's Purple machine will arrive at Livermore in July 2005. Purple will fulfill the goal set in 1996 to achieve 100 teraops by mid-decade for prototype full-system stockpile stewardship simulations.

In addition to ASC scientists, researchers working in almost every other program at Livermore need to run unclassified simulations on ASC-class supercomputers. The Multiprogrammatic and Institutional Computing (M&IC) Initiative has made this class of platform available to a wide spectrum of scientific investigators at Livermore since the mid-1990s. Most recently, the M&IC platforms have been deployed using Linux cluster technology. (See *S&TR*, June 2003, pp. 4–13.)

M&IC is so named because it serves both mission programs (multiprogrammatic) and individual (institutional) researchers. A mission program can purchase a block of time on existing machines and share in the investment in new equipment. In addition, M&IC grants Livermore scientists engaged in leading-edge research access to computer time, independent of the program to which they belong. Researchers who are funded by Livermore's Laboratory Directed Research and Development (LDRD) Program, an institutional sponsor of individual researchers pushing the state of science in diverse fields, have significant access to M&IC machines.

Seager recalls, "We mounted an effort in the late 1990s to bring large-scale supercomputing to non-ASC scientists by leveraging everything we learned from using ASC machines and developing codes for them." Over the years, he says, the NNSA-funded ASC Program

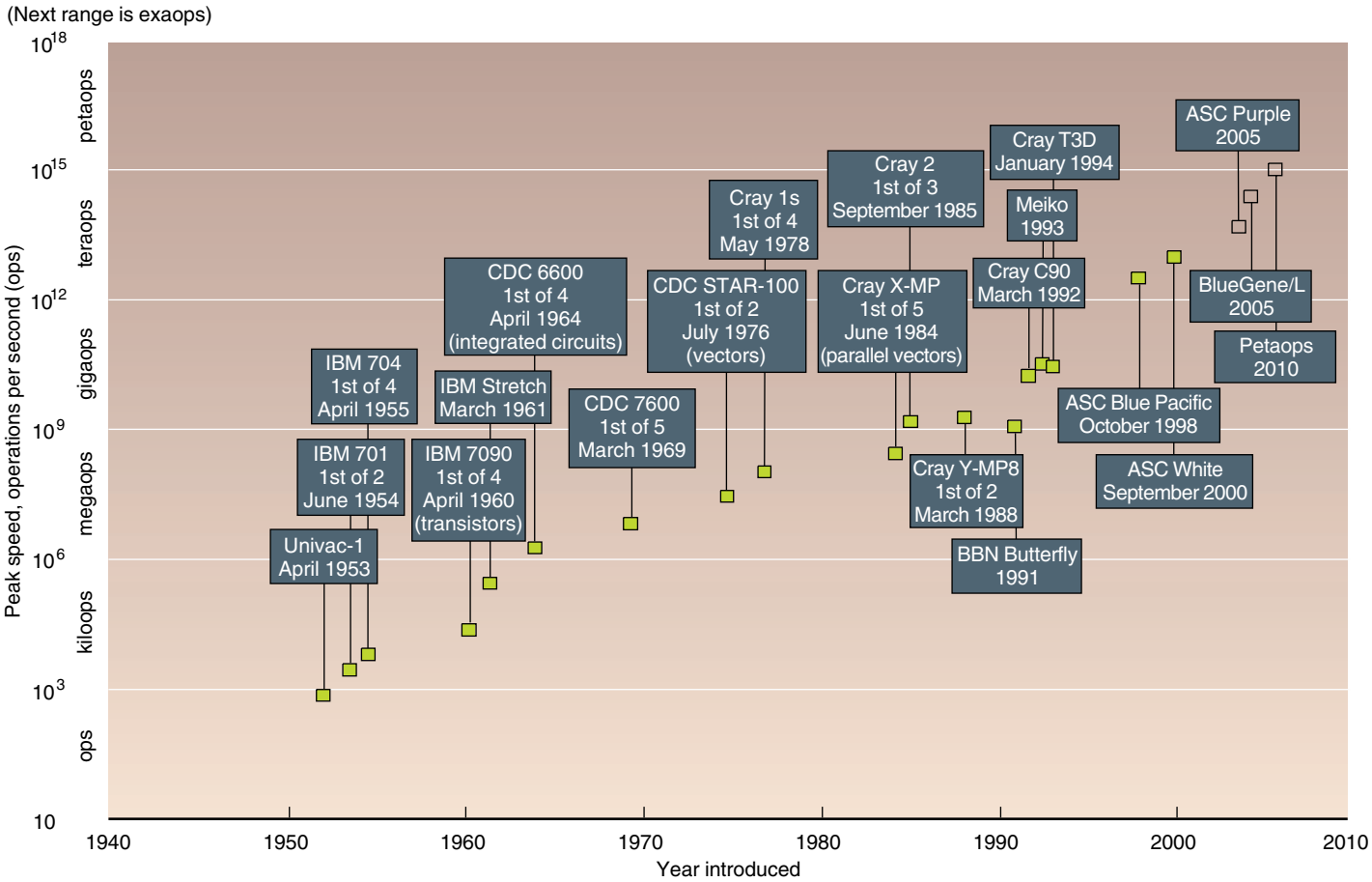
The White supercomputer is a current "workhorse" of the National Nuclear Security Administration's Advanced Simulation and Computing (ASC) Program, performing 12.3 billion operations per second (nearly 31 billion times faster than Livermore's first supercomputer). Another ASC supercomputer, Purple, is scheduled for demonstration in June 2005 and delivery to Livermore in July 2005. Purple will have a peak performance of 100 trillion operations per second (teraops) and, as with White and the other ASC machines, will be dedicated to research for the nation's nuclear stockpile. (inset) Livermore's first supercomputer, the Remington-Rand Univac-1, was delivered in 1953. It had over 5,600 vacuum tubes and a memory that could store 9 kilobytes of data—a fraction of what today's handheld devices can hold.

and the institutionally funded M&IC Initiative have cooperated and leveraged their cumulative expertise. For example, unclassified simulations for stockpile stewardship–related projects run on M&IC machines.

Bruce Goodwin, associate director for Defense and Nuclear Technologies, notes, "Livermore has pioneered the development of a cost-effective, terascale Linux cluster technology that provides the high-performance computing environment required by the weapons program." The unclassified computers, Goodwin points out, are an essential part of Livermore's strategy to provide computing for both weapons science and weapons simulation. "As Linux cluster technology continues to advance, we expect it to help shoulder our most demanding requirements as well as more routine uses."

When acquiring new machines for unclassified research, the developers of the M&IC Initiative took a different approach from the ASC Program beginning in 2000. At the time, in what appeared to be a bold gamble to acquire and run supercomputers at much less cost, Livermore assembled Linux clusters, composed of commercial microprocessors running on the open-source Linux operating system. The results were so impressive that other institutions, from universities to

Thunder, the latest of the Multiprogrammatic and Institutional Computing (M&IC) Initiative's Linux clusters, is composed of commercial microprocessors running on the open-source Linux operating system and cluster software. The 23-teraops Thunder machine runs simulations for scientists from a broad range of scientific disciplines.



A timeline shows Livermore's key supercomputers and their peak computing power.

corporations, followed Livermore's lead. Today, Linux clusters make up more than one-half of the nation's top-performing supercomputers.

Livermore's Linux clusters range from small platforms, such as the Intel Linux Cluster and Compaq GPS Cluster, that run one-dimensional (1D) codes useful for initial research, to the much more powerful 11-teraops Multiprogrammatic Capability Resource (MCR) and 23-teraops Thunder machines that run 3D codes for ASC-class simulations. MCR and Thunder will be joined later this year by ASC's computational science research machine: BlueGene/L (at 360 teraops).

BlueGene/L is under construction by IBM and recently took over the title of the most powerful supercomputer in the world from the Japanese Earth Simulator. When fully assembled at Livermore in June 2005, the 131,072 microprocessors of BlueGene/L will drive the next generation of simulation codes to advance stockpile stewardship on a path toward petascale (a quadrillion operations per second) computing.

The simulations on MCR and Thunder benefit many scientific disciplines, such as laser physics, materials science, computational biology, computational physics, and astrophysics. "The breadth and scope of applications are amazing," says Seager.

Making New Science Possible

"The real story is not about the machines but about advancing science," says Brian Carnes, who leads the Services and Development Division in ICC. "Simulations on both ASC and M&IC machines are showing insights and proving new things."

For example, geologist Lew Glenn is using the MCR machine to do fundamental research on damage to large underground structures subjected to shock waves or explosives. "We have developed codes that analyze the behavior and simulate the response of the structures. These codes require the scalable parallel-computing platforms of M&IC," says Glenn.

Large seismic modeling efforts at Livermore include earthquake hazards, oil exploration, nuclear nonproliferation, underground-structure detection, and nuclear test readiness. Geophysicist Shawn Larsen says, "Without M&IC, a significant number of seismic modeling efforts in multiple directorates would not have been initiated and conducted." In addition M&IC has aided in collaborative research at external institutions. For example, he notes, several University of California graduate students, postdoctoral researchers, and faculty owe much of their research to the computers' availability.

Researchers in Livermore's Biology and Biotechnology Research Program Directorate are using supercomputers to solve biochemical problems related to human health and national security. Projects include designing anticancer drugs, developing detection systems for protein toxins, and investigating the mechanisms of DNA repair and replication. The simulation work includes molecular dynamics software that mimics how individual atoms interact. "We use M&IC computers for simulations that will not fit on our own modest workstations," says biomedical researcher Mike Colvin. "These computers have been crucial to our scientific progress, which has led to dozens of publications in peer-reviewed literature, invited talks, and external collaborations."

Livermore simulations have extraordinarily broad time scales.

Sixteen racks of BlueGene/L (one-quarter of the system) are shown here being assembled at IBM in Rochester, Minnesota. The racks consist of 16,000 nodes with 32,000 microprocessors and have achieved a peak computing speed of 90 teraops. At press time, the racks had been moved to Livermore and were being reassembled in the Laboratory's new Terascale Simulation Facility. BlueGene/L is expected to be fully assembled in June 2005.

For example, physicists often probe the intricacies of nuclear detonations nanosecond by nanosecond. At the other extreme, geologists monitor the slow changes in nuclear waste repositories over centuries. Geologist Bill Glassley says, "M&IC has provided the computational horsepower that enabled us to tackle otherwise intractable simulation." Sponsored by the LDRD Program, Glassley's group conducted the world's only 3D simulations of how a nuclear waste repository would evolve over thousands of years. The group also conducted the world's first thorough simulations of the long-term response of soil water to climate change.

Gygi's simulations model atoms and molecules accurately by using the laws of physics and quantum mechanics. "With these simulations, we can address questions that are difficult to answer even with advanced experiments," he says. In a simulation funded by LDRD, Gygi followed the propagation of a shock front in liquid deuterium. By learning that the propagation of the front is related to the front's electronic excitation, scientists were able to better plan future experiments and understand past experiments. "This was the first time we could describe a shock in a molecular liquid in such detail," says Gygi.

Physicist Giulia Galli says that quantum simulations are playing an increasingly important role in understanding matter at the nanoscale and in predicting the novel and complex properties of nanomaterials. In the next few years, Livermore researchers expect these simulations to acquire a central role in nanoscience and allow them to simulate a variety of alternative nanostructures with specific, targeted properties. In turn, this work will open the possibility of designing optimized materials entirely from first principles.

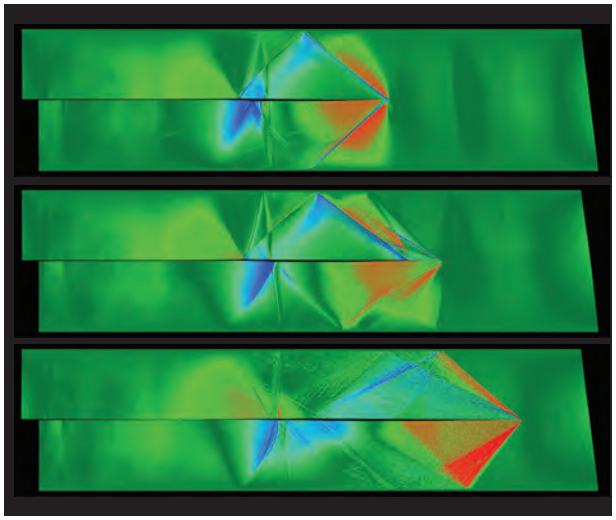
"Although the full accomplishment of this modeling revolution will be years in the making, its unprecedented benefits are already becoming clear," says Galli. Indeed, simulations based on quantum mechanics are providing key contributions to the understanding of a rapidly growing body of measurements at the nanoscale. "Quantum simulations provide simultaneous access to numerous physical properties such as structural, electronic, and vibrational, and they allow one to investigate properties that are not yet accessible for experiments," she says. A notable example is represented by microscopic models of the structure of surfaces at the nanoscale, which cannot yet be characterized experimentally with today's imaging techniques. The characterization of nanoscale surfaces and interfaces is important to predicting the function of nanomaterials and eventually their assembly into macroscopic solids.

Planning for NIF

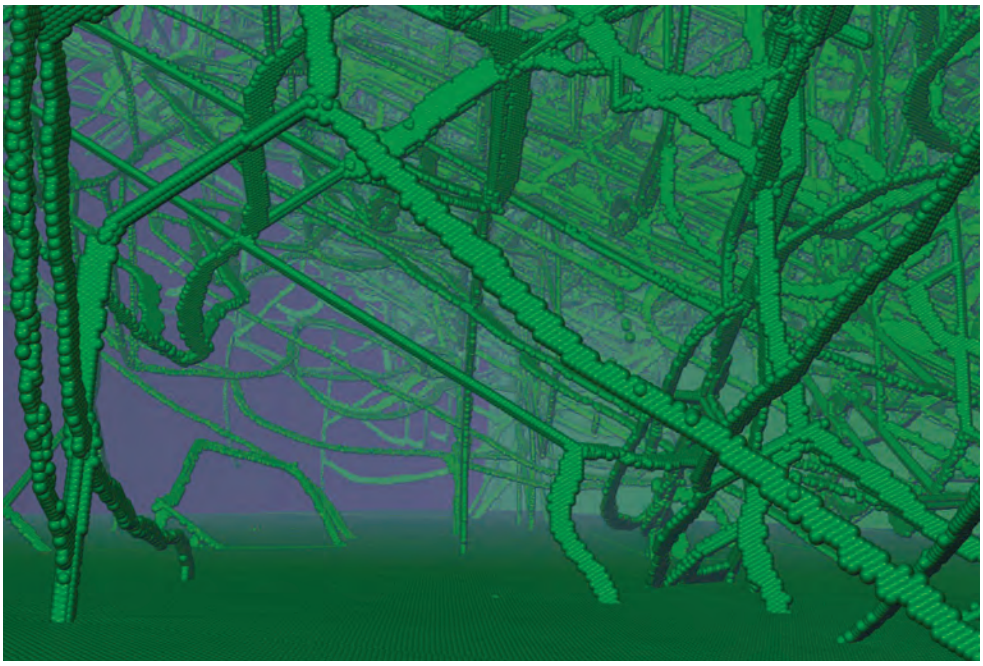
Simulations by physicists Bert Still and Steve Langer are playing an essential role in carrying out the first experiments at the National Ignition Facility (NIF) at Livermore. According to Still, "Simulating 1 cubic millimeter of plasma may not seem like a big task, but it requires a supercomputer to track 6.8-billion zones nanosecond by nanosecond." Still and Langer used 3,840 microprocessors of Thunder (94 percent of the machine) to model laser–plasma interactions in the first 4.2 millimeters of a 7-millimeter-long "gas pipe" experiment on NIF. Carbon dioxide gas was ionized in a plastic bag by laser beams, thereby creating plasma similar to that which will be formed by targets in future NIF experiments.

The Thunder simulation unexpectedly showed a delay in the time taken for the laser beam to burn through the plasma at the far end of the gas pipe, when compared to predictions from previous, lower resolution design calculations. One possible explanation for this phenomenon is laser–plasma instabilities. The burn-through-delay issue did not arise in a simulation conducted in August 2003 on MCR. This simulation used 1,600 processors (69 percent of the machine) to model 2.7 millimeters of a similar experiment that used carbon dioxide. A previous simulation, conducted in February 2003, used 1,920 processors of MCR (83 percent of the machine) to model the first 4.5 millimeters of a gas pipe experiment involving neopentane. This simulation turned up another surprise: Scattered light from the neopentane plasma showed strong variability at subpicosecond time scales.

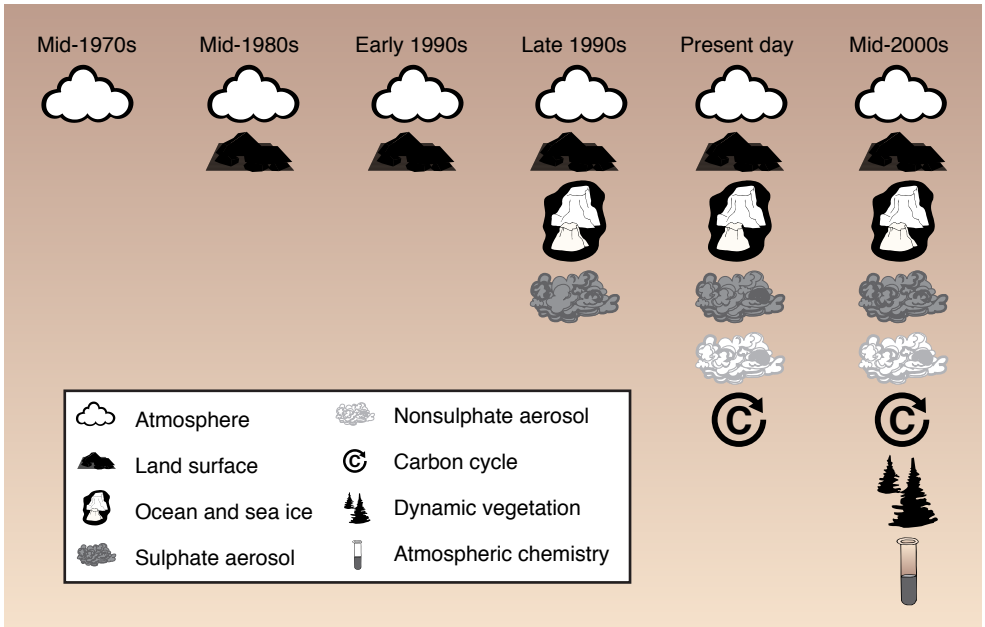
"MCR- and Thunder-class systems make it possible to simulate effects like these for the first time. Earlier systems could not model a NIF-scale plasma," says Still. "These scalable clusters are indispensable. Few platforms exist that can run such simulations, and many of them are located at Livermore, either



A Livermore multimillion-atom simulation to study crack propagation in rapid brittle fracture was performed on the 12.3-teraops ASC White supercomputer to help answer the question, Can crack propagation break the sound barrier? The simulations showed that crack behavior is dominated by local wave speeds, which can be faster than the conventional sound speeds of a solid. The snapshot pictures represent a progression in time (from top to bottom) of a crack traveling in a harmonic wave.



In another study of materials failure, scientists using ASC White examined what happens in ductile failure; that is, what happens when tough materials like metals bend and fail. A close-up snapshot from a simulation of more than one billion atoms shows the true complexity of propagating dislocations and rigid junctions in a crystal structure subjected to ductile failure and work hardening.



Climate models over the past 30 years have become more complex and detailed and can now include more variables as the codes and the machines they run on have become increasingly more powerful.

as ASC or M&IC machines. Such large calculations help us identify and assess plasma physics issues relevant to NIF experiments and dramatically contribute to achieving ignition."

Still points out that advanced simulations have 1,000 times more resolution than the detectors that will be used on NIF experiments. As a result, Still and Langer have advised NIF experimenters where best to locate the detectors.

Cracks Break the Sound Barrier

Two landmark simulations, conducted in late 2000, demonstrated the power of advanced simulations to the world's materials science community. The simulations were performed by Livermore physicist Farid Abraham (at the time working for IBM), computer scientist and visualization expert Mark Duchaineau, Díaz de la Rubia, and Seager.

The simulations, completed on the then newly installed ASC White computer, provided insights into how materials fail. The simulations used molecular dynamics to predict the motion of large numbers of atoms based solely on interatomic forces. "The simulations showed how it is possible to use molecular dynamics to design and perform mechanical tests that complement laboratory experiments," says Abraham.

The first simulation was a 20-million-atom study of crack propagation in the fracture of brittle materials. The researchers unexpectedly observed the birth of a crack traveling faster than the speed of sound. "Theory stated cracks could move only up to the speed of sound," says Abraham. He notes that researchers can't possibly see cracks forming and spreading during experiments. As a result, the simulations serve as a "computational microscope," in which researchers can see what is happening at the atomic scale.

The second simulation investigated ductile failure by using a record-smashing

1 billion atoms. The study simulated the creation and interaction of hundreds of dislocations. In ductile failure, metals bend instead of shatter as a result of plastic deformation, which occurs when rows of atoms slide past one another on slip planes (dislocations).

The simulations, which have been used to produce a 3D movie (www.llnl.gov/largevis/atoms/ductile-failure/index.html), show how a lattice of rigid junctions forms. "We see dislocation moving along, like a little wave, as atomic planes slide over one another," says Abraham. Dislocations move, interact with one another, and finally become rigid as they stick to one another. This rigidity causes the material to change from ductile to brittle, a phenomenon also called work hardening. The phenomenon had been known for a long time but had never been understood on the atomic level.

Climate Study Needs Simulations

Researchers in climate change have long been avid users of the most powerful supercomputers available. "Supercomputer calculations have altered the direction of climate change research," says Doug Rotman, head of Livermore's Carbon Management and Climate Change Program. Rotman says the latest M&IC machines have helped simulation science in three ways.

First, they have increased the number of runs atmospheric scientists can do in a reasonable amount of time. "Climate is a statistical science," he says. "We have to do ensembles of runs to discover what is happening. Starting with slightly different conditions leads to different weather patterns."

Second, the machines provide increasing resolution, both horizontally and vertically. He notes that until recently, most climate change research has focused on the global scale at low resolution (100 kilometers at best). The computational power of MCR and Thunder is permitting researchers to focus for the first time on the regional scale at higher resolution. "We'll be looking at how certain emissions from a city, for example, affect air quality in a particular region," says Rotman. "And we'll be able to see, for the first time, how rain fluctuations affect snow packs in selected mountain ranges and also see the effects in other areas, such as reservoirs."

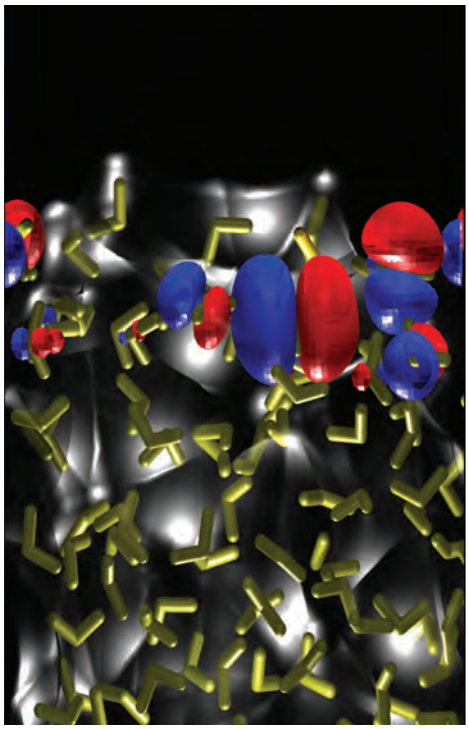
Finally, the machines permit codes to incorporate an unprecedented amount of chemical and physical reactions and chemical species. "The computational power of M&IC computers has enabled Livermore to develop the IMPACT chemistry model and to push the scientific edges of atmospheric chemistry modeling," adds Rotman. IMPACT is the only atmospheric model capable of interactively modeling the combined troposphere and stratosphere, which together make up Earth's atmosphere. IMPACT can examine the processes that determine the distribution of ozone and other chemicals in the tropopause (the boundary between troposphere and stratosphere).

Rotman points out that Livermore is the only U.S. institution that can simulate carbon as it cycles through the planet in different forms, including sequestration in the oceans. "We've used every machine and are ramping up to use BlueGene/L," he says.

Simulating Liquid–Vapor Interfaces

Chemist Chris Mundy and postdoctoral researcher I-Feng Kuo simulated the interface between liquid water and water vapor in a landmark simulation published in *Science* last year. Their results are important to both biologists and atmospheric scientists because knowledge of the reactions on surfaces and interfaces of liquid water are important in both fields. The pioneering study was made possible by using 440 microprocessors on MCR (63 percent of the machine) to simulate, over several picoseconds, 200 water molecules comprising a film of water 3 nanometers deep.

"Recent experiments are probing the surface of liquids, and Livermore is playing a vital role in providing a microscopic picture using these terascale simulations," says Mundy. He and colleagues are using Thunder to investigate the liquid–vapor phase interfaces of other species. The potential applications of these techniques include homeland security, such as calculating the physical characteristics



A snapshot is shown of the calculated aqueous liquid–vapor interface, as simulated in an ab initio molecular dynamics study. The individual water monomers are represented by the yellow cylinders. The top isosurface shows an area of the water slab that is reactive to excess protons and electrons. This pioneering study used 1,440 microprocessors on the Multiprogrammatic Capability Resource (63 percent of the machine) to simulate, over several picoseconds, 200 water molecules comprising a film of water 3 nanometers deep.

of a possible terrorist chemical weapon without having to test an actual sample.

"When one has access to these kinds of computational resources, one's first inclination may be to take a normal system and double it, but one doesn't often find new physics by taking that approach," says Mundy. "Livermore's terascale resources allow us to turn quantity, that is, system size, into a new quality—understanding complex chemistry in different environments. We couldn't simulate interfacial systems via first principles without MCR and Thunder. These resources enable us to answer many important scientific and programmatic questions from first principles. It's very exciting!

Making Breakthrough Science Possible

Breakthrough computer simulations that lend new insight or reveal new physics require the most powerful machines and advanced codes available. For Livermore scientists running unclassified simulations, those machines have recently become Linux clusters.

The previous generation of scalable parallel supercomputers rely on vendor-integrated systems using high-performance proprietary microprocessors (the type found in expensive servers), proprietary interconnects and vendor (Unix-based) system software. This approach has matured to the point where the cost per teraops (trillion operations per second) improves only slowly.

In the late 1990s, Livermore experts turned to Linux cluster technology, in which large groups of commodity microprocessors (the type found in inexpensive desktop personal computers) are combined with third-party interconnects and open-source (Linux-based) system software. The result has been extraordinary advances in cost-effective computing, with Livermore taking the lead in harnessing this cluster technology for programmatic needs. Computer scientist Mark Seager says, "By using the economic force of nature known as a commodity ecosystem, we've changed the way scalable systems are architected, procured, and used. We invented the methods and the partnerships to scale these machines way beyond the previous state of the art."

The first cluster to gain national recognition was the Multiprogrammatic Capability Resource (MCR) scalable parallel supercomputer, with 2,304 processors capable of 11.2 teraops. This system began running large-scale applications in December 2002. In June 2003, MCR was ranked as the world's third fastest computer, the first time that a computer based on Linux-cluster technology was one of the top 10 computers in the world. The machine dramatically increased Livermore's unclassified computing capability. MCR nearly matched the Advanced Simulation and Computing (ASC) Program's 12.3-teraops White machine in power, but at $1.2 million per teraops, it was 10 times less expensive than White. Seager notes that MCR would not have been possible without the ASC Program's investments in technology developed at Livermore.

In 2004, as the competition for access to MCR increased, Livermore procured a more powerful system called Thunder. This machine features a peak speed of 22.9 teraops and uses 1,024 high-performance nodes each with four Intel Itanium2 processors (4,096 processors total) and 8 gigabytes of memory. The machine debuted as the world's second fastest computer. Most simulations on Thunder—and MCR—support projects in biology, materials science, lasers, and atmospheric science as well as unclassified simulations for stockpile stewardship.

A new generation of supercomputers uses system-on-a-chip technology and low-cost, low-power embedded microprocessors. This technology is embodied in BlueGene/L, which is scheduled to arrive at Livermore this summer. The machine will have 131,072 advanced microprocessors and a peak computational rate of 367 teraops.

Physicist Steve Langer says, "Clusters seem to be the way to go for massively parallel codes. There are a few problems that we can still cram into a single SMP (a computer architecture in which memory and other components are shared), but we're not going to put in billions of zones and have enough memory and computing capacity to get a simulation done anytime soon. The performance-to-cost ratio of clusters is higher than we've had on any other machine."

The software running on Multiprogrammatic and Institutional Computing (M&IC) Initiative computers consists of three major components: an operating system, a parallel file system, and a resource management system. The Clustered High Availability Operating System, developed at Livermore, augments the standard Linux system with modifications for high-performance networks, cluster management and monitoring, and access control.

LUSTRE is an open-source parallel file-sharing system developed in part through a collaboration between Livermore, ClusterFile Systems, Hewlett-Packard, Intel, and the ASC Program. Langer says, "LUSTRE ties everything together with a unified file system: multiple Linux clusters, visualization resources, and the archive. Before we had to copy data multiple times and then keep track of it."

Simple Linux Utility for Resource Management (SLURM) is a tool developed in a collaboration between Livermore, Linux Networx, Hewlett-Packard, and others to manage a queue of pending work, allocate access to nodes, and launch and manage parallel jobs. SLURM has proven to be reliable and highly scalable. As a result of its success on Linux-based systems, it is being deployed on ASC platforms.

"To do these problems, you need to be at a place like Livermore," says Mundy. "It takes not only the machines but also the staff of experts who can run the machines and write new software." He notes that the newest generation of machines allows scientists to simulate a new class of physical reactions, which replace homogeneous systems with heterogeneous systems. "Most things in life are heterogeneous."

Hydrogen Meltdown Uncovered

The October 7, 2004, cover of *Nature* reported a new melt curve of hydrogen at extremely high pressures predicted by Livermore scientists using the ab initio molecular dynamics code GP. This new curve—the result of nearly two years of work on an LDRD-funded project by physicists Stanimir Bonev, Eric Schwegler, Tadashi Ogitsu, and Galli—presents the melting point of hydrogen at pressures from 50 to 200 gigapascals at temperatures from 600 to 1,000 kelvins.

At about 80 gigapascals, the melt line hits a maximum and goes from a positive to a negative slope. This maximum, the scientists say, relate to a softening of the intermolecular interactions and to the fluid and solid becoming similar in structure and energy at high pressure. Melting point maximums are unusual but are also found in water and graphite. In these materials, liquid is denser than solid when they coexist.

The extremely complex simulations were run on several Livermore machines including MCR, Frost, and other Linux clusters. The GP code calculated the interactions of 720 atoms over time spans from 5 to 10 picoseconds. Thanks to the power of the code and machines, scientists were able to perform numerous simulations under varying thermodynamic conditions.

Results from these first-principles simulations provided strong evidence of the existence of a low-temperature quantum fluid in hydrogen, notes Bonev. These findings led the team to propose new experimental measurements that could help verify the existence of a maximum melting temperature and the transformation of solid molecular hydrogen to a metallic liquid at pressures close to 400 gigapascals.

The success of the project, Galli notes, is due to a combination of codes, machines, and expertise accumulated over the years. "Results such as these do not just happen," she emphasizes. "You need all three elements—people, codes, and machines—in place."

Amazing Progress in 10 Years

Seager summarizes that simulation science at Livermore has gone from about 50 gigaops in 1995 to 12.3 teraops on ASC White in late 2000 to 100 teraops on ASC Purple. Later this year, BlueGene/L, with 360 teraops of processing power, will begin its shakedown. Seager says, "It's been an amazing ramp-up from the first clusters, and all those systems have had direct and measurable impact on programs at this Laboratory."

Mike McCoy, head of ICC and deputy associate director for Computation, calls today's simulations "science of scale" because they are predictive. "The computing is performed at a resolution and degree of complexity, with inclusion of sufficient physics, that scientists have confidence they can predict the outcome of an experiment. This is an exciting time to be at Livermore," he says.

These examples show over and over, in multiple physical disciplines and programs at the leading edge of scientific discovery, the tight coupling between experiment and simulation at the Laboratory. Simulation is essential in the design of modern experiments. In addition, simulations are now of sufficient resolution and size and contain enough physics that their results can be directly compared with experimental results. Hence, simulations are essential to understand the physical phenomena involved in experiment.

Even with all this progress, Díaz de la Rubia notes that much work still needs to be done. Many fields, such as computational biology, are still in their infancy in taking advantage of the simulation power of the latest machines. "Supercomputers are helping us tremendously to solve problems we couldn't attack otherwise," he says, "but we can't claim victory yet." He sees a need for improved models and for coupling experiments with simulations more tightly.

With ASC Purple and BlueGene/L coming on line this year, Livermore computer experts are preparing for the newest generation of scalable parallel supercomputers. In addition, these systems position the ASC Program and the Laboratory for the next leap forward to petascale computing. For Livermore researchers, another generation of these systems means an even more powerful tool for understanding—and predicting—the physical universe.

—Arnie Heller and Ann Parker

Key Words: Advanced Simulation and Computing (ASC) Program, atmospheric chemistry modeling, BlueGene/L, climate change, crack propagation, ductile failure, GP code, hydrogen melt curve, IMPACT code, laser–plasma interactions, Linux clusters, liquid–vapor interfaces, molecular dynamics, Multiprogrammatic and Institutional Computer (M&IC) Initiative, Multiprogrammatic Capability Resource (MCR), National Ignition Facility (NIF), Purple, seismic wave analysis, supercomputers, Thunder, White.

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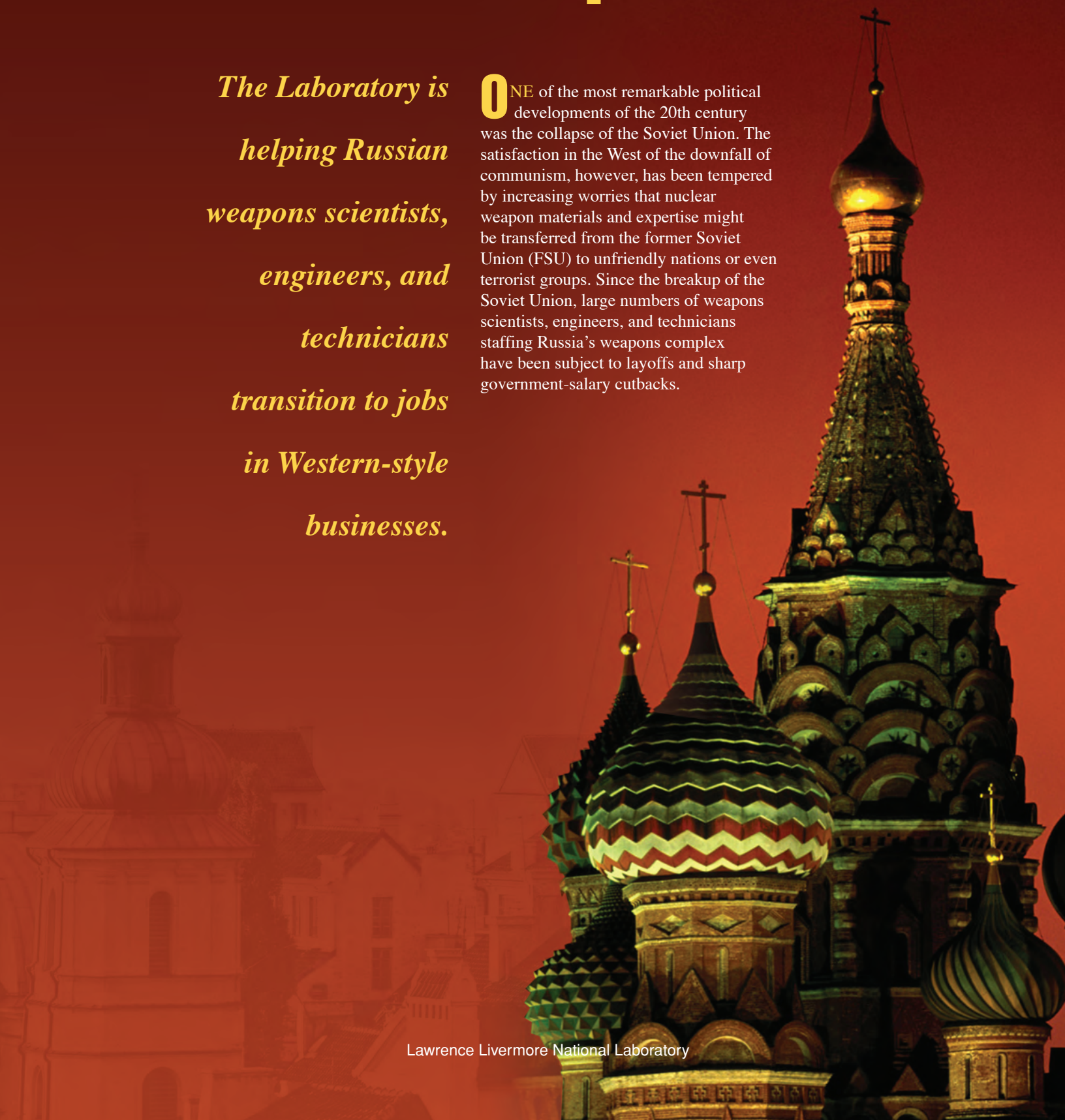
Russian Weapons Workers

The Laboratory is helping Russian weapons scientists, engineers, and technicians transition to jobs in Western-style businesses.

ONE of the most remarkable political developments of the 20th century was the collapse of the Soviet Union. The satisfaction in the West of the downfall of communism, however, has been tempered by increasing worries that nuclear weapon materials and expertise might be transferred from the former Soviet Union (FSU) to unfriendly nations or even terrorist groups. Since the breakup of the Soviet Union, large numbers of weapons scientists, engineers, and technicians staffing Russia's weapons complex have been subject to layoffs and sharp government-salary cutbacks.



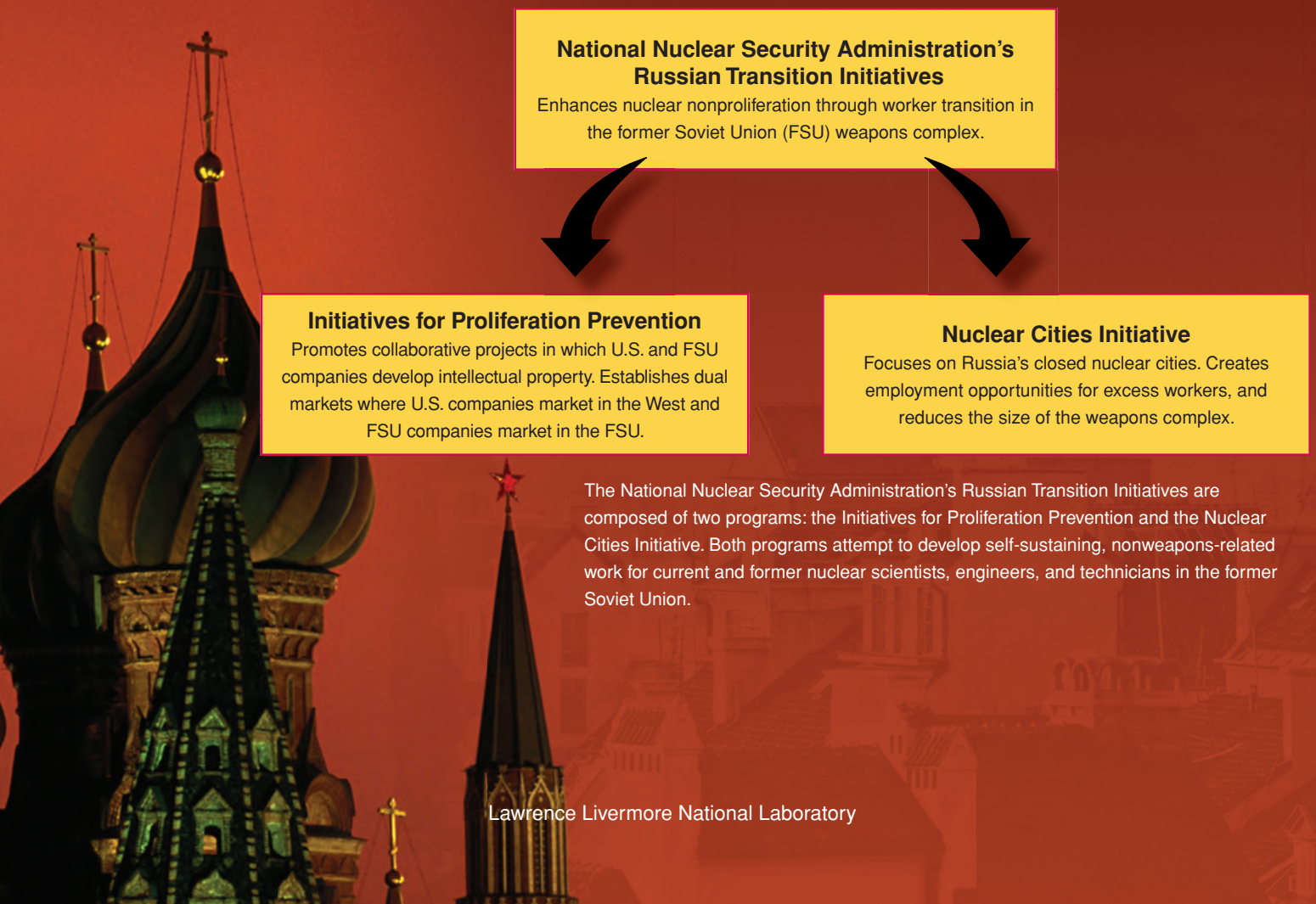
Begin New Commercial Venture

In response to the nuclear proliferation danger, the Department of Energy's (DOE's) National Nuclear Security Administration (NNSA) created nonproliferation programs focused on the states of the FSU. "We want to keep workers in the FSU with nuclear expertise employed by helping them create viable jobs in the high-technology sector," says Livermore seismologist Jay Zucca, a leader in the Laboratory's Proliferation and Terrorism Prevention Program, which is part of the Nonproliferation, Arms Control, and International Security Directorate.

NNSA's Russian Transition Initiatives are composed of two programs: the Initiatives for Proliferation Prevention (IPP) and the Nuclear Cities Initiative (NCI). Both programs attempt to develop self-sustaining, nonweapons work for current and former weapons scientists, engineers, and technicians. Zucca notes that Livermore's long-standing knowledge of FSU nuclear facilities and its scientists makes the Laboratory an excellent resource for both FSU scientists and American companies interested in forging partnerships.

Established in 1994, the IPP promotes collaborative projects among DOE national laboratories, U.S. private-industry partners, and institutes in the FSU. Projects are selected for their commercial potential and are designed to lead to long-term employment in the civilian sector for former weapons workers.

The NCI was established in 1998 under a government-to-government agreement to help Russia reduce the size of its nuclear weapons complex, which is about three times the size of the U.S. complex. The NCI is active in three of Russia's ten "closed" nuclear cities—Sarov, Seversk, Snezhinsk—and is planning to work with a fourth, Zheleznogorsk. These closed cities have populations ranging from 30,000 to



The National Nuclear Security Administration's Russian Transition Initiatives are composed of two programs: the Initiatives for Proliferation Prevention and the Nuclear Cities Initiative. Both programs attempt to develop self-sustaining, nonweapons-related work for current and former nuclear scientists, engineers, and technicians in the former Soviet Union.

120,000. Until about 15 years ago, Western researchers were not allowed to visit them. In fact, the cities were not even on maps.

Livermore participates in both the IPP and NCI programs. Zucca notes that there is not a strict division in activities between the two programs. For example, more than 25 percent of the IPP's activities take place in Russia's closed nuclear cities.

Role of the IPP

The IPP creates new jobs through projects that commercialize expertise and products in FSU scientific institutes involved in weapons technologies. Today, 11 organizations belonging to DOE are involved in the IPP program—10 national laboratories and NNSA's Kansas City Plant. Almost two dozen Livermore workers, mostly engineers, are involved in about 20 different IPP projects.

"The IPP is the broker between the Russians and private industry," says Don Lesuer, a materials engineer and program manager for the Livermore IPP. "We validate what the Russians are doing, and that gives their technical expertise and products credibility to American firms. These firms are recognizing the possible business and technical advantages of developing concepts and prototypes in the FSU."

Since its inception, the IPP program has funded more than 750 projects involving more than 15,000 weapons scientists, engineers, and technicians at more than 200 institutes in Russia, Ukraine, Kazakhstan, Georgia, Uzbekistan, and Armenia. American companies match U.S. government funds to develop and commercialize projects that are not military-related. Seventy percent of these funds is spent in the FSU, and 30 percent is spent in the U.S. for technical contributions and project management.

Two entities carefully review proposed commercialization projects. The Inter-Laboratory Board, whose members are from the national laboratories and the Kansas City Plant, reviews the proposals generated by DOE laboratories for technical content and economic viability. The U.S. Industry Coalition evaluates the commercial viability of proposed projects. NNSA gives final approval before a project is funded.

An Initiatives for Proliferation Prevention project is developing pain-blocking devices that use low-level electrical pulses. A wireless device (shown here) won an R&D 100 Award for being one of the most important industrial inventions in 2002. Livermore scientists partnered with the U.S. firm Cyclotec and the Russian firm Biofil to develop and miniaturize the control module (inset) for the device.

Focus on Medical Technology

Several IPP projects involving Livermore and a U.S. private-industry partner focus on medical technology and biological research. One project is developing pain-blocking devices that use low-level electrical pulses. The Russian firm is Biophysical Laboratory (Biofil) Ltd., a company spun off from the All-Russian Research Institute of Experimental Physics in Sarov. Biofil conducts research and development on biomedical devices. The U.S. partner is Cyclotech Advanced Medical Technologies (Cyclotech), Inc.

The partners formed a joint cooperative research agreement to develop the advanced, easy-to-use pain-blocking device. The device won an R&D 100 Award for being one of the most important industrial inventions in 2002. (See *S&TR*, October 2002, pp. 12–13.) Livermore scientists partnered with Cyclotec and Biofil to develop and miniaturize a control module for the device.

Another project involving Biofil focuses on a breast cancer probe that resulted from work done at Livermore in its Medical Technology Program. Russian researchers are developing data-analysis algorithms and software for a probe that uses the electrical and optical properties of tissue to identify malignant tumors in the breast.

The project, which began in 2004, is one of the first to be sponsored jointly by the IPP and NCI programs.

"Because of the work that Biofil has done with Livermore, the company is making significant strides to becoming a self-sustaining business," says Lesuer. Biofil has received more than $350,000 from several U.S. biomedical companies for research and development on biomedical devices.

A project that began in 2003 involves collaborative work between Livermore and the National Center for Disease Control (NCDC) in Tbilisik, Georgia. This project, which is relevant to U.S. counterterrorism efforts, conducts molecular fingerprinting and DNA decoding of strains of *Yersinia pestis* and *Francisella tularensis*, the bacteria that cause plague and tularemia, respectively. DNA from strains at NCDC was transferred to Livermore for study, and, in August 2003, two NCDC scientists worked at Livermore to learn DNA decoding.

Another IPP project focuses on commercializing a Russian device called an alternating current (ac) plasma torch to completely destroy hazardous and medical waste. Participating Russian institutes include the Institute for Problems of Electrophysics and Soliton-NTT (a spin-off company of Russia's Kurchatov Institute). The U.S. private-industry partner is Scientific Utilization of Huntsville, Alabama. The torch is a commercial version of a waste destruction system used by the Russians for a number of applications, including the destruction of chemical weapons and bioagents. The device being developed under the IPP program is intended for destroying medical waste. It creates plasma temperatures between 2,500 and 6,000 kelvins and can process 150 kilograms of waste per hour.

Three ac plasma torches and power supplies were manufactured in Russia and sent to the U.S. for evaluation. Livermore contributions included studying the electrode materials and evaluating torch performance. Plans are under way for the first Russian medical waste plant in St. Petersburg, which will use the ac plasma torch. Livermore scientists, in collaboration with the County of Alameda in California, have submitted a proposal for a waste disposal plant that would generate 20 megawatts of power while destroying 500 tons of municipal waste a day. The plant design would use high-temperature gases produced by the plasma torch for the co-generation of electricity.

In another IPP project, Livermore is teaming with Cryocarbon (another spin-off company of Russia's Kurchatov Institute), the Polish Academy of Sciences' Institute of Molecular Physics, and Spectra Gases of New Jersey to design and produce isotope-manufacturing facilities at Kurchatov. The project is developing facilities to manufacture two isotopes, carbon-13 and oxygen-18. Carbon-13 is used for labeling urea and glucose as markers of medical conditions, such as ulcers and diabetes. Applications for oxygen-18 include medical diagnostic imaging, such as positron emission tomography imaging, and medical research studies.

At the project's start, Kurchatov had no experience in the production of these medical isotopes. To aid this effort, Livermore applied its technical expertise in isotope separation technologies and complex systems analysis. Full production of isotopes began in December 2004. At the project's conclusion, the goal is for Kurchatov weapon scientists and engineers to be permanently employed producing the isotopes and developing and marketing other labeled compounds derived from carbon-13 and oxygen-18.

Launching Commercial Products

One of the most promising IPP projects involves manufacturing and evaluating advanced aircraft and space-launched vehicle components. The project teams Livermore, Boeing, and five institutes in Russia and Ukraine for the study of advanced Russian metal-forming and welding technologies and their possible application to Boeing products.

As part of the IPP project, prototype cryogenic tanks for a Boeing Delta-series launch vehicle and airplane fuselage sections were fabricated and sent to Livermore for analysis. In October 2003, Boeing representatives visited the Laboratory to study the hardware and discuss the application of Russian manufacturing technologies to future Boeing products.

Boeing is studying the possibility of establishing a permanent manufacturing capability in the FSU for next-generation aircraft parts. Lesuer says a manufacturing

Livermore is teaming with Cryocarbon, a spin-off company from Russia's Kurchatov Institute, and Spectra Gases of New Jersey to design and produce manufacturing facilities for two medical isotopes, carbon-13 and oxygen-18. Shown here are distillation columns at Kurchatov for manufacturing carbon-13.

plant could employ hundreds of scientists, engineers, and technicians.

Several IPP projects exploit Russian expertise in high explosives. One effort is developing a rarefaction shock-wave cutter for removing offshore oil and gas platforms at the end of their useful lives. The cutter uses special explosives technology to cut thick-walled pipes. The device can be deployed without divers, and its explosive impacts are less damaging to marine life than current technology. Halliburton Energy Services Inc. has entered into a commercialization option agreement with scientists from the All-Russian Institute of Experimental Physics in Sarov. "This IPP project has been a resounding success," says Lesuer.

In 2004, work began on a project to develop and evaluate an explosives detection system for use on checked airline baggage and cargo. The project is a collaborative effort between five Russian institutes, Livermore, and Valley Forge Composites of King of Prussia, Pennsylvania. The explosives detection system is based on a small-scale accelerator developed by P. N. Lebedev Physical Institute, the lead Russian partner. The device analyzes gamma radiation resulting from photonuclear reactions in explosive compounds. Livermore engineers will be evaluating the accelerator and system performance.

"Through these projects, the Russians learn what it takes to launch a Western-style commercial project. They're also understanding the need to keep costs low to stay competitive," says Lesuer.

Opening Closed Nuclear Cities

Since 1999, NNSA and the Federal Atomic Energy Agency (formerly the Russian Ministry of Atomic Energy) have jointly implemented the NCI program. Their objective is to reduce Russia's enormous nuclear weapons complex by helping former weapons experts in closed nuclear cities make the transition to civilian employment.

The program's primary focus was on three closed cities: Sarov, Snezhinsk, and Zheleznogorsk. These cities were formerly known by the mailing addresses of nearby cities: Arzamas-16, Chelyabinsk-70, and Krasnoyarsk-26, respectively.

Sarov is the site of the All-Russian Research Institute for Experimental Physics (VNIIEF), which was Russia's first nuclear weapons laboratory, and the Avangard weapons assembly plant.

Snezhinsk is the home of the All-Russian Research Institute for Technical Physics (VNIITF), which was Russia's second nuclear weapons laboratory. Zheleznogorsk is home to the Mining and Chemical Combine, which is one of Russia's three plutonium production complexes. In Zheleznogorsk, the NCI is supporting Russian efforts to shut down the plutonium production reactors.

Both the VNIIEF in Sarov and the VNIITF in Snezhinsk have identified scientists, engineers, and technicians with special weapons design knowledge who will be released from their institutes over the next few years. The NCI is working to convert their government jobs to ones

Prototype cryogenic tanks are manufactured in Russia as part of an Initiatives for Proliferation Prevention project involving five Russian institutes, Lawrence Livermore, and Boeing. Livermore and Boeing workers are shown with the tanks at Livermore.

in commercial companies. Lawrence Livermore is a key national laboratory for NCI projects in Snezhinsk, which is the sister city to Livermore, California.

According to Livermore NCI program manager Ann Heywood, the program develops physical and business infrastructure in the cities, helps establish sustainable enterprises, creates good jobs, and advances Russian business development and diversification. The goal is a smaller Russian weapons complex and increased U.S. and international security. Private U.S. businesses often participate in projects, but their participation is not required, as it is with IPP projects.

In 1999, an important NCI project began when Livermore helped create the Open Computing Center in Snezhinsk for commercial computing and software development. The project was attractive to NCI managers because of Russian computer programming expertise and the small capital investment required. A modern, permanent facility was completed in 2003; two-thirds was paid for by the VNIITF and the remaining third by NCI.

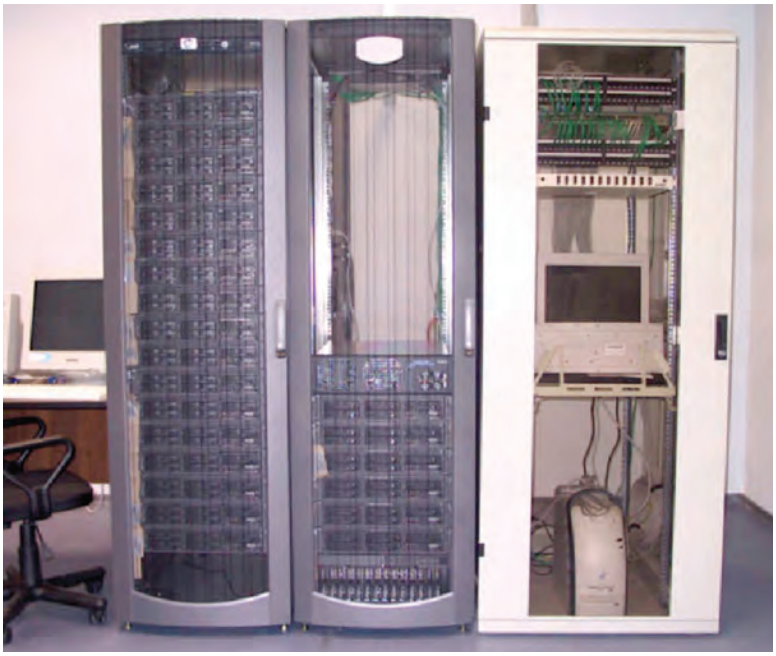
As the center grew, it was renamed STRELA, which means "arrow" in Russian and is the name of the first computer that operated in the Urals. Livermore helped STRELA obtain U.S. Department of Commerce approval for acquiring the center's principal computer, an American-made Linux cluster. The computer has 20 nodes, each containing two Intel Pentium-4 microprocessors connected by high-bandwidth Infiniband networking.

In addition, the Russians adopted Western companies' best practices for data protection and archiving. STRELA currently employs about 60 programmers. "They find most of the software projects just as challenging as their old weapons-related work," says Livermore physicist Dale Nielsen, Jr., who has helped oversee STRELA's development.

Although STRELA initially worked on a large set of projects, it now focuses on five commercialization efforts. For example, the company is the sole official distributor in Russia for LS-DYNA, a software product of Livermore Software Technology Corporation. The code is a commercial version of DYNA, which was developed at Livermore, and has evolved into the world standard for simulating vehicle crashes. STRELA sells licenses to other companies and does consulting work. Nielsen explains that Russian car companies are modifying their designs to meet European Union standards for crash-worthiness, so they need better simulation software and expertise. Livermore has trained STRELA engineers to use the code.

STRELA also operates a document-processing center to help institutions digitize paper-based data, such as card catalogs in Russian libraries. The NCI program helped STRELA to obtain high-end scanning equipment, storage devices, and software to efficiently convert paper documents to electronic files. "There is a

The Nuclear Cities Initiative is active in three of Russia's ten closed nuclear cities—Sarov, Seversk, Snezhinsk—and is planning to work with a fourth, Zheleznogorsk. A few Initiatives for Proliferation Prevention projects are also being carried out in the closed cities.



The STRELA company in Snezhinsk employs about 60 programmers who work on commercial computing and software development. Livermore helped the center acquire its Linux cluster computer, which consists of 20 computing nodes.

At the Spektr-Conversion company, the oil-well perforator business is growing. (a) A final inspection of a perforator is performed before field-testing in Russian oil fields. (b) The successful field tests led to the first commercial production of perforators.

tremendous business potential in Russia for this kind of work," says Nielsen.

A similar effort involves working with the Association of Small and Medium-Size Towns in Russia to help cities manage their official data. STRELA has partnered with the Russian firm ARSINT for sales, installation, and support of technology to transfer data electronically.

The NCI program is also helping Spektr-Conversion, a growing engineering services company of 50 employees who formerly worked on nuclear weapons at the All-Russian Scientific Research Institute of Technical Physics in Snezhinsk. Spektr-Conversion engineers have developed advanced oil-well perforators.

The perforators use shaped charges to fracture the surrounding rock and allow the liberation and extraction of more oil and gas. Tests conducted in December 2003 showed the perforators outperformed other units of both Russian and Western design. Livermore and Spektr-Conversion jointly designed the perforator, charges, detonators, and metal parts.

Last year, the company produced its first 160 units, and their goal is 20,000 units per year. The company's products also include custom auto parts, a dynamic wheelchair device, and electronic knee prostheses. Their business plan forecasts the creation of more than 230 jobs in three years. "Spektr-Conversion is becoming comparable to major companies, such as Halliburton, in product design," says Heywood.

Imaging Technology Shows Promise

One notable NCI-supported project in the FSU is a positron emission tomography (PET) center being established with Snezhinsk scientists. PET is an imaging technology for diagnosing cancer. It uses sugars tagged with isotopes, which are injected into a patient. These glucose molecules preferentially flow to tumors because of their extensive vascular systems. Because a PET scan shows where

glucose molecules concentrate, it is a sensitive indicator for tumors.

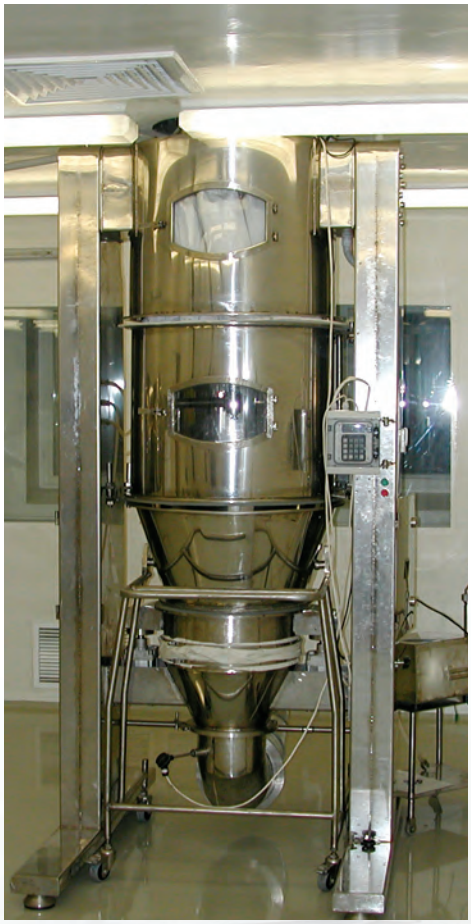
Livermore formed a PET team that includes the Biomedical Research Foundation of Northwest Louisiana, the VNIITF in Snezhinsk, and the Chelyabinsk Oblast Oncology Center. Livermore helped create a strong business model that included a market analysis. The NCI program is funding the building of a major PET center in Snezhinsk. The facility should provide high-tech employment for many scientists and engineers who have imaging science, accelerator, and chemical expertise.

This project has strong support from Russian authorities. Because many health problems in the area have been attributed to the nuclear weapons industry, local governments have a keen interest in diagnosing and treating cancer. Russian medical experts estimate that the PET center, which would be the only such center in the Urals, could reduce surgeries by 30 percent.

Heywood says the project will benefit many people in the area and generate significant revenue. Project planners are discussing the installation of PET scanners in other cities in the Urals and providing PET consulting to other cities and regions.

In another health-related project, Livermore is helping to bring cost-effective antibiotics to the Urals. Previously, the Snezhinsk Pharmaceutical Company was repackaging drugs to distribute to regional hospitals and physicians. Because the NCI program was able to procure machinery for the company that gave them the capacity to form pills from bulk materials, the company is now selling antibiotics in pill form across the Urals and working on contracts to supply developing nations.

Heywood notes that no single business model for NCI projects exists. Joint ventures, not-for-profit centers, companies formed directly out of a laboratory, and partnerships with the West can all be successful. She also says that the NCI program is changing its focus to those cities where plutonium reactors are shutting down, such as Zheleznogorsk and Seversk. Livermore has a 12-year relationship with Seversk and is coordinating an effort to develop catalysts from uranium oxide. The pilot plant and the anticipated manufacturing plant will be located at Seversk's Siberian Chemical Combine. Additional funding sources are under evaluation.



The Nuclear Cities Initiative helped the Snezhinsk Pharmaceutical Company obtain machinery that forms pills from bulk materials. The company is now selling antibiotics in pill form across the Urals and working on contracts to supply developing nations.

Mutual Gains

Zucca says the growing number of partnerships between Livermore, former Russian nuclear weapons workers, and, in many cases, American companies has shown that the two programs have been successful in growing businesses in the FSU and providing new careers. The programs have helped foster an openness to change among Russian scientists, technicians, engineers, and government officials.

Both the West and Russia benefit, says Zucca. Russian weapons workers and institutes gain from commercial relationships with established U.S. private-industry firms and DOE national laboratories, exposure to Western commercial business practices, and employment and income opportunities in nonmilitary high-technology fields. Livermore scientists are learning from their foreign counterparts, as well. For example, they are learning new manufacturing and welding techniques, such as superplastic forming, which deforms metal as if it were plastic or glass. Livermore researchers are also learning about Russian technology to detect explosives.

"Good things are happening," says Zucca. The payoff is increased international security.

— Arnie Heller

Key Words: Federal Atomic Energy Agency, former Soviet Union (FSU), Initiatives for Proliferation Prevention (IPP), nonproliferation, Nuclear Cities Initiative (NCI), Proliferation and Terrorism Prevention Program, Russian Ministry of Atomic Energy, Russian Transition Initiatives.

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Terascale Simulation Facility: Built for Flexibility

The Terascale Simulation Facility's four-story office tower will house more than 250 workers. Behind the office structure is a two-story wing (unseen) built for the Laboratory's new terascale supercomputers: Purple and BlueGene/L. Data-visualization, conference, and computer- and network-operations facilities will also be housed in the 23,504-square-meter building.

AS design and construction manager for the Laboratory's new $91-million Terascale Simulation Facility (TSF), Anna Maria Bailey found herself in a gratifying, although unusual position for an electrical engineer: overseeing construction of a building in which electrical and mechanical systems took precedence over the traditional interests of architects.

"Most architects want to dictate the design," says Bailey. In the case of TSF, it didn't work that way. Programmatic electrical and mechanical requirements controlled the design. "The architectural features had to take a back seat."

Architects were told to approach their design by thinking of TSF as a large electrical–mechanical system surrounded by an architectural skin. This message was conveyed early in the design process to underscore the importance of the supercomputer systems that are vital for national security and will reside in TSF. The result is a facility that emphasizes function over form.

Ahead of Schedule

Groundbreaking for the 23,504-square-meter (253,000-square-foot) TSF was held in April 2002. Built by M. A. Mortenson Construction Company of Minneapolis, Minnesota, TSF was completed ahead of schedule in late 2004 and within budget. TSF will house two supercomputers being built by IBM to perform trillions of operations per second (teraops). The new machines—Purple and BlueGene/L—will support the Advanced Simulation and Computing (ASC) Program, a part of the Department of Energy's National Nuclear Security Administration and an important component of stockpile stewardship.

Purple, with a peak computational rate of 100 teraops, will perform sophisticated physics and engineering simulations to help researchers better gauge the safety and reliability of aging nuclear weapons in the absence of nuclear testing. Purple will contain more than 12,000 next-generation IBM Power5 microprocessors, 50 terabytes of memory, and 2 petabytes of globally accessible disk space. The supercomputer will be delivered in phases with the first pieces arriving in April 2005.

The 360-teraops BlueGene/L will handle a variety of challenging ASC-related scientific simulations, including ab initio molecular dynamics for materials science; three-dimensional (3D) dislocation dynamics for materials modeling; and turbulence, shock, and instability phenomena in hydrodynamics. BlueGene/L will also serve as the ASC platform for evaluating advanced architectures for computational science. In October 2004, the supercomputer attained a record-breaking performance running at one-quarter its final size. BlueGene/L will arrive in three increments, with the second two expected in January and March 2005.

The machines will reside in the two computer rooms dominating the second level of the two-story supercomputer wing. The west room will house Purple, and the east will house BlueGene/L. A nonload-bearing wall separating the two rooms can be removed to create one large room should the need arise for more floor space for future ASC computers. Located on the ground floor beneath each computer room is a mechanical utility room. A total of 28 air-handling units blow cool air up to the second level, each at a rate of 80,000 cubic feet per minute. After cooling the computers, the air continues to rise upward and is forced into large return-air plenums for recirculation.

Housing for 250 Workers

TSF's four-story office tower provides research and development areas for visualization and hardware prototyping, a 150-seat auditorium and visualization theater for unclassified presentations, a second visualization theater for classified reviews, an operations

hub that will eventually control the Computation Directorate's high-performance computers across the Livermore site. It also includes three small computer rooms to support facility infrastructure, an atriumlike lobby, conference rooms, and a classroom.

The facility will house more than 250 employees, most of them from the Computation Directorate's Integrated Computing and Communications Department (ICCD). The employees are expected to begin moving into the building in February 2005. The third and fourth floors will be mainly offices, while the second will be a combination of offices, laboratory space, computer rooms, and space for the vendors and computer engineers who will maintain and service the machines.

To provide natural light for interior office areas, the architects designed TSF with an array of floor to ceiling windows at the end of corridors. Barbara Atkinson, associate deputy head of ICCD and the TSF construction liaison for the ASC Program, says, "In most cases, when one steps out of an office, one enters a bright hallway. The architects did a good job."

Three Design Requirements

At the start of facility design, the ASC Program defined three broad requirements that guided the architects in their approach to TSF: flexibility, scalability, and reliability. "These are competing factors that can be difficult to achieve," says Bailey. "Yet, the program wanted these factors to be addressed and implemented across all design disciplines."

The Computation Directorate wanted a facility built in such a way that modifications could be made to permit the siting in TSF of computer systems that today are only a gleam in the eyes of supercomputer designers. "We wanted a facility that would have a 35-year lifetime," says Atkinson. Don Davis, a long-time Computation facilities manager who served as a technical representative to TSF, adds, "We don't get the opportunity to construct a building very often. We had to design and build this one to last."

High among the factors driving the design of TSF, says Bailey, was the anticipated power requirements for teraops-scale computers and the next-generation systems that will eventually succeed them. Specifications called for a 7.5-megawatt computer load per machine room. Purple is expected to consume a peak-power load of 4.8 megawatts. Total power consumption for computations and cooling will be approximately 8 megawatts. BlueGene/L, by comparison, will draw about 1.6 megawatts of power. The designed power capacity at TSF is 25 megawatts, great enough to power a city between 16,000 and 20,000 people and slightly less than half the current Laboratory peak-power demand of 60 megawatts on the hottest day of summer.

Nearly 5 kilometers of trenches were dug for underground power lines. A trench on the west side of TSF stretches beyond the Laboratory's property line to the east to tie into the Laboratory's northeast substation. Another trench heads south to link with the south substations. "The redundant sources of power guarantee a backup source in the event we lose one," says Davis. "We don't want TSF off-line."

Overcoming Cable Limitations

Strategic placement of electrical–mechanical systems and clear-span construction with a deep subfloor in the terascale machine rooms helped to overcome problems created by the use of copper connector cables, which have a 25-meter-length limitation.

Atkinson explains, "Clear-span construction eliminates columns and opens up space on the computer floor. If we were forced to go around an impediment, 25 meters would suddenly become very short. We couldn't throw in a 50-meter cable, because it would alter the communication timing. Computer manufacturers connect hardware with communication cables that are all the same length. That way, it takes a predictable amount of time for a signal to go from one place to another in a machine."

When the distance between components is less than 25 meters, excess communication cable is placed in coils beneath the machine room floor. However, placing excess cables beneath the floor can create its own problems if the coiled cables block the flow of air needed to cool the supercomputers. The design solution was to provide a 1.2-meter raised floor for the computer rooms. Perforated and grated tiles sit atop the floor, allowing 13°C air from below to enter the hot intake sides of the computers and cool the machines. Both the computer room and office tower cooling systems are supported by four 1,200-ton chillers, one 400-ton chiller, and cooling towers capable of handling 8,176 liters of water per minute.

Clear-span construction techniques were used for the Terascale Simulation Facility's supercomputer rooms (approximately 2,230 square meters), opening up floor space by the elimination of columns and other impediments that could hinder placement of computer components. The grated floor tiles allow for chilled air to rise from air handlers on the first level, cooling the supercomputers that will be housed in the facility.

Large water pipes suspended beneath the ceiling separate the electrical–mechanical room from the second-level computer floor and are another example of flexibility designed into TSF. “Our computers are air-cooled now, but if we ever switch to water-cooled computers, we can easily tap into those pipes,” says Davis.

Workers install the raised floor for the west computer room, which is slated to house Purple. The 1.2-meter raised floor allows for the convenient placement of copper computer cables and the free circulation of chilled air to cool the supercomputer.

The architectural signature of the Terascale Simulation Facility is a structure known as the Armadillo Room, which features a 150-seat data-visualization theater and auditorium. The structure is shown here covered in waterproof sheathing before the installation of zinc roof panels. (inset) A powerwall inside the Armadillo Room displays a simulation to the audience. Powerwalls work by aggregating, or “tiling,” the separate images from many projectors to create one seamless image.

Visualization on a Large Scale

A prominent architectural feature of TSF is what has been named the Armadillo Room—a zinc-clad structure resembling an armadillo’s armored body that abuts the east side of the glass-fronted lobby. “The architects were adamant about keeping this unusual-shaped structure,” says Atkinson. “It is their architectural moment, their signature.”

Inside the Armadillo is a 150-seat auditorium for unclassified presentations. Scientists can display 3D simulations on an immense 1.2-centimeter-thick Plexiglas screen called a powerwall. The screen has eight projectors behind it in a 4-by-2 array. “Visualization is the only way we can understand the huge quantities of data being generated by the ASC supercomputers,” says Atkinson. (See *S&TR*, November 2004, pp. 12–19.)

TSF has a similar visualization theater for displaying classified data but in a program-review-style setting where core participants can gather around a table to offer technical critiques.

As the ASC Program liaison, Atkinson says, “My job was to field requests from program personnel and the TSF design and construction team and to translate these requests from ‘computereze’ to terms engineers and architects could understand.”

The program, she says, is pleased with TSF. “We have a great deal of flexibility to handle different technologies that will come our way. In terms of power capacity for supercomputers, TSF should accommodate anything that will be in the marketplace for a long time to come.”

—Dale Sprouse

Key Words: Advanced Simulation and Computing (ASC) Program, BlueGene/L, data visualization, Purple, supercomputer, Terascale Simulation Facility (TSF).

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Mining Geothermal Resources

Adam Wallace (former Livermore employee and now a Ph.D. candidate at Virginia Polytechnic Institute) keeps an eye on the 19-liter stirred reactor used to test silica precipitation in Livermore's mobile laboratory at the Mammoth Pacific LP geothermal power plant in Mammoth Lakes, California.

IT'S beautiful on beaches and receives kudos for its use in paint, tires, paper, toothpaste, and even in kitty litter—but it's a real pain in geothermal power plants. It's silica, and 6 million pounds of it is refined from beach sand every day and used to extend the life of tires and soles of shoes, to control the physical properties of paint, to increase the opacity and improve the adhesion of ink to paper, and much more. Unfortunately, in geothermal power plants, as a component of the heated underground fluids, silica clogs pipes, wells, and heat exchangers.

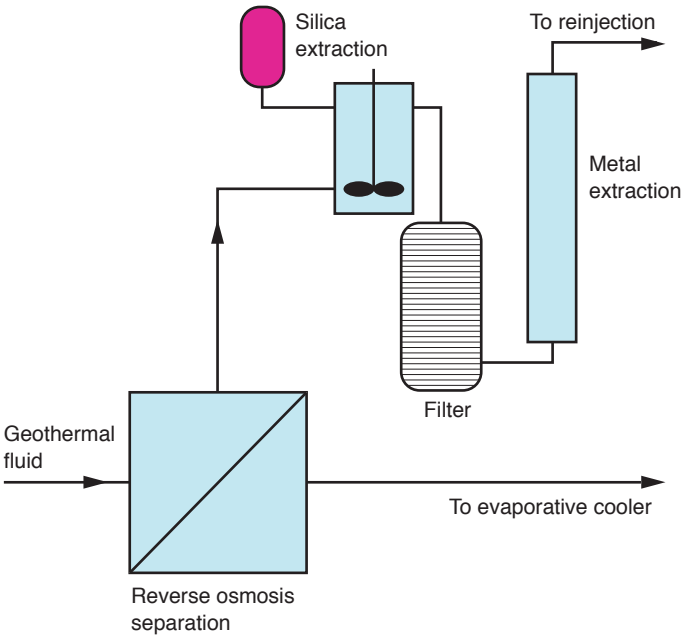
Lawrence Livermore has developed a technology for extracting silica from geothermal fluids, allowing plants to work more efficiently and have a marketable silica by-product. Once the silica is removed, the door is open to mining other metals from the geothermal brine as well, including lithium (used in ceramics and batteries) and tungsten. Another benefit to silica extraction is the production of freshwater that can be used as a heat exchanger coolant to further increase power production.

A New Bonanza?

The silica-mining story got a big boost three years ago when the California Energy Commission staff suggested to Livermore geochemists Bill Bourcier and Carol Bruton that it would be advantageous to find a way to extract lithium from geothermal resources. On the commercial market, a pound of lithium commands as much as $2.50. Some geothermal systems bring to the surface and then reinject over 50 metric tons of lithium per day, which means a mineral by-product worth upward of $500 million per year is being thrown away.

"Before considering lithium extraction," says Bourcier, "we had to deal with the silica in the geothermal fluid, which clogs up tanks, pipes, and other equipment. Finding a way to extract silica from the fluid is key to this type of 'cascaded use' of geothermal energy—that is, extracting not only heat for energy but also marketable by-products, such as silica and other minerals, for resale."

In 2002, Livermore scientists were able to pursue this concept when they were awarded a $669,683 grant from the California Energy Commission's (CEC's) Public Interest Energy Research (PIER) Program with cofunding from the Department of Energy's Geothermal Technologies Program. Livermore and Mammoth Pacific LP formed an agreement allowing the scientists to conduct their research at the geothermal power plant in Mammoth Lakes, California.



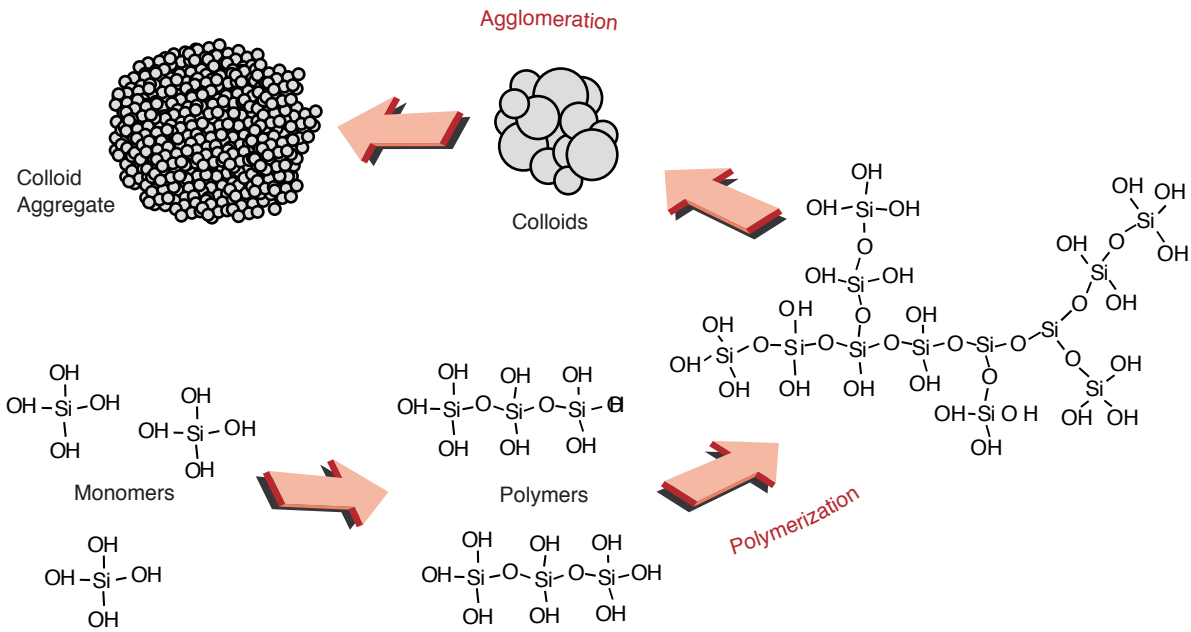
The Livermore extraction process involves running a geothermal fluid through a reverse-osmosis separation process to create freshwater and concentrated brine. The freshwater is used for evaporative cooling, and the concentrated brine is pumped into a reactor where chemicals are added and silica is extracted. The silica-free brine can then be pumped through another process for extraction of other metals before the fluid is pumped to a surface pond and reinjected into the subsurface.

"Power plant managers wanted freshwater for cooling and a silica by-product that could be resold," says program leader Bruton. "Production of marketable by-products reduces the cost of geothermal power, which is a goal of the CEC's PIER Program. Mammoth Pacific was willing to let us come test our process at their facility in return for our results. With these results, their managers could evaluate the economic benefits of full-scale implementation. So we set up a small field station and mobile laboratory at the geothermal plant for our experiments."

The Livermore-developed extraction process begins with geothermal fluid obtained upstream from the power plant's air-cooled heat exchangers. The silica is concentrated in the fluid using reverse osmosis—the same process used at water treatment plants to purify water. (See the box p. 27.) The concentrated fluid then flows through a stirred reactor where salts or polyelectrolytes are added to induce silica precipitation. The simple silica molecules bond together to form colloids—silica particles about 10 to 100 nanometers in size. These larger molecules cluster to form particles that can be removed by filters downstream from the reactor.

The scientists discovered that the properties of the silica can be varied by changing the silica's residence time in the reactor, varying the pH of the fluid, changing the amounts of additives, and changing the silica concentration. The variables interrelate—for example, shorter residence times produce smaller silica particles that are more difficult to filter but are of higher value. Longer residence times and higher additive concentrations

The Livermore extraction process allows scientists to control the size of colloids and agglomerates so that their surface areas and pore sizes match those of commercially useful silicas. The compound involved consists of silicon (Si) atoms surrounded by hydroxyl (OH) groups composed of oxygen and hydrogen.



produce more firmly agglomerated particles that are relatively easy to filter but less suited to high-end commercial applications. Bourcier notes, "The properties of the silica must match the particular market needs. For instance, the size of the silica clusters and the silica purity are important when silica is used to increase rubber lifetime or as a polishing agent for silicon wafers in the electronics industry."

Presently, the Livermore scientists can produce silica with a purity of greater than 99 percent and surface areas ranging from 50 to 150 square meters per gram. In addition, the water obtained from the reverse-osmosis process has less than 100 parts per million total salt and less than 20 parts per million silica, making it ideal for cooling applications at the power plant.

Minerals for the Mining Industry

The market value of silica that could potentially be produced from the Mammoth plant is about $10 million per year, based on both the typical market price of 70 cents per pound for precipitated silica used in rubber manufacturing and a recovery rate of 7,200 tons per year. For the process that treats and extracts silica from the entire fluid stream, a preliminary economic evaluation suggests the equipment would be paid for in 7 years, and the rate of return on the investment would be about 16 percent.

To date, the researcher's work has focused on silica extraction, but extracting other mineral by-products, including lithium, is not far behind. "Many other metals could be 'mined' at Mammoth," says Bourcier. "In addition to lithium, the geothermal fluid contains tungsten and two materials with no other known sources in the U.S.—cesium and rubidium."

The silica extraction project has been funded by the CEC at $737,000 for the next steps, which are to conduct a continuous pilot-scale process test and an economic analysis of the results. "So far, so good," says Bruton. "For Mammoth Pacific, we've developed an extraction process for silica, and a source of clean water for cooling. For the geothermal industry as a whole, we've found a way to create a new geothermal revenue stream through mineral extraction and a methodology for making silica with tailored properties. Other U.S. industries can look forward to a source of low-cost silica as well as a domestic and 'green' source for other metals."

—Ann Parker

Key Words: cascaded use, geothermal energy, geothermal mining, Mammoth Lakes, silica extraction.

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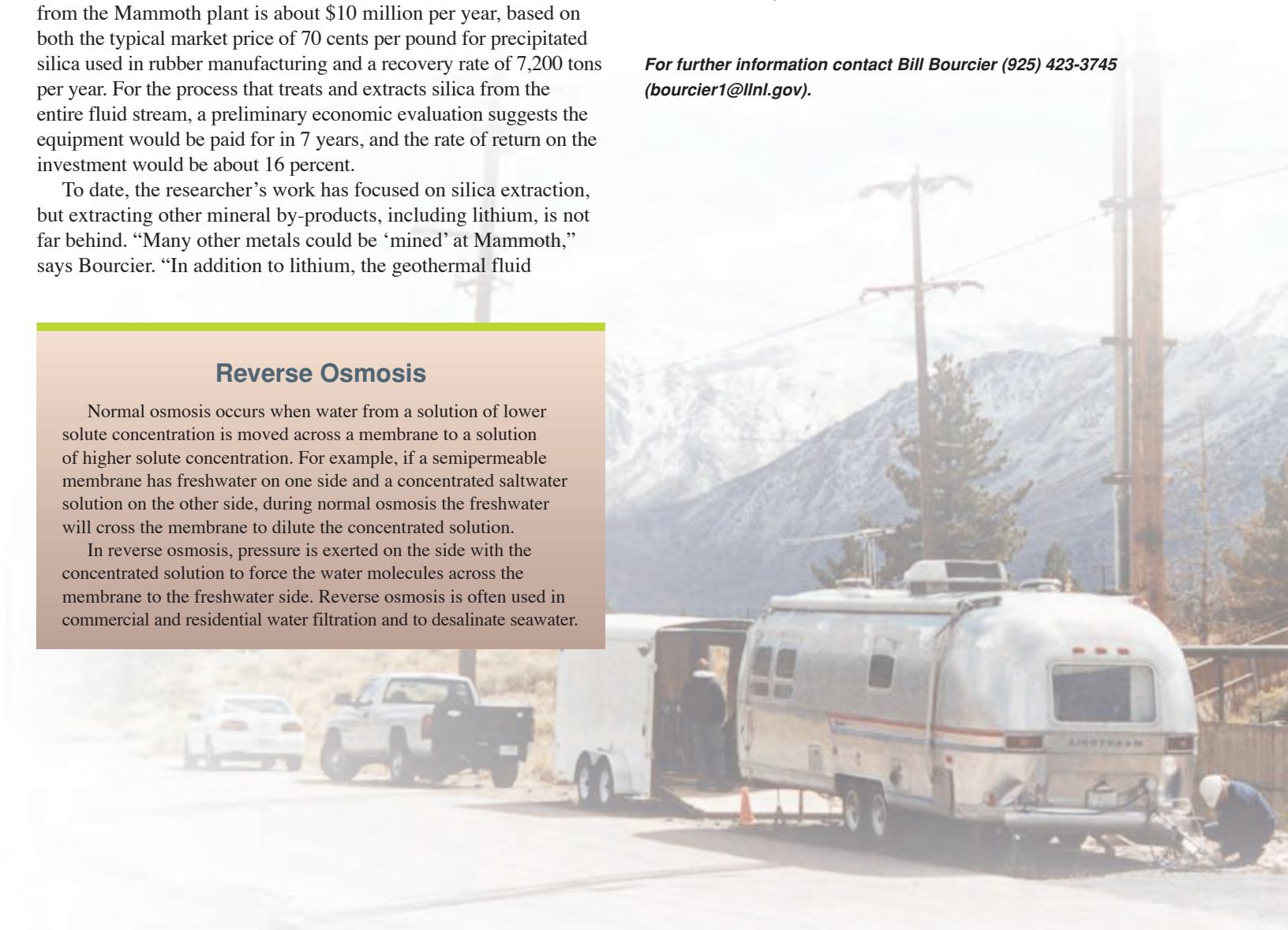
Reverse Osmosis

Normal osmosis occurs when water from a solution of lower solute concentration is moved across a membrane to a solution of higher solute concentration. For example, if a semipermeable membrane has freshwater on one side and a concentrated saltwater solution on the other side, during normal osmosis the freshwater will cross the membrane to dilute the concentrated solution.

In reverse osmosis, pressure is exerted on the side with the concentrated solution to force the water molecules across the membrane to the freshwater side. Reverse osmosis is often used in commercial and residential water filtration and to desalinate seawater.



Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Laser Peening of Thin Cross-Section Components

Lloyd A. Hackel, John M. Halpin, Fritz B. Harris, Jr.
U.S. Patent 6,805,970 B2
October 19, 2004
The properties of a metal piece are altered by laser peening the piece on the first side using an acoustic-coupling material connected to the second side and then laser peening the piece on the second side using an acoustic-coupling material connected to the first side.

Solid Materials for Removing Metals and a Fabrication Method

Paul R. Coronado, John G. Reynolds, Sabre J. Coleman
U.S. Patent 6,806,227 B2
October 19, 2004
Solid materials were developed to remove contaminating metals and organic compounds from aqueous media. The contaminants are removed by passing the aqueous phase through the solid materials, which can be in molded, granular, or powder form. The solid materials adsorb the metals and organics, leaving a purified aqueous stream. The solid materials consist of solgel or solgel and granulated activated carbon mixtures. The species-specific adsorption occurs through specific chemical modifications of the solids tailored toward the contaminant(s). The contaminated solid materials can then be disposed, or the contaminant can be removed and the solids recycled.

Preparation of Hydrophobic Organic Aerogels

Theodore F. Baumann, Joe H. Satcher, Jr., Alexander E. Gash
U.S. Patent 6,806,299 B2
October 19, 2004
These synthetic methods are used to prepare hydrophobic organic aerogels. One method involves the solgel polymerization of 1,3-dimethoxybenzene or 1,3,5-trimethoxybenzene with formaldehyde in nonaqueous solvents. In a procedure analogous to the preparation of resorcinolformaldehyde aerogels, this approach generates wet gels. These gels can be dried using either supercritical solvent extraction to generate new organic aerogels or air-dried to produce an xerogel. Other methods involve the solgel polymerization of 1,3,5-trihydroxybenzene (phloroglucinol) or 1,3-dihydroxybenzene (resorcinol) and various aldehydes in nonaqueous solvents. These methods use a procedure analogous to the one- and two-step base acid–catalyzed polycondensation of phloroglucinol and formaldehyde, but the base catalyst is triethylamine. The methods can be applied to a variety of other solgel precursors and solvent systems. These hydrophobic organic aerogels have numerous applications for material absorbers and waterproof insulation.

Awards

Director Emeritus **Bruce Tarter** was awarded the **Department of Energy**'s (DOE's) **Gold Award**, its highest honorary award, during a special ceremony October 25, 2004, at the Woodrow Wilson Center for Scholars in Washington, DC. Former Energy Secretary Spencer Abraham presented the award to Tarter. The award was given in recognition of outstanding contributions to DOE while serving as director of Lawrence Livermore from 1994 through 2002.

Under Tarter's leadership, the citation reads, "the Lab demonstrated extraordinary achievement in its mission to ensure national security and apply science and technology to the important problems of our time. A driving force in the Lab's transition to a post–Cold War nuclear weapons world, [Tarter] helped transform the nuclear weapons program from a 'design, test, and build' approach to a science-based Stockpile Stewardship effort focused on assessment, safety, reliability, and performance of the Lab's designed warheads." Tarter "also initiated impressive programs in areas of nonprofliferation and counter-terrorism and in energy, environment and bioscience."

Ron Hafner of Livermore's Engineering Directorate is one of the 25 recipients of the **National Weather Service**'s (NWS's) annual **Holm Award**. Named after John Campanius Holm, the award was created in 1959 as a way for NWS to honor cooperative accomplishments in the field of meteorological observation. More than 11,000 people and organizations across the nation participate in NWS's cooperative observer program, which began 120 years ago.

In June 1981, Hafner began taking daily measurements. He became the seventh person to participate in the unbroken chain of continuous weather readings in Livermore, which date back to March 1870. Hafner sends his monthly data to NWS in Ashville, North Carolina, where it combines the statistics from all of the cooperative weather observers throughout the nation. The data provide the historical climatological record for the U.S.

Abstracts

Experiment and Theory Have a New Partner: Simulation

From the beginning, Lawrence Livermore has invested in supercomputers, with each generation bringing scientific insights. Today's scientists use powerful machines and codes for computer simulations that have changed the way science is done at Livermore—with experiment and simulation more tightly coupled than ever, as are theory and computation. Simulations can now mimic the physical world down to the interactions of individual atoms, allowing scientists to conduct electronic "experiments" where real experiments would be too difficult or expensive to perform or would raise environmental or safety issues. The design of anticancer drugs, the slow changes that occur in nuclear waste repositories over centuries, the interactions of plasma with laser light from nanosecond to nanosecond, the discovery of a new melt curve of hydrogen at extreme pressures—all of these and more are the results of complex simulations on Livermore's supercomputers.

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Russian Weapons Workers Begin New Commercial Ventures

The National Nuclear Security Administration's Russian Transition Initiatives comprise two nonproliferation programs focused on the states of the former Soviet Union (FSU). Both of these programs, the Initiatives for Proliferation Prevention (IPP) and the Nuclear Cities Initiative (NCI), attempt to develop self-sustaining, nonweapons work for current and former weapons scientists, engineers, and technicians. Established in 1994, the IPP promotes collaborative projects among Department of Energy national laboratories, U.S. private-industry partners, and weapons institutes in the FSU. Projects are selected for their commercial potential and are designed to lead to long-term employment in the civilian sector for former weapons workers. The NCI was established in 1998 under a government-to-government agreement to help Russia reduce the size of its nuclear weapons complex. The program is active in three of Russia's ten closed nuclear cities—Sarov, Seversk, Snezhinsk—and is planning to work with a fourth, Zheleznogorsk.

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U.S. Government Printing Office: 2005/783-059-10003

Finding the Source of Nuclear Materials

Nuclear forensics researchers are developing methods to analyze intercepted nuclear materials and trace them back to the source.

Also in March

- *Livermore scientists are fostering communication among scientists in two critical regions—Central Asia and the Middle East.*
- *Computer models indicate that gamma-ray bursts from dying stars may be important sources of elements such as iron, zinc, titanium, and calcium.*
- *Earth scientists are answering geologic and environmental questions by examining complex geophysical conditions in a laboratory setting.*

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