June 2003

Science & Technology REVIEW

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

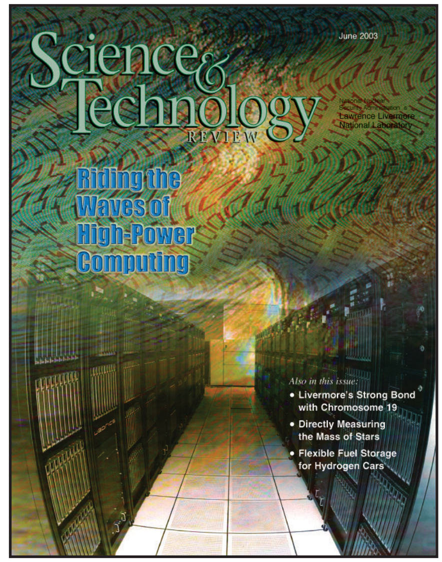
Riding the Waves of High-Power Computing

Also in this issue:

- Livermore's Strong Bond with Chromosome 19
- Directly Measuring the Mass of Stars
- Flexible Fuel Storage for Hydrogen Cars

About the Cover

Since the Advanced Simulation and Computing Program began in 1995, Livermore has been a leader in the push to develop massively parallel scalable supercomputing systems to support the nation's Stockpile Stewardship Program. To continue to meet these and other supercomputing needs, the Laboratory is pursuing a three-pronged strategy to provide increasingly powerful, cost-effective high-performance computational capability and capacity to a variety of users. The article beginning on p. 4 reports on this strategy and reveals how Livermore is supporting the goal of providing multiple-petascale (quadrillion calculations per second) computing power by 2010.



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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 assuring 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.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str/.

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Lawrence Livermore National Laboratory

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Features

Research Highlights

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Space technologies adapted to fight terrorism

Detection technologies developed by Livermore researchers to study astrophysical phenomena such as black holes and supernovas have a new down-to-earth application—helping to fight terrorism. Now, technologies for finding and imaging space phenomena are assisting in the detection of nuclear materials or devices.

One such technology is the High-Energy Focusing Telescope (HEFT), scheduled to be launched in the fall of 2003. HEFT will be used primarily to study how supernovas create and distribute most of the elements heavier than helium. The telescope's integrated circuits work in conjunction with cadmium–zinc–telluride crystals to detect and measure faint gamma-ray signals. HEFT's mirrors focus the gamma rays into imaging detectors to produce clear pictures with high spectral resolution.

Simon Labov, the director of Livermore's Radiation Detection Center, explains that "In both astrophysics and nuclear materials, the emissions are faint, and there is a lot of background noise. Having advanced high-sensitivity detectors can solve both problems. In effect, the efforts of about 50 researchers and $20 million spent during the past 5 years is being leveraged for detecting nuclear materials" to combat terrorism and support homeland security.

Detector technologies for studying black holes in space will also be used in small hand-held detectors for finding and analyzing nuclear materials on Earth.

Contact: Simon Labov (925) 423-3818 (labov1@llnl.gov).

Uncertainties found in global warming satellite data

Using a new analysis of satellite temperature measurements, a research team including Livermore scientists has discovered that satellite data used to measure temperature changes in various layers of the atmosphere contain uncertainties that may hamper the detection of human effects on climate change.

Since 1979, microwave sounding units (MSUs) flown on 12 polar-orbiting U.S. weather satellites have measured the microwave emissions of oxygen molecules, which are related to atmospheric temperature. By monitoring these emissions at different frequencies, researchers can work backward to determine temperature changes in various layers of the atmosphere.

Analysis of MSU data, which until recently was done solely by researchers from the University of Alabama at Huntsville, has indicated little or no warming of the troposphere (the lowest layer of the atmosphere) since 1979. These findings bring into question both the reality of human-induced global warming and the reliability of computer climate models that predict tropospheric warming in response to increases in greenhouse gases. The University of Alabama results are also at odds with thermometer measurements indicating pronounced warming of Earth's surface during the satellite era.

Analysis of MSU data is, however, complicated by factors such as the gradual decay and drift of satellite orbits, which affect the time of day at which MSUs measure atmospheric temperatures, and by problems with MSU calibration.

Recently, a group of researchers led by Carl Mears, Matthias Schabel, and Frank Wentz of Remote Sensing Systems in Santa Rosa, California, conducted an independent analysis of the raw MSU data. Using different methods to correct for satellite orbital drift and calibration problems, they found that the troposphere probably warmed by roughly 0.18°F per decade from 1979 to 2001, for a total rise in tropospheric temperature of 0.4°F over that period.

Livermore scientists Benjamin Santer, Karl Taylor, James Boyle, and Charles Doutriaux, along with researchers from Remote Sensing Systems, the National Center for Atmospheric Research, Lawrence Berkeley National Laboratory, and the University of Birmingham in England, are exploring the implications of these uncertainties for the study of human effects on climate. Their findings are reported in the May 1, 2003, edition of *Science Express*, the online publication of *Science* magazine.

The team's modeling yielded detailed patterns, or fingerprints, of tropospheric temperature change. These fingerprints are identifiable in the Remote Sensing Systems analysis of MSU data showing a warming troposphere, but not in the University of Alabama analysis.

According to Livermore's Santer, lead author of the *Science Express* paper, "In the last 24 years, satellites have helped us observe the climate of our planet more intensively and systematically than at any other time in Earth's history. Yet even over the satellite era, there are still large uncertainties in our estimates of how tropospheric temperatures have changed. It's important to take these uncertainties into account in evaluating the reliability of climate models. . . . Our detection results point toward a real need to reduce current levels of uncertainty in satellite temperature measurements."

Contact: Benjamin Santer (925) 422-7638 (santer1@llnl.gov).

Livermore's Three-Pronged Strategy for High-Performance Computing

IN 1995, the Advanced Simulation and Computing (ASC) Program (originally the Accelerated Strategic Computing Initiative, or ASCI) was formed as a critical element of the Stockpile Stewardship Program. ASC's purpose is to accelerate the development of the simulation capabilities needed to analyze the performance, safety, and reliability of nuclear weapons.

At the beginning of the ASC Program, we looked at the kinds of problems we would need to solve, when we needed to be able to solve them, and how quickly we would need to get calculation results back. This analysis determined the size of the computers we set out to acquire through partnerships with computer industry leaders. Our goal was to obtain a a computer system by 2004 that could process 100 trillion floating point operations per second (teraflops). In the past 8 years, Livermore, Los Alamos, and Sandia—the three national laboratories involved in ASC—have fielded a number of increasingly powerful massively parallel scalable supercomputers, that is, large numbers of processors working together on complex calculations. ASCI Purple, arriving at Livermore next year, will be the fulfillment of the original ASC 100-teraflops goal. But the story does not end there.

As the supercomputers came on board, researchers in stockpile stewardship and other programs developed increasingly complex codes to take advantage of them. One-dimensional codes gave way to two- and three-dimensional codes, and some science simulations were developed based on first-principles physics. Users needed more from the supercomputers—more capability to run scientific calculations at large scale and more capacity to simultaneously handle multiple calculations and diverse workloads. As our users' needs have evolved, so has our strategy described in the article beginning on p. 4.

In brief, our strategy is to work with the U.S. supercomputer industry to pursue three technology curves, separately and at times in tandem. The three curves are current scalable multiprocessor technology, open-source (nonproprietary) cluster technology, and cell-based (computer-on-a-chip) technology. The goal is to deliver platforms best suited to the work at hand. The supercomputing industry has chosen to pursue massively parallel scalable architectures, and it is spending billions of dollars exploring technologies in this arena. We work with these companies to leverage their advances and investments, bringing more capability and capacity cost-effectively to our users. We are constantly on the lookout for "what's next" and what's "after next" to meet future workloads. Our goal is to find an affordable path to the petaflops (1,000 teraflops) level for the ASC Program by 2010—beating the speed of Moore's Law (capacity doubling every 18 months) not just by a little but by a lot.

Today's ASC Program uses proven and mature technologies, because there's no room for risk in system functionality and reliability when simulating on tight programmatic schedules the behavior of nuclear weapons. To determine our next-generation supercomputer, we have been investigating machines featuring open-source cluster technology. This technology is the basis of our recently deployed Multiprogrammatic Capability Resource (MCR) machine, which is being used by Laboratory researchers who can tolerate some problems with functionality as we work out the bugs and add features for a production environment. In preparation for what's after that, we are researching technology that's farther out on the horizon—cell-based supercomputers. Assuming that budgets and the technology hold, we will acquire such a cell-based machine, BlueGene/L, in late 2004 or early 2005. BlueGene/L will be used to improve physics models in ASC codes and to evaluate the technology for suitability to a broader workload.

This is our strategy for staying ahead of Moore's Law—a strategy that is absolutely crucial to the Laboratory. Here at Livermore, we have a culture that supports and embraces simulation, which, with experimentation and theory, forms the scientific discovery process. A successful simulation environment requires more than a huge computer with maximum peak speeds. It requires code development, physics models, code validation, and an infrastructure—storage systems, visualization capabilities, networks, compilers, debuggers—all working together. We must balance all these factors to maintain a computing environment that has the power, capability, and capacity to serve the Laboratory's needs in stockpile stewardship, energy and environment, biotechnology and bioresearch, chemistry and material science, and more.

Pursuing three technology curves—what's current, what's next, and what's after next—and working with U.S. industry to bring the technologies to the nation's critical missions is Livermore's computing strategy. This three-pronged strategy allows us to deliver robust production-level computing to meet today's programmatic needs while looking ahead to provide for the demands of tomorrow.

■ Dona Crawford is associate director for Computation.

Riding the Waves of Supercomputing Technology

Looking toward the future, Livermore's Computation Directorate leverages three high-performance, cost-effective technology curves to deliver computing capability at a faster rate than described by Moore's Law.

BUILDING supercomputers powerful enough to run complex simulations of the performance of nuclear weapons is a challenge that the National Nuclear Security Administration's (NNSA's) Advanced Simulation and Computing (ASC, formerly ASCI) Program has met full on since its beginning in 1995. But even as the capabilities of the ASCI machines—Red, Blue, White, Q, and the upcoming Purple—have grown, so have the sophistication of the applications and the number of users eager to run their simulations.

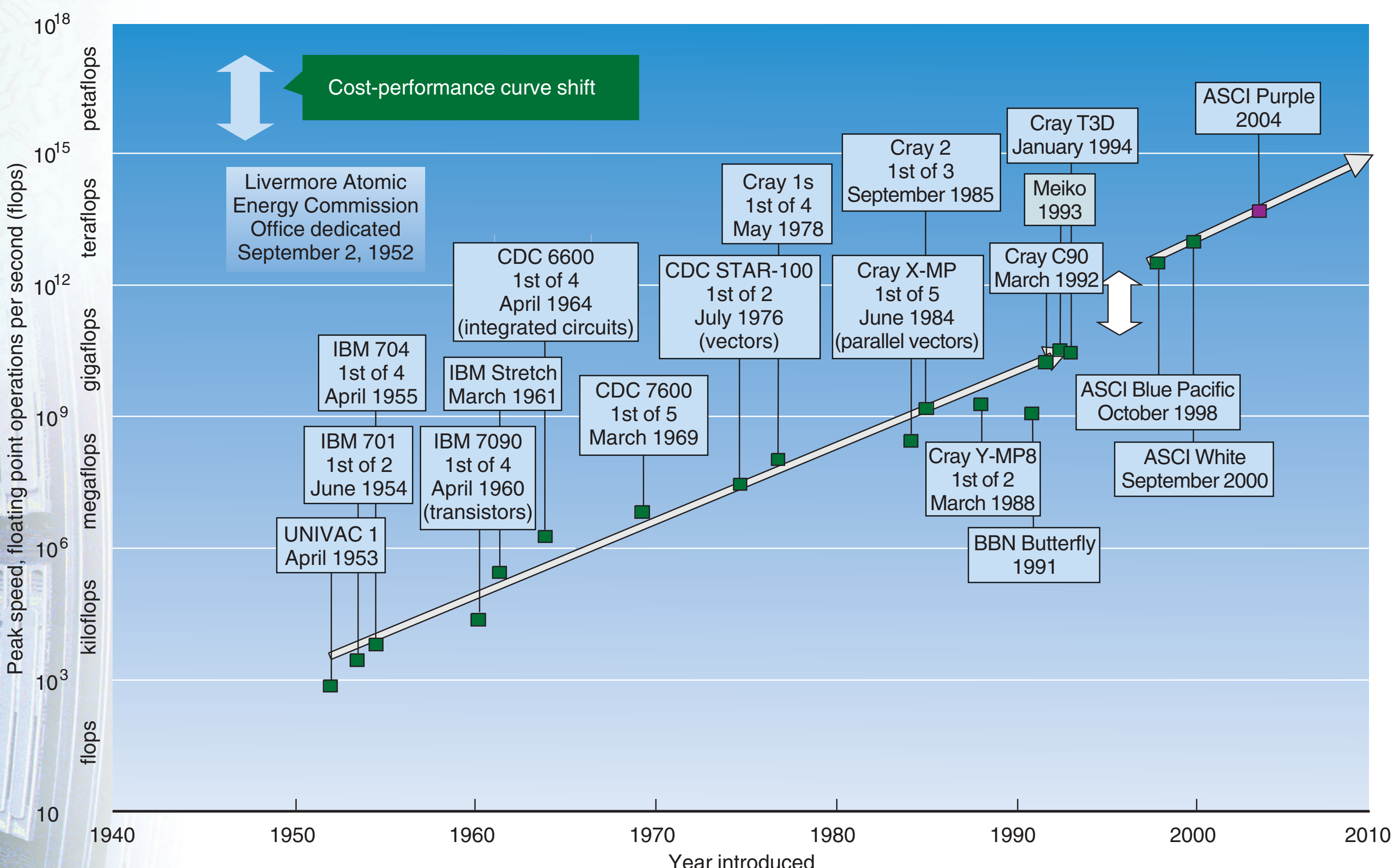
Livermore's users, like their counterparts at Los Alamos and Sandia, include not only weapons scientists who run simulations for NNSA's Stockpile Stewardship Program, but also researchers whose simulations of, say, plasma instabilities or the performance of insensitive high explosives feed vital information into stockpile stewardship efforts. In addition, other scientists working on research important to Livermore's overall national security mission—for example, nuclear nonproliferation, detection of underground structures, nondestructive evaluation, earthquake hazard analysis, or oil exploration—want to run simulations on ASCI-caliber supercomputers available through Livermore's Multiprogrammatic and Institutional Computing (M&IC) Initiative. With ASC and ASCI-class machines, there always seems to be a need for more—more capability to run scientific calculations at large scale and more capacity to process a varied workload from many users simultaneously.

As Michel McCoy, head of the Integrated Computing and Communications Department (ICCD), notes, Livermore is in many ways a victim of its own success. "Because three-dimensional code development funded by ASC and other programs has been so successful at Livermore," he explains, "the demand for supercomputing capability and capacity to explore complex scientific issues has become enormous. Someday, even the 100-teraflops [trillion floating point operations per second] Purple machine will not be powerful enough to help us answer these big science questions. The demands of classified stockpile stewardship simulations, which have the highest priority, can crowd out the classified basic science calculations related to stockpile stewardship that run on ASCI machines. We're also faced with the issue of how to accommodate unclassified basic science applications that are, nevertheless, important to the ASC Program's mission. Add to all of this the science problems from a multitude of Laboratory programs that can't be solved without help from ASCI-class supercomputers, and the need for more supercomputing capability and capacity increases further."

The only way to generate the type of capability required, says McCoy, is to deliver computing capability faster than the rate described by Moore's Law, which states that processing power doubles every 18 months. And the rate must be faster not just by a little, but by a lot. "If we continue to follow the existing technology curve, namely, vendor-integrated multiprocessor platforms, we will not get to multiple petaflops by 2010."

To meet the ever-growing needs of the ASC Program and the rest of the scientific community, Livermore's Computation Directorate is implementing a computing strategy that promotes switching to and straddling new cost–performance computer technology curves, or waves—a balancing act of timing, prescience, and prediction. To get where it needs to be and deliver capacity and capability at low cost, Livermore must jump from the wave of present technology to the next new technology wave at the right time—and ride not just one wave, or two, but three of these technology waves simultaneously. Each wave can provide benefits to some area of scientific research, even when the technology is new and unproven. As the technology matures, the new system becomes useful to additional kinds of research.

McCoy points out that the tri-laboratory ASC Program and the institutionally funded M&IC program have cooperated and leveraged expertise to exploit the various capability–capacity technology curves. In particular, ASC has funded Livermore's Computer Center and its



The history of supercomputing at Livermore includes jumps between technology curves to gain cost effectiveness and increased speed and capability. If supercomputing continues on the present curve, it will approach a quadrillion floating point operations per second (petaflops) by 2010 but will not reach the goal of multiple petaflops.

large base of expertise in the field of ASCI computers, and the Laboratory has leveraged this expertise and funded alternative high-performance, cost-effective supercomputing technologies for institutional users. "This synergy benefits both parties," says McCoy. For ASC, it accelerates the rate at which the new technologies mature. For the institution, it provides cost-effective supercomputer capacity and capability across the Laboratory.

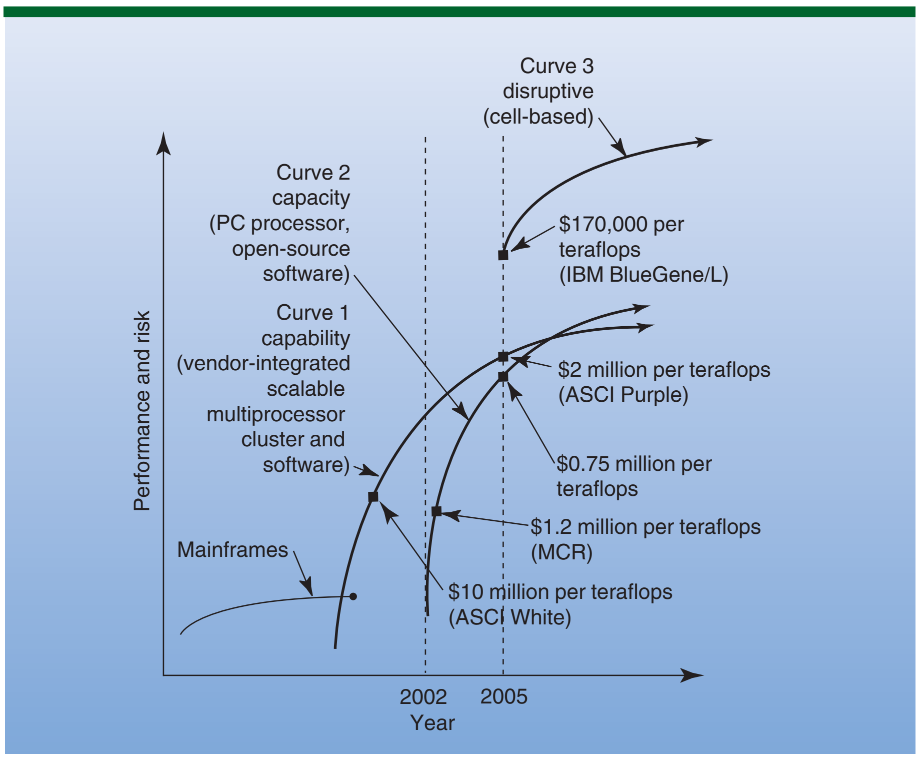
This type of synergy is not new at Livermore. Earlier, the Laboratory worked with Compaq and Quadrics to develop the TeraCluster2000 (TC2K) which is part of M&IC. (See *S&TR*, October 2001, pp. 4–12.) The partnership with Compaq on TC2K made possible Compaq's successful bid for ASCI Q at Los Alamos and the computer funded by the National Science Foundation at the Pittsburgh Supercomputing Center.

Riding the Technology Waves

Livermore has made jumps from one computing technology to another in the past. First were the mainframes, followed in the 1970s by vector supercomputers and in the late 1980s by massively parallel processing supercomputers. With the cessation of underground testing of nuclear devices in 1992 and the birth of the Stockpile Stewardship Program the following year came the need for much better computer simulations to help ensure that the nation's nuclear weapons stockpile remained safe, reliable, and operational.

The ASC Program was created to provide the integrating simulation and modeling capabilities and technologies needed to combine new and old experimental data, past nuclear test data, and past design and engineering experience. The result is a powerful tool for future design assessment and certification of nuclear weapons and their components. ASC required machines that could cost-effectively run simulations at trillions of floating point operations per second. This requirement forced a sea change in the supercomputing industry and a jump to another technology wave—massively parallel scalable supercomputers.

The ASCI machines use many thousands of reduced instruction set computer (RISC) processors—a class of processors found in workstations—working in unison instead of the more expensive, one-of-a-kind specialized processors characteristic of earlier parallel processing. ASCI machines delivered "more bang for the buck." Code developers benefited as well. "In about six years," adds McCoy, "we went from systems where one-dimensional codes were routine and two-dimensional codes were possible, but a stretch, to ASCI systems where



Since any given computing technology curve is ultimately limited by Moore's Law, Livermore's Computation Directorate is embracing a strategy to straddle and, when the time is right, switch to new technology curves. Vendor-integrated massively parallel ASCI machines are the current workhorses of the ASC Program. The Linux cluster machine typified by Multiprogrammatic Capability Resource (MCR) will lead to the next-generation production systems. Cell-based technology, such as that to be used in BlueGene/L, appears to be an affordable path to petaflops systems. Only time will tell whether other cost-effective paths will emerge that might lead to the petaflops regime.

2D is the norm and 3D calculations are done, but are sometimes a stretch."

By all accounts, the ASC Program has been remarkably successful in meeting its goals. Its machines are the workhorse computers for running the complex two-dimensional and three-dimensional codes used to meet the nation's most demanding stockpile stewardship requirements. "These machines and their codes are proven," says Mark Seager, assistant department head for platforms in ICCD. "They are used routinely for stockpile stewardship and for must-have deliverables. These machines and the codes that run on them are reliable and trusted, both of which are a necessity for stockpile stewardship. There's no room for error when simulating nuclear weapons."

With each ASCI system, the cost per teraflops fell as technology advanced. For Livermore's ASCI White, the cost was $10 million per teraflops. For ASCI Q, a Los Alamos machine, the cost is $7 million per teraflops. For ASCI Purple, an upcoming Livermore machine, the estimate is $2 million per teraflops. But now, this particular technology curve—vendor-integrated systems using high-performance workstation processors and proprietary vendor software—has matured to the point where the cost per teraflops improves at only a slow exponential rate as dictated by Moore's Law. So people such as McCoy and Seager are looking at technologies that can be exploited at better cost performance after the 100-teraflops Purple. They are also interested in building smaller-capacity machines at much lower cost.

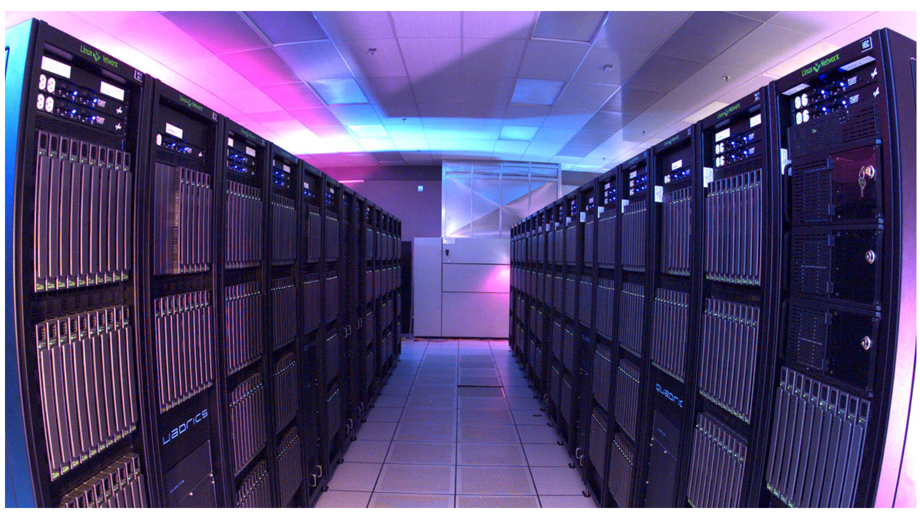
Two new technologies hold promise. A near-term technology based on cluster architecture—that is, large groups of interconnected commodity microprocessors (the type found in desktop personal computers and laptops)—combined with open-source, or nonproprietary, software is epitomized in the Multiprogrammatic Capability Resource (MCR) system. Farther in the future are cell-based supercomputers that would use system-on-a-chip technology and low-cost, low-power embedded microprocessors. This third technology is embodied in BlueGene/L, a system designed by IBM and slated for delivery to Livermore in December 2004.

Next on the ASCI Crest

ASCI Purple will the fulfill the goal set in 1996 to achieve 100 teraflops by mid-decade for stockpile stewardship use. Purple will have a peak performance (100 teraflops) equivalent to 25,000 high-end personal computers. It will have 50 trillion bytes of memory and 2 petabytes of disk storage capacity, the equivalent of a billion books or about 30 times the contents of the Library of Congress. About the size of two basketball courts, Purple will have more than 12,000 IBM Power5 microprocessors. It will allow scientists to run a full-physics, full-system model of a nuclear weapon in three dimensions.

ASCI Purple will be eight times more powerful than ASCI White, which was the first ASCI system powerful enough to investigate crack propagation in the materials of a nuclear weapon in three dimensions. A major step forward, Purple will allow designers and code developers to focus increasingly on improving physics models. For instance, if weapon designers need to change some element of the weapon, they can insert this change into the initial conditions of the simulation, and the recalculation will show them the effect of the changes. One three-dimensional simulation representing the operation of the weapon system for a fraction of a second will still take about eight weeks of computing time.

Sometime between October and December 2003, the Early Delivery Technology Vehicle (EDTV) will be available at Livermore as part of the Purple contract. EDTV will consist of at least 32 nodes and feature the new IBM Federation switch, the node interconnect that is being used on Purple. "Having EDTV here first will help us avoid some issues we faced



The Multiprogrammatic Capability Resource at Livermore combines open-source software and cluster architecture to provide Advanced Simulation and Computing–level supercomputing power for unclassified research.

Simulating Laser–Plasma Interactions

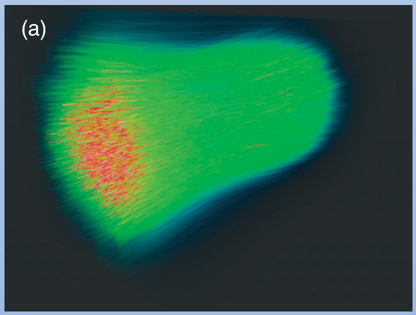
Using the Laboratory's recently installed Multiprogrammatic Capability Resource (MCR) system, physicists Steven Langer and Bert Still spent the early part of 2003 simulating an experiment scheduled to occur this summer on the National Ignition Facility's (NIF's) Early Light (NEL) system. NEL consists of the first four beams of NIF and was first fired at high power in December 2002.

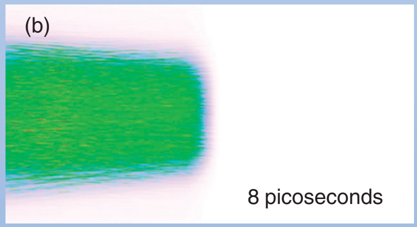
The experiment simulated by Langer and Still will study laser–plasma interactions under conditions similar to those that will be found in hohlraum targets in future NIF ignition experiments. (A hohlraum is a small, cylindrical chamber used to enclose the target in experiments on high-power lasers.) A NIF laser beam has to cross roughly 5 millimeters of plasma between the laser entrance hole and the gold wall of the hohlraum. The laser heats the wall so much that the wall emits x rays in a configuration designed to uniformly bombard a spherical capsule at the center of the hohlraum, squeezing it down until it reaches fusion temperatures and pressures.

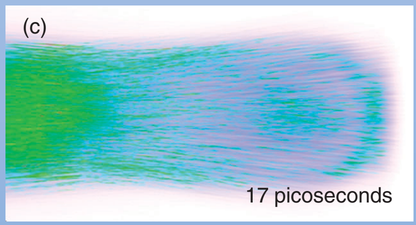
The experiment will use a 4.5- by 4.5- by 5.5-millimeter plastic bag filled with neopentane gas. The gas inside the bag will be quickly ionized, creating a plasma that will be a reasonable surrogate of that in the actual NIF target, and the NEL beams will pass through it. It is this interaction of light and plasma that Still and Langer sought to simulate with the code PF3D, which Still and others began developing in the mid-1990s.

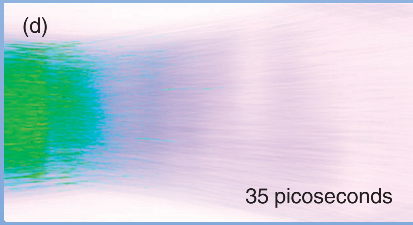
In the simulation, the laser beam passes through the central portion of a 1- by 1- by 5-millimeter plasma. "Our physics algorithms constrain a computational cell, or zone, to be only slightly larger than the wavelength of the laser light, which is 0.35 micrometers," explained Langer. "We ended up using 6.8 billion cells in the calculation, which is an enormous number of cells."

The simulation ran for 10 days on 1,920 of MCR's processors to simulate 35 picoseconds, the time it will take for the laser light to travel 5 millimeters twice. Results from the simulation occupy about 14 terabytes of archival storage, which, Langer notes, was roughly 25 percent of all the information written to storage at the Laboratory in February 2003. None of Livermore's existing volume visualization programs could handle a 6.8-billion-zone simulation with a lot of fine-scale structure. Mark Duchaineau, supported by the Advanced Simulation and Computing Program's Visual Interactive Environment for Weapons Simulation project, wrote a software volume visualization program that would handle the data.







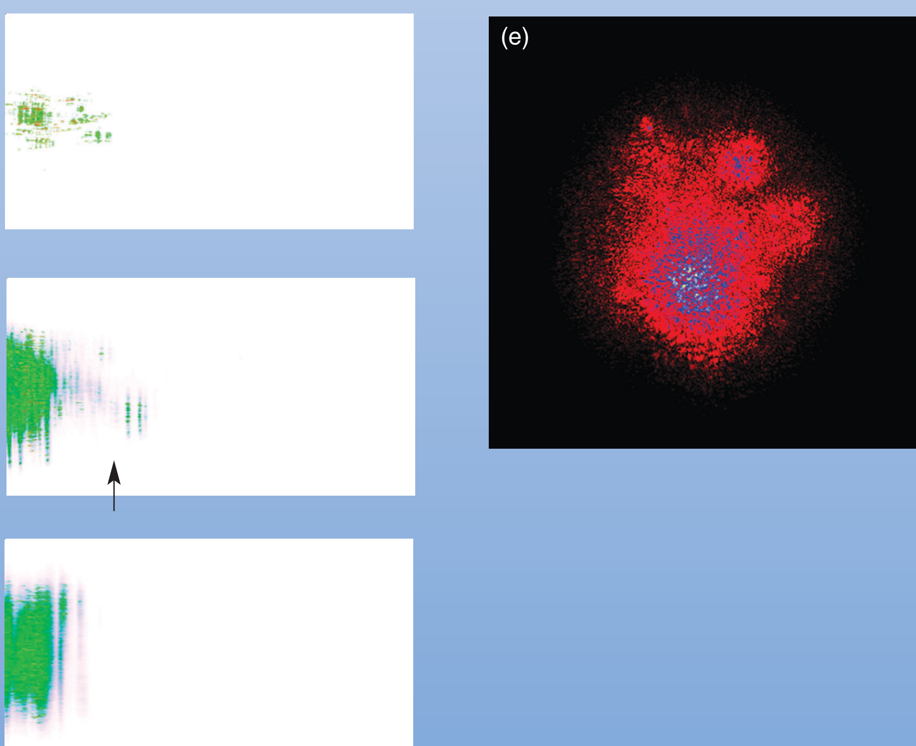


This volume visualization of a simulation done on the Multiprogrammatic Capability Resource shows a National Ignition Facility laser beam as it passes through a hot plasma. A cross section of the laser beam has many small, bright spots. These bright spots form long, thin filaments as they pass through the plasma. The lowest intensities are blue, intermediate intensities are green and yellow, and the highest intensities are red. (a) This oblique view shows that the brightest (red) filaments are concentrated in the core of the beam. (b) This side-on view shows that after 8 picoseconds, the laser (left) has penetrated halfway through the plasma. Scattering (right) is weak. (c) After 17 picoseconds, the laser beam (left) has almost reached the back of the simulation volume. Scattered light (right) is strong, and most of the laser light is absorbed or scattered (as intended in the experimental design). (d) After 35 picoseconds, the transmitted laser light (left) is spread into a wider cone, and the scattered light (right) is still strong. (e) Scattered light comes in bursts. The arrow in the scattered light (right) part of (c) points at one burst. The view in (e) shows the intensity of the burst in a plane perpendicular to the beam direction. Low intensity in (e) is shown in red, intermediate intensity in blue, and high intensity in white. The scattered light starts as a narrow spot and becomes wider as it passes through the plasma. The largest blob in (e) becomes nearly as wide as the simulation volume by the time it leaves the plasma volume.

The results, notes Langer, were a real eye-opener. "We found that the laser beam penetrates most of the way through the 5 millimeters of plasma, then the backscattered light becomes strong, and the forward beam broadens as it transverses the plasma. We can see in detail how the bursts of scattered light grow stronger as they move through the plasma."

On the basis of their simulation, Langer and Still can make some predictions about the upcoming experiment that will help designers fine-tune NEL systems. For example, they can provide information about where to put detectors on the target chamber walls to pick up transmitted light and what detector sensitivity settings are appropriate for measuring backscattered and transmitted light.

"This was a great example of how, at Livermore, simulation and experiment work hand-in-hand," says Langer. "The work of planning and building NIF and developing ASCI computers and massively parallel computer codes such as PF3D are now coming to fruition. We have the results of simulations, showing us what we expect will occur in the gas bag experiments and providing information that will help guide design of the first NEL experiments. We're eager to see what the data show when the experiments run this summer."



with White, when switch, node, and file systems were all brand new to us at one time," says McCoy. Delivery of all of Purple's 197 refrigerator-size processing units is scheduled to be completed by December 2004. Once up and running, Purple will be the primary supercomputer for the tri-laboratory ASC Program and a production resource to stockpile stewardship.

Catching the Next Wave

The time to move to the next technology wave, one that can deliver increasingly cost-effective capability and capacity for running the next generation of simulations, is nearing for the ASC Program.

Currently, ASCI machines use vendor-designed and -maintained operating software, computers, and processors. All that service doesn't come cheap. "We pay for this service and intellect," says McCoy. So the second technology curve, which Livermore is now exploring at scale using institutional funding, features open-source, not vendor-proprietary, software; cluster architecture; and microprocessors of the kind found in personal computers and laptops (32-bit Pentium-4 Xeon processors, in particular, although 64-bit processors are also being evaluated).

"The result is that we won't have to buy the software, and we'll be using much less expensive components, but we'll own all the problems," notes McCoy. "Owning problems is expensive and psychologically unsettling, of course, so there are pluses and minuses to this approach. But our experience, as we move forward cautiously, is that it is better to be in control than to be dependent. If this fails, we will also know whom to blame."

The first step is to build capacity systems and mid-level capability systems with open-source cluster technology. Livermore is securely positioned on this second computer technology wave with its new 11.2-teraflops MCR system. It nearly matches the 12.3-teraflops ASCI White in power, but at $1.2 million per teraflops, its cost per teraflops is 10 times less than ASCI White's.

MCR is a 32-bit microprocessor-based cluster built by Linux NetworX for M&IC. Cluster computers are composed of many identical or similar types of machines that are tightly coupled by high-speed networking equipment and message-passing interface software. The MCR cluster uses an open-source software environment based on Linux and the Lustre global file system.

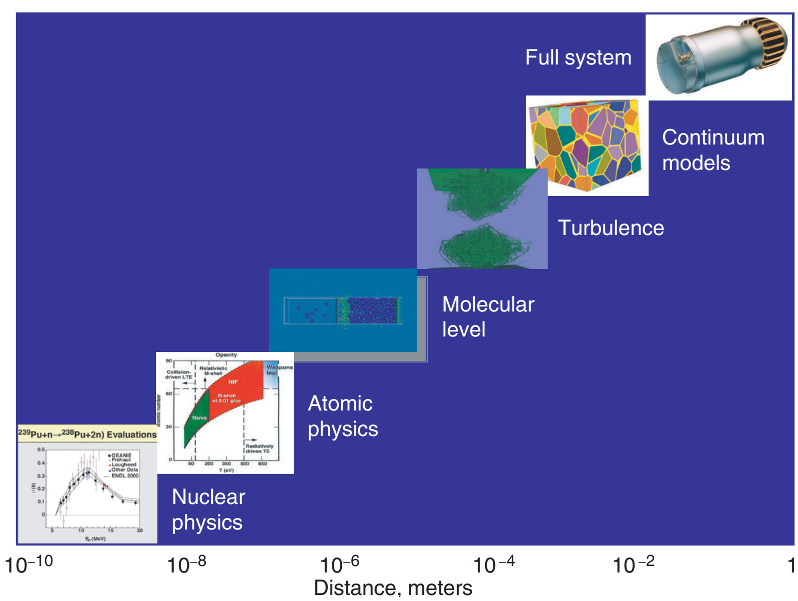
"Using open-source software," says Seager, "means we can often fix or address our own problems rather than hand them over to a vendor, which we have to do for systems that run proprietary software. The vendor, however, may not even be able to reproduce our problems because of a difference in scale between the vendor's systems and ours. So MCR is a much more efficient proposition for us." Seager adds that the other advantage to running open-source software is that many open-source developers are creating codes and software that end up in a big pool of open-source development. Jumping into that pool means that finding areas of mutual interest and setting up collaborations may become easier.

MCR arrived at Livermore in the summer of 2002 and started running large-scale applications in December 2002. MCR is now running select unclassified science simulations for stockpile stewardship and other Livermore programs. The system will go into full production mode as soon as the new file system is stabilized. McCoy points out that MCR's arrival represented a second example of the synergy between the Laboratory and the ASC Program. "The MCR system incorporates a new technology ideal for basic science investigations, but it is not yet ready to approach the scale of problems presented by ASC weapons codes," he says. "Yet, MCR would not have been possible without ASC's investments in technology and the expertise developed at Livermore."

The goal is to provide scientists throughout Livermore with stable Linux clusters for a general scientific workload. "MCR is a capability and capacity machine for running large-scale parallel scientific simulations. The plan is to get it into the hands of scientists quickly," adds Seager.

The system was upgraded to its current size in early 2003. Since that time, a handful of scientific teams have been using it to run codes, large and small, to help get the system ready for general availability at 11.2 teraflops this summer. Among the early users were physicists Bert Still and Steven Langer, who used MCR to simulate one of the first experiments scheduled to be performed on the National Ignition Facility this summer. (See the box on p. 8.) Geophysicist–computer scientist Shawn Larsen also acquired time on MCR to run his seismic wave analysis code E3D for exploring issues related to test readiness, nuclear nonproliferation, and earthquake prediction. (See the box on p. 11.)

"This open-source, cluster curve will almost certainly provide the transition to the next generation of ASC computers," says McCoy. "We plan to ride this curve now and shake down these new, unproven machines with our unclassified science codes. Then, in the coming months when we're convinced it's ready, we can shift this technology to stockpile stewardship by introducing moderate-size clusters into the classified environment for mid-sized problems."



BlueGene/L may offer a rapid path to the multiple petaflops level, allowing scientists to finally address a number of complex physics issues from the atomic scale (on the order of nanometers) to the macroscale (on the order of meters).

New System Heightens Three-Dimensional Reality in Seismic Simulations

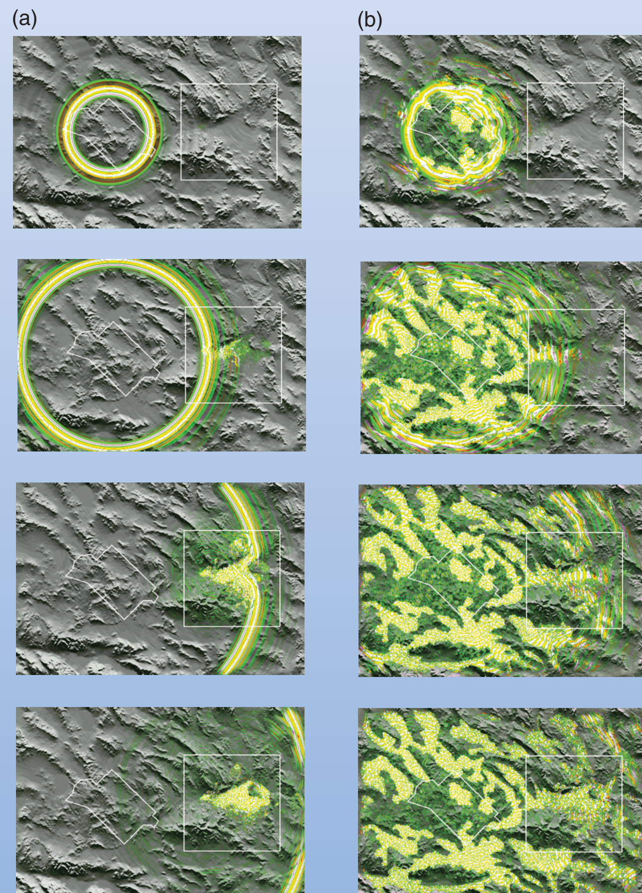
Geophysicist–computer scientist Shawn Larsen was a member of one of the science teams that put the Multiprogrammatic Capability Resource (MCR) through its paces when it first became available in December 2002. He used his E3D code, a powerful seismic code that incorporates three-dimensional information about the propagation of seismic waves, to get a more detailed picture of how these waves interact with different geologies and topographies in their path. His results contribute to a number of Livermore's efforts, including test readiness, earthquake hazard analysis, and nuclear nonproliferation.

A 1993 Presidential Decision Directive requires that the national laboratories shall be ready within a specified amount of time if the nation decides to resume underground nuclear testing. Larsen's task was to use a three-dimensional geologic model developed at the University of Nevada at Reno to simulate the seismic shaking that would occur in the Las Vegas area from a nuclear underground test at the Nevada Test Site. "Las Vegas sits in a basin," says Larsen. "Since the last test in 1992, Las Vegas has grown considerably to the north, into deeper parts of the basin. We wanted to look at the different types of seismic waves and see how they all propagated from the source of an explosion, through the intervening geology, to the basin."

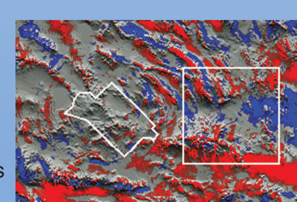
Running simulations that include hills, mountains, valleys, and other topography required a larger supercomputer than previously available. With the arrival of MCR, this kind of complex three-dimensional simulation became possible. (See top figure at right.) "For practical purposes, most of these simulations need over 6 billion zones," explains Larsen. To complete the 16 simulations needed required about 300 hours and 1,600 processors. "We could have easily used the entire machine," says Larsen, "but we left some of it free for others." Each simulation used about 1.5 terabytes of memory.

Using MCR, the team observed details that had never before been revealed by modeling. The energy from the point source of the simulated underground explosion no longer radiated in neat rings, as in previous calculations. It scattered. Also, the topography caused some of that radial energy to "leak" into the transverse direction, creating ground motion perpendicular to the radial direction. "This is the first time we've seen this leaking in a model," says Larsen. "We have seen it in the data and measurements, and now we're finally able to simulate it. The topographic simulations indicated that ground motions can be amplified at the tops of ridges, hills, and mountains, which is important to know when looking at earthquake hazards." (See bottom figure at right.)

For the nuclear nonproliferation effort, knowing how seismic energy propagates is also important. The emphasis is on understanding the seismic signal: Does it come from a mining blast or underground nuclear explosion? "We need to understand the complexity of propagation, and how topography affects propagation," he said. "The kind of modeling we're doing on MCR brings us one step closer to being able to fully understand and discriminate a seismic source."



Seismic energy moving in (a) a simple geologic model and (b) a Multiprogrammatic Capability Resource model using complex geology. Note the vastly increased level of detail in (b).



Results from a Multiprogrammatic Capability Resource simulation show seismic shaking on the tops of hills and in valleys, as well as the more intense shaking on ridges compared with that in valleys.

Growing on the Horizon

The third wave, cell-based computer technology, is even farther out on the technical horizon. It shows great promise of yielding machines that are even more powerful and less expensive than their predecessors. However, since the technology is unproven, investing in this technology today involves high risk. For example, cell-based technology would feature systems using low-cost, low-power embedded microprocessors. Embedded microprocessors, Seager notes, are everywhere—in cars, CD and DVD players, telephones, and other consumer electronics. Livermore and IBM are working together to use this technology to produce systems on a chip—that is, to combine most of the features of a node (microprocessor, memory controller, network, for instance) into a single chip, or cell, instead of the many chips that perform these functions in present-day ASCI computers. Combining node features in a cell reduces power consumption and cost and permits more nodes to fit in a given amount of floor space.

This third curve will be realized through BlueGene/L, a computational sciences research and evaluation machine that IBM will build in parallel with ASCI Purple and deliver in 2005. BlueGene/L will be used for unclassified research into areas such as first-principles molecular dynamics for materials science, three-dimensional dislocation dynamics of materials, high-explosives, and turbulence.

Like MCR, BlueGene/L will run the open-source Linux operating system to take advantage of all the pluses in the open-source arena of code development. The machine will be based on

Supercomputer Characteristics

	Curve 1 technology			Curve 2 technology	Curve 3 technology	Currently world's fastest
Machine	ASCI White	Q	Purple	MCR	BlueGene/L	Earth Simulator
Machine peak speed, teraflops	12.3	20.0	100.0	11.1	180.0 to 360.0	40
Total memory, terabytes	8	33	50	4.6	16 to 32	10
Footprint, square meters	930	1,266	1,115	465	230	3,200
Total power, megawatts	1.0	2.5	4.5	0.3	1.2	10.0
Cost, millions of dollars	100	160	240	13.9	less than 100	about 350 (Does not include maintenance or nonrecurring engineering costs.)
Number of nodes	512	2,730	197	1,152	65,536	640
Total central processing units	8,192	10,922	12,608	2,304	130,000 microprocessors	5,120

Key characteristics of the computers belonging to Livermore's three technology curves compared with each other and with those same features of the Earth Simulator, currently the world's fastest computer.

130,000 advanced microprocessors and have a theoretical peak computational rate of 367 teraflops, with a cost per teraflops of $170,000. When it's up and running, it promises a major advantage in peak speed over present-day computers, including Japan's Earth Simulator, currently the fastest supercomputer. BlueGene/L could be the "next bigthing." If all goes well, the next-generation system, BlueGene/P, could be the first petaflops machine performing a quadrillion calculations per second.

Scientists and researchers are looking forward to BlueGene/L and pondering what it may mean to them and their research. Larsen, who does seismic wave modeling, says, "On MCR, we can create a limited number of complex simulations, one after the other. BlueGene/L will allow us to do hundreds or even thousands of simultaneous simulations, in which we can more easily vary the physical parameters by considering many types of geologies using a statistical approach."

Physicists Langer and Still are also intrigued with the possibilities of BlueGene/L. "By industry standards, the average life of supercomputers like MCR is about 200 weeks," says Langer. "So simulations like our 10-day run on laser–plasma interactions for the National Ignition Facility can't monopolize the machine, much as we'd like to. Others are waiting their turn. But BlueGene/L has the potential to make runs such as ours routine by the time NIF comes fully online in 2008."

Balancing on Technology Waves

"We see cell-based BlueGene/L delivering an affordable means to petaflops supercomputing, which is where we need to be in 2010," says Seager. "But we have to stay open to other possibilities and not commit entirely too early. In the next few years, other technology curves may become apparent—disruptive technologies we can't predict—that will lead to a breakthrough regime by the year 2006 or 2007."

Disruptive technologies are those that change the game quickly and unexpectedly—the Internet, for example. The trick is to gauge when the time is right—if it ever is—to switch to a disruptive technology. "Some technologies make it, some don't, and it's important not to switch too early to something that may not be there in the longer term," says Seager. However, says McCoy, "An institution such as the Laboratory needs to pursue at least one of these new approaches whether or not it works out in the end, because experimentation is necessary for evolution."

For the ASC Program and for the Laboratory, the goal is to cost-effectively deploy advanced, high-performance computing architectures. The first wave of these systems is the current reliable one, with the massively parallel, scalable ASCI Purple next in line.

The second wave, which is based on open-source codes and cluster architecture, is embodied in Livermore's MCR. In January 2003, MCR was ranked the fifth fastest supercomputer in the world on the TOP500 supercomputing list, the first time ever that a computer based on Linux cluster technology broke into the list's top 10. In addition, it was the only Linux-based supercomputer to appear in the top 5, leading industry experts to note that MCR is an important step in supercomputing history because it demonstrates the potentially large effect Linux clusters will have in the high-performance computing community.

The emergence of Linux clusters is just the latest wave on the horizon, gaining speed as it roars to prominence. As high-performance technical users such as Lawrence Livermore and researchers such as Still, Langer, and Larsen move to clustered solutions, the technology will be tested and it will mature in reliability and functionality.

The third wave, which includes cell-based design using system-on-a-chip technology and embedded microprocessors, will be explored in BlueGene/L. With petaflops potential, this machine promises to open a new universe of scientific simulation. Seager says, "Having Blue Gene/L will be like having an electron microscope when everyone else has a magnifying glass."

When Purple and BlueGene/L are both fully operational, which is expected before the end of 2005, they will, combined, have a higher theoretical peak capacity than the 500 fastest supercomputers in the world today. Then, it will be time to catch that breaking wave and ride it to shore.

—Ann Parker

Key Words: Advanced Simulation and Computing (ASC) Program, ASCI Purple, ASCI supercomputers, BlueGene/L, computation strategy, E3D, laser–plasma interactions, Linux clusters, Multiprogrammatic Capability Resource (MCR), National Ignition Facility Early Light (NEL), PF3D code, seismic wave analysis.

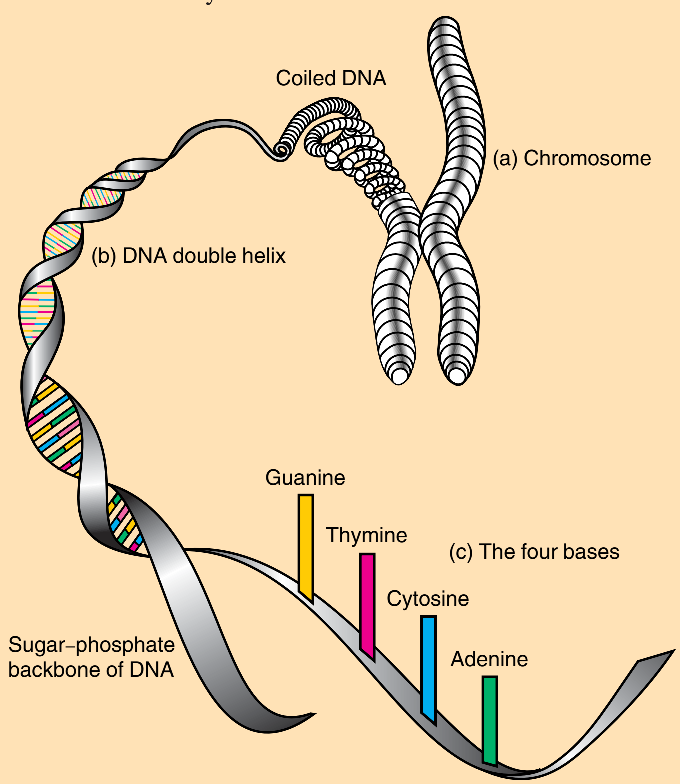
For further information contact Michel McCoy (925) 422-4021 (mccoy2@llnl.gov).

Chromosome 19 and Lawrence Livermore Form a Long-Lasting Bond

Livermore researchers join in the worldwide celebration of meeting the goals of the Human Genome Project.

THIS year marks the 50th anniversary of the discovery of DNA by researchers James Watson and Francis Crick. It seems historically fitting, then, that the complete sequence of all 23 human chromosomes was published earlier this year, thereby fulfilling the ultimate goal of the Human Genome Project, the most ambitious research effort in the history of the life sciences.

Biomedical scientists at Lawrence Livermore have played a prominent role in the Human Genome Project through their study of chromosome 19. Over the past two decades, dozens of Livermore researchers have discovered important new information about the 1,400 genes belonging to this chromosome. They determined the location of hundreds of genes (a process



Every cell in the human body (except red blood cells) contains 23 pairs of chromosomes. (a) Each chromosome is made up of a tightly coiled strand of DNA. (b) DNA's uncoiled state reveals its familiar double helix shape. If DNA is pictured as a twisted ladder, its sides, made of sugar and phosphate molecules, are connected by (c) rungs made of chemicals called bases. DNA has four bases—adenine, thymine, guanine, and cytosine—that form interlocking pairs. The order of the bases along the length of the ladder is the DNA sequence.

called mapping) on chromosome 19, discovered the function of many of its genes, and began the enormous task of sequencing the chromosome, that is, determining the exact order of its DNA base pairs. Later, they participated in the complete sequencing effort as part of the Department of Energy's Joint Genome Institute (JGI) in Walnut Creek, California.

With the sequencing of chromosome 19 complete, Livermore scientists are helping to shape a new era in which the function of all genes and the proteins they produce are understood and medical professionals will be able to diagnose, treat, and perhaps cure the approximately 5,000 known hereditary diseases. To accomplish these ambitious goals, the researchers are comparing the human genome to that of other organisms such as the mouse, rat, chicken, and pufferfish. They are also studying the complex mechanisms that govern how some genes regulate the actions of others. Finally, they are building new computer tools to help make sense of the human genome.

Draft Sequence in 2001

It was barely two years ago, in April 2001, that DOE announced the draft decoding of chromosomes 5, 16, and 19 by JGI. Livermore biomedical scientist Lisa Stubbs notes that the historic milestone was only a first step because the draft sequence contained gaps and errors. Nevertheless, because the draft covered 90 percent of the human genome, it allowed scientists to identify thousands of genes, some of them responsible for inherited diseases.

The final sequencing steps, done at 20 genome centers worldwide, filled most of the gaps in the sequence and increased the overall accuracy to 99.99 percent, or one error per 10,000 bases. "It's really good to have the sequencing finished," says Stubbs. She says the final sequencing steps performed at JGI and Stanford University show that the draft sequence "pretty much got it right."

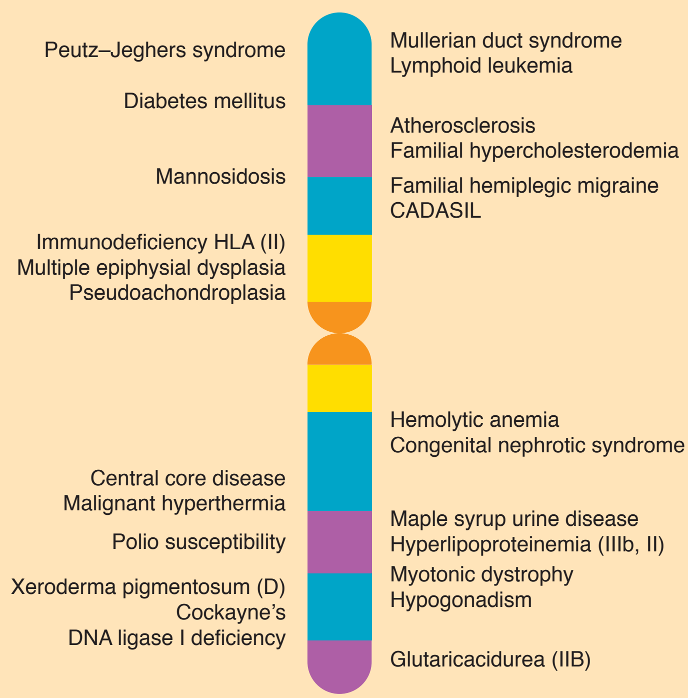
All chromosomes are numbered according to their length, with chromosome 1 being the longest. Chromosome 19 is one of the smallest and, with about 65 million bases, most gene-dense of the human chromosomes. It is home to the genes that are linked to lymphoid leukemia, myotonic dystrophy, diabetes mellitus, atherosclerosis, and a susceptibility to polio along with dozens of other heritable conditions.

Livermore's chromosome 19 research was a natural outgrowth of the work in its biomedical department, which was chartered in 1963 to study the radiation dose to humans from isotopes in the environment. Radiation was known to cause damage in chromosomes, and scientists believed that a useful way to learn about the effects of radiation and other environmental toxins was to study DNA directly. (See *S&TR*, November 2002, pp. 22–30.)

Early Start on Chromosome 19

Livermore researchers chose chromosome 19 to study because, of all 23 human chromosomes, it has the highest concentration of guanine–cytosine base pairs, long thought to imply a higher concentration of genes. That hunch proved to be correct. "The density of genes on chromosome 19 is one of the highest of all chromosomes," says Livermore biomedical scientist Laurie Gordon.

One early Livermore research project examined three genes on chromosome 19 that are involved in the repair of DNA damaged by radiation and environmental pollutants. DNA repair genes produce proteins that "cruise" the



Dozens of genes associated with heritable diseases are located on chromosome 19.

length of DNA, removing unwanted proteins and looking for any mistakes that might disrupt the smooth functioning of a cell. These repair gene studies, which still continue, may lead to insights about the development of cancers, many of which are caused by defects in DNA repair pathways. Another Livermore project studied a family of about 60 genes on chromosome 19 involved in detoxifying and excreting chemicals foreign to the human body.

Livermore research on chromosome 19 accelerated when, in 1986, DOE launched a major initiative to completely decipher the human genetic code. Soon, Livermore researchers were studying all of chromosome 19, with Lawrence Berkeley researchers focusing on chromosome 5 and Los Alamos scientists on chromosome 16. In 1990, DOE joined the National Institutes of Health to launch the U.S. portion of the Human Genome Project with the goal to discover all the human genes and to determine the complete sequence of the genome's 3 billion DNA base pairs. The project soon drew additional collaborators worldwide.

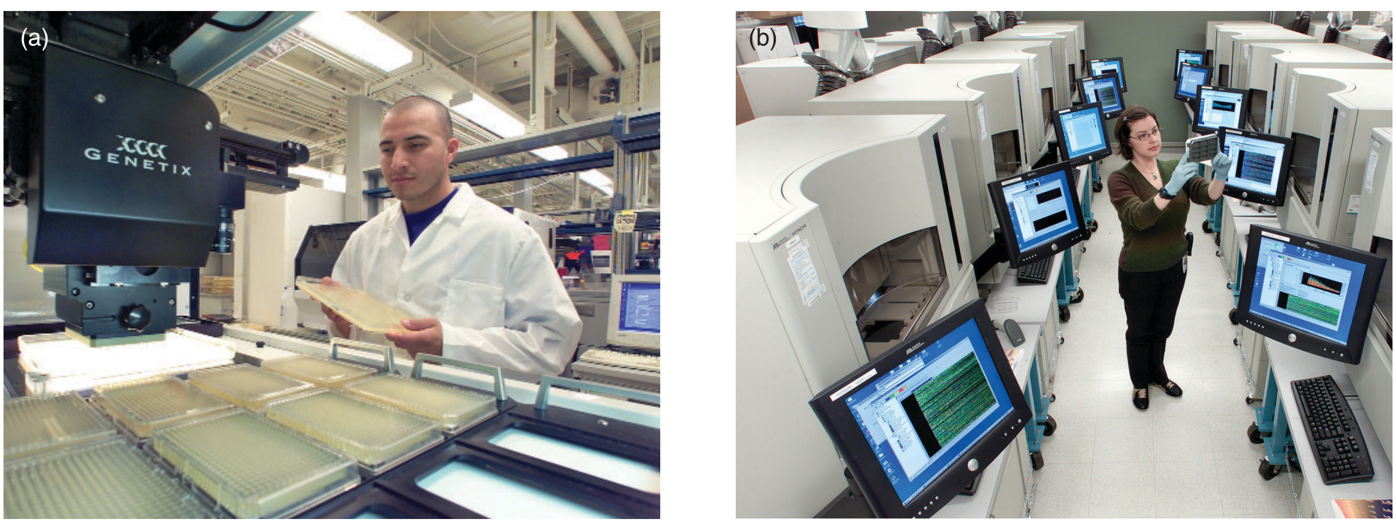
Biomedical scientist Linda Ashworth worked on chromosome 19 for 14 years before retiring in 2001. "When I first got involved in the mid-1980s, genome science was a very small field," she recalls. Ashworth, Anne Olsen, and others started mapping chromosome 19 in the mid-1980s to understand the location of hundreds of genes that were then known to reside on the chromosome and to prepare for the sequencing effort that lay ahead.

Mapping Effort Not Easy

The tedious process, which Ashworth describes as "putting Humpty-Dumpty together again," involved breaking up thousands of chromosome 19 molecules into small pieces of the same size; producing exact copies, called clones, of each piece with bacterial colonies; and then fitting the pieces together in the correct order. The technique was the only option available at the time because scientists were (and still are) unable to sequence an entire chromosome from end to end. "Our goal was to create a high-resolution sequence-ready map," says Olsen, who also retired recently.

Olsen says that chromosome 19 was not easy to map. It contains a large number of repetitive sequences that are interspersed throughout its DNA. Another factor, which complicated accurate sequencing later on, is that the chromosome is more tightly bonded than other chromosomes because of its high instances of guanine–cytosine bonds. As a result, a single strand of the double-stranded molecule can loop back on itself to form confusing secondary structures.

During the mapping effort, Livermore researchers tapped the latest tools and techniques in the fledgling biomedical industry, such as automated pipettes, and invented a few of their own. One important technique, developed at the Laboratory to locate short pieces of DNA and establish their relative position on an individual chromosome, is called fluorescence in



(a) Robots have revolutionized many formerly labor-intensive activities at the Joint Genome Institute. A robot selects bacterial colonies with large amounts of cloned human DNA and transfers to machines that will sequence the DNA. (b) These high-speed DNA sequencers at the Joint Genome Institute can sequence 2 billion base pairs per month.

situ hybridization (FISH). Researchers improved the resolution of FISH by using hamster eggs fused with individual human sperm, which caused the sperm DNA to extend in length. This extension allowed investigators to see the molecule in much greater detail than was previously possible.

Sequencing Begins

In the late 1980s, armed with their map of known genes along the chromosome, Livermore scientists started sequencing the 65 million base pairs of chromosome 19. Ashworth recalls, "When we started sequencing, it took about 14 hours to sequence 400 bases, but that was considered state of the art."

As the mapping efforts continued, other Livermore researchers discovered more about the location and function of chromosome 19's genes. In 1992, Livermore researchers, collaborating with colleagues in Canada and Europe, discovered the genetic defect that causes myotonic dystrophy, the most common form of muscular dystrophy.

When the Joint Genome Institute was established in 1997 as a collaboration between Livermore, Los Alamos, and Lawrence Berkeley national laboratories, Livermore researchers sequenced 200 million raw base pairs in one year—that is, they gave the DNA its first rough reading. JGI can currently complete 200 million raw bases in less than 3 days.

With JGI's production facility in full swing by mid-1999, sequencing took on an industrial character by centralizing and largely automating the effort that was being done individually at the three laboratories. JGI personnel, including a team led by biomedical scientist Susan Lucas, worked to complete the sequencing of chromosomes 5, 16, and 19.

JGI transferred the final sequencing work to a group at Stanford University

The Joint Genome Institute: From Virtual Facility to Gene Research Powerhouse

Located in Walnut Creek, California, the Department of Energy's Joint Genome Institute (JGI) is one of the largest publicly funded genome sequencing centers in the world. The institute was founded as a virtual entity on January 1, 1997, as a collaboration between Lawrence Livermore, Lawrence Berkeley, and Los Alamos national laboratories. Livermore scientists initially mapped and began to sequence chromosome 19, while Los Alamos scientists worked on chromosome 16, and Lawrence Berkeley worked on chromosome 5 before joining forces through the JGI. (See *S&TR*, April 2000, pp. 4–11.)

The main work of the JGI is done at its 5,600-square-meter Production Genomic Facility (PGF). Secretary of Energy Bill Richardson was keynote speaker at the April 19, 1999, formal PGF dedication. Its staff of about 150 includes 40 Lawrence Livermore researchers.

The PGF uses an automated process during which the samples pass through capillaries as a laser scans them. After DNA bases are read, computers reassemble the overlapping fragments into long, continuous stretches of sequenced DNA, which are analyzed for errors, gene-coding regions, and other characteristics. This process is repeated many times for all of the sections of DNA that make up a genome. The front end of the operation, where the pieces of DNA are cut, involves the most skilled handwork. Virtually all other facets of the process have been automated.

Livermore biomedical scientist Elbert Branscomb served as JGI's first director. Edward Rubin, an internationally known geneticist and medical researcher, was named the current director in January 2003. Funding is provided mainly by the Office of Biological and Environmental Research in DOE's Office of Science, with additional funding from the National Science Foundation, the U.S. Department of Agriculture, and other agencies.

JGI's initial goal was completing the DNA sequencing of chromosomes 5, 16, and 19, which together constitute 11 percent of the human genome. In April 2001, JGI announced the completion of the draft of JGI's three chromosomes. JGI was the first large genome center to make such an announcement, several months ahead of schedule.

After completing the final sequencing, JGI researchers sent their data to a team at Stanford University for "finishing," that is, closing the gaps and resolving any discrepancies in the draft sequence. To be considered finished, the sequence must be completely contiguous, be confirmed by at least two templates, have no gaps, and have a final estimated error rate of less than 1 out of 10,000 bases.

The center has taken advantage of innovations and breakthroughs in the bioresearch field, which have resulted in remarkable increases in the amount of DNA that is sequenced. Since 1999, the JGI has increased its production rates more than 20-fold to sequencing about 35 million bases per day.

JGI is in the process of becoming a more research-oriented facility. It has established whole genome sequencing programs that include vertebrates, fungi, plants, and bacteria.

for what is known as finishing. This process improves accuracy and closes small gaps in the known sequence. Stubbs notes that because the human genome will be used as a reference for all scientists, it is essential that it be as accurate as possible.

Entering a New Era

With the final decoding of the human genome, scientists are entering the postgenomic era. The new focus, says Stubbs, is on understanding the function, regulation, and evolution of genes. After a gene is precisely located on a chromosome and sequenced, researchers can easily predict the primary structure of the protein that the gene encodes. But in only a few cases do scientists have an idea what that protein does. Sometimes basic function can be deduced by similarity to other known proteins. For example, protein structure may suggest a role in detoxification or as a structural component.

"We know what only a handful of genes are doing in the organism," says Stubbs. "In most cases genes are like black boxes. What kinds of toxins do they metabolize? In which cells, and when do the cells require them? A small number of genes do not encode proteins at all but are suspected of producing RNA products that help regulate other genes."

Stubbs says that scientists also need to explore the largely uncharted noncoding region, sometimes called junk DNA, which makes up about 95 percent of human DNA. Although junk DNA looks like nonsense coding, it may have regulatory functions, or it might be necessary for the structural integrity of the DNA double helix. Gordon believes that junk DNA may yield surprising functions. Curiously, yeast and bacteria do not have junk DNA.

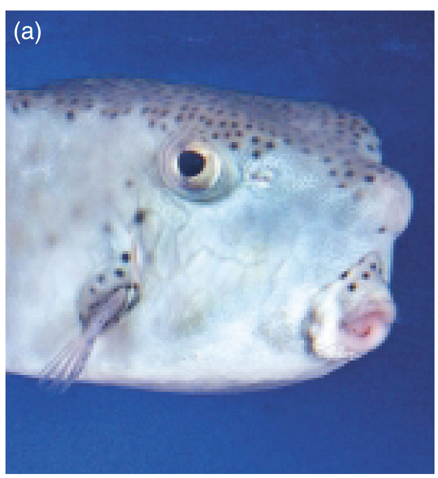
Many scientists like Stubbs and Gordon are interested in how genes are regulated. Two genes may have almost identical sequences, yet one may be active only in skin and the other only in bones. What determines the tissue-specific activity are DNA elements linked to the genes. These so-called regulatory elements serve as docking sites for proteins that determine the "on–off" state of every gene. Understanding gene regulation is important to a broad range of applications, ranging from human susceptibility to disease to managing microbes in the environment.

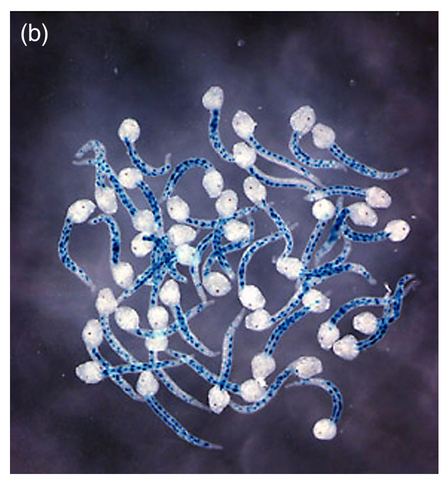
Livermore researchers have discovered possible regulatory sequences for genes throughout chromosome 19. "The complexity involved in gene regulation becomes exponential the more we look into it." says Gordon. " The cascade of reactions is fascinating."

Comparing Genomes

To gain further understanding of the human genome, many scientists are looking to comparative genomics. This relatively new field analyzes and compares the genetic material of different species to study evolution and gene function. A key goal is to find the five percent of most complex genomes that serve critical roles in cell development, maintenance, and health.

A pioneering study led by Livermore researchers showed the high degree of similarity between the mouse and human genomes.





In 2001, the JGI led a consortium that sequenced (a) the Japanese pufferfish, *Fugu rubripes*, and (b) the sea squirt, *Ciona intestinalis*. The pufferfish is the first vertebrate genome after human to be draft sequenced. The sea squirt is a primitive chordate and has a small genome.

Comparative genomics focuses on identifying DNA sequences that are shared between two or more diverse species. These conserved elements (that is, those that aren't reinvented for each species) include genes that produce key proteins and enzymes and the genes that establish basic features of the organism such as body shape during development. "If you really want to discover the genes that are most critical to basic life, you have to look at other genomes," says Stubbs.

Livermore scientists are discovering that humans share a surprising number of genes with mice, fish, chickens, and even primitive bacteria. A Livermore–JGI team led by Stubbs compared human chromosome 19 with similar sections of mouse DNA and detailed its findings in the July 2001 issue of *Science*. The article, the first major example of the power of large-scale genomic comparisons, described clues to the mechanisms of gene evolution in mammals. The research was also helpful because the mouse is often used as a model for studying diseases and testing medicines. (See *S&TR*, May 2001, pp. 12–20.)

The researchers found that functional counterparts of about 90 percent of the human genes in chromosome 19 are also located in similar sections of mouse DNA. However, against this backdrop of amazingly high similarity, they also found some significant differences. Most of the differences are due to the active copying of certain genes over 80 million years of evolution. Both rodents and primates have copied genes from the earliest chordates (animals with backbones), but not the same genes. As a result, rodents have multiple copies of some genes that are found only once in human DNA, and vice versa.

"Duplicated genes will often specialize, with each copy taking on parts of the original gene's function," says Stubbs. "For example, one copy may take over duties in the liver, while the other one specializes for work in the brain. This specialization is a way to build more complexity over time. As the genes mutate and additional duplications take place, completely new functions may arise. Gene duplication is therefore a major source of genetic variation, the critical fodder for evolution."

One group of genes that has duplicated especially frequently is called zinc finger genes, which produce proteins that bind to elements allowing them to regulate the activity levels of other genes. A significant fraction of the roughly 800 human zinc finger genes are found on chromosome 19.

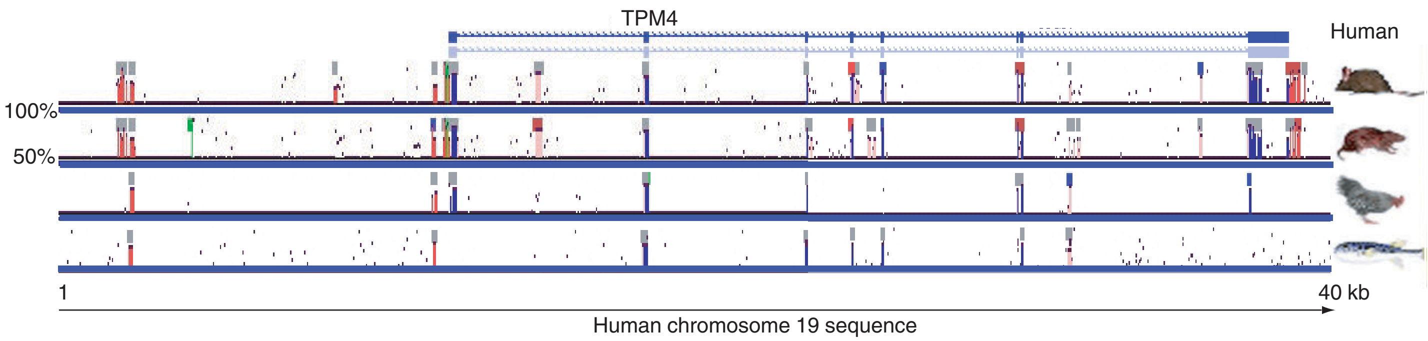
Gaining Insight with Pufferfish

Stubbs says that scientists need to look at genomes of organisms farther away evolutionarily from humans to gain further insight into the human genome. In early 2001, JGI led a consortium that sequenced the Japanese pufferfish, *Fugu rubripes*. It was the first vertebrate genome to be sequenced after the human genome. The pufferfish genome is known as the *Reader's Digest* version of the human genome because it is one-eighth the size. Nevertheless, it contains a gene set that is highly similar to the human genome, and its sequence is helping scientists to further identify regulatory genes in humans.

Later in 2001, JGI sequenced the genome of the sea squirt, *Ciona intestinalis*. This organism, a primitive chordate, has a small genome (165 billion base pairs) and therefore holds important information about how genes evolved over time.

Stubbs, Gordon, and other Livermore researchers have begun analyzing portions of the chicken genome and comparing it to the human genome. They chose the chicken because it sits on the evolutionary tree between the mouse and the pufferfish. Gordon points out that Livermore

Livermore researchers have begun analyzing the chicken genome and comparing it to the human genome because the chicken sits on the evolutionary tree between the mouse and the pufferfish.



A linear map (top) of a 40-kilobase (kb) region of human chromosome 19 containing the tropomysin 4 (TPM4) gene. Nucleotide positions 1 to 40,000 are represented by the horizontal axis of each panel. The seven segments, or exons, of the gene sequence are shown by boxes joined by a blue line. The four panels below the TPM4 sequence summarize the results of aligning this human sequence with similar regions of the genome of the mouse, rat, chicken, and pufferfish. Wherever matches greater than 50-percent identity are found between the human and other sequences, a dot is plotted in each panel at a height that corresponds to the percentage. A series of clustered dots may coalesce into a larger, evolutionarily conserved region (ECR). Blue ECRs correspond to gene exons; red ECRs correspond to nongene regions. The nongene regions are likely to represent regulatory sequences that control gene expression. TPM4 is well conserved between human and mouse, rat, birds, and fish. The figure is taken from the ECR browser designed by collaborator Ivan Ovcharenko of Lawrence Berkeley National Laboratory (nemo.lbl.gov/~ovcharen/).

researchers do not work among chicken coops. Instead, they use chicken genes that are available as clones produced by bacterial colonies. The chicken study, as with the mouse effort, largely involves complex computational analyses of the different genomes.

Indeed, computational genomics has become essential. These powerful computer tools allow users to ask complex questions and extract meaningful answers rapidly from massive amounts of genome data. Some of the tools have been developed by Livermore researchers such as bioinformaticist Paramvir Dehal, who is helping to compare different species' DNA, and computer scientist Art Kobayashi, who is developing new ways to analyze larger pieces of sequenced DNA than is now possible.

Smart Choice

Many new projects to better understand the human genome are just beginning. Gordon says that it's quite likely that more human genes will be discovered and their functions elucidated. "We have years and years of work ahead of us," she says. Increasingly, that work is done as collaborative efforts with other institutions.

Gordon notes that another large task is understanding the many variations among genes. Every human has a slightly different genome than everyone else. Just as certain genes determine the blood types A, B, AB, and O, other genes are responsible for proteins that are slightly different from each other.

In retrospect, says Stubbs, selecting chromosome 19 was an excellent choice for Livermore bioresearchers. It is small, therefore manageable, and twice as gene-dense as many other chromosomes. Working on the chromosome led to Livermore's present stature as a world leader in genomics, bioinformatics, and comparative genomics, and to its full participation in JGI. Knowledge about chromosome 19 and other chromosomes will speed the understanding of how genes influence disease development, contribute to the discovery of new treatments, illuminate how species evolved, and help scientists form a molecular understanding of life.

Many researchers, even those who have retired, still have strong feelings about chromosome 19. "Those of us who have worked with chromosome 19 for so many years have an emotional attachment to it," says Olsen.

—*Arnie Heller*

Key Words: chromosome 19, comparative genomics, DNA, gene mapping, gene sequencing, Human Genome Project, Joint Genome Institute (JGI), pufferfish, regulatory genomics, sea squirt.

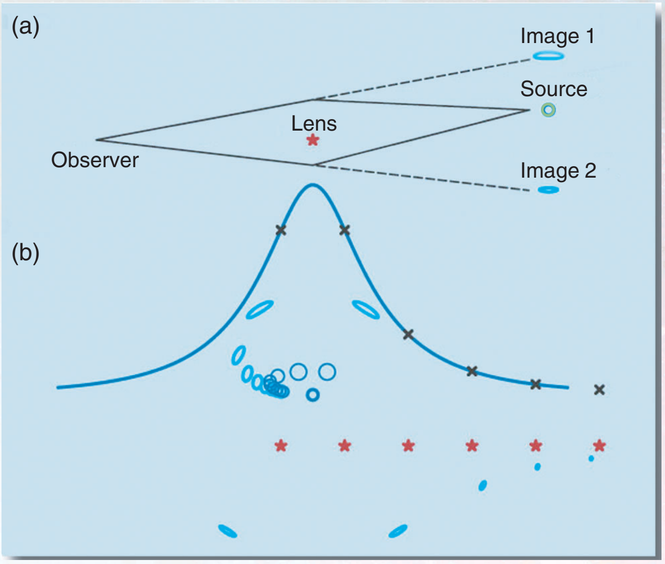
For further information contact Lisa Stubbs (925) 422-8473 (stubbs5@llnl.gov).

A New Way to Measure the Mass of Stars

WHEN an international collaboration began a search for dark matter in the Milky Way Galaxy, measuring a star's mass was not the goal they had in mind. But as the team examined more closely the massive compact halo objects (MACHOs) they had found, they realized that all the information they needed for measuring a single, isolated stellar mass was right in front of them.

Measuring the mass of a star or a satellite such as planets or moons used to be a relative affair: How does the presence of one body affect the position of the other? The movement of the Sun as the Earth and other planets revolve around it is largely a function of their relative masses. The same is true for our Moon as it revolves around our home planet. New discoveries about the existence of planets around other stars are inferred by observing wobble in a star's position. More wobble means more mass is revolving around it. Careful observations of the wobble can reveal how many planets are acting on the star.

Astrophysicist Kem Cook, who leads the Livermore contribution to the team, notes, "Measuring the mass of a star has never been possible when it was in physical isolation. Always before, we were looking at two bodies—the Sun and Earth or binary stars. Now we can do just one, but it takes lots of time and data."



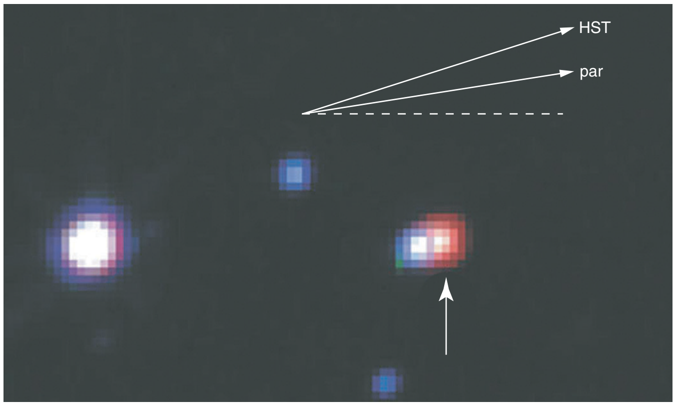
A step-by-step guide to gravitational microlensing. (a) Light from the source star (green) is deflected by the lens (red), creating two enlarged and distorted images (blue). (b) As the lens passes in front of the source, the pair of images becomes first larger and then smaller, so that the observed light flux (blue curve) becomes brighter and then fainter.

The Critical Image

From 1992 to 2000, the MACHO collaboration, including researchers from the U.S., Australia, Chile, Germany, Britain, and Canada, searched the outer regions of the Milky Way for MACHOs using the Large Magellanic Cloud (LMC) as a backdrop (see the box on p. 22). They were looking for events in which the gravitational field of a MACHO came between their detector and a distant star, causing the distant star to brighten significantly. Gravity acts as a lens in a process called microlensing. Six years of observational data have been analyzed thus far, revealing 17 microlensing events in the Milky Way's halo, including the first event ever positively identified.

Of particular interest was the brightest event, known as LMC-5. The distant, or source, star became at least 15 times brighter when it was behind the microlensing object. The unmagnified color of the patch of sky occupied by both the lens and the source star was redder before and after the peak of the microlensing event. Researchers suspected that the source star was a blue star in the LMC that, because of atmospheric blurring, was confused with a red star, whose color and brightness suggested a red dwarf star in the Milky Way.

To better characterize the source stars of all microlensing events, the team obtained images taken by the Hubble Space Telescope, which operates well above Earth's atmosphere. The 1999 Hubble image for the LMC-5 region, taken 6.3 years



A three-color composite image from the Hubble Space Telescope (HST) of the brightest microlensing event. The microlensing source star is the blue star at the right of the figure, which is partially blended with a much redder object (indicated by the arrow) displaced by 0.134 arcseconds. The directions of motion of the lens on the sky derived from the HST (–92 degrees) and from the unconstrained parallax (par) fit (–100 degrees) are shown.

after the peak of the LMC-5 microlensing event in February 1993, revealed a faint red object in addition to the source star. The two stars were still so close to one another that even on the Hubble image, they appeared slightly blended.

The team went back to reexamine the details of the LMC-5 microlensing curve. By analyzing perturbations in the curve caused by Earth's movement around the Sun, they were able to predict the direction that the lens would move across the sky. They found that the red star shown in the Hubble image was in the place that their calculations predicted and must be the lens. But the team didn't stop there.

Adding It All Up

Over 30 years ago, researchers suggested that gravitational microlensing could be used to measure the masses of nearby stars, although no one had yet seen a microlensing event in action.

Data collected in microlensing events are insufficient to measure the mass of the lens: The duration is proportional to the mass of the lens, the relative distances of the lens and the

The Search for MACHOs

Massive compact halo objects (MACHOs) are thought to be one kind of the invisible dark matter that surrounds and permeates our galaxy and other galaxies like it. Astronomers have determined that the Milky Way Galaxy must be much more massive than the amount of mass that is visible. Without the additional mass, the galaxy would fly apart. In fact, as much as 90 percent of the Milky Way's mass cannot be detected with available techniques. There is no question that dark matter exists. Finding it is the challenge.

Earlier studies suggested that MACHOs would produce gravitational microlensing, a process by which the gravity of one object comes between an observer and a distant star and causes the light of the distant star to be briefly magnified. Because a microlensing event requires that the two bodies be lined up almost perfectly, microlensing events are quite rare. Although a star could act as a microlens, the relative lack of stars in the outer regions of the Milky Way made it likely that any microlenses seen would prove to be MACHOs.

Using the Large Magellanic Cloud (LMC) Galaxy as a backdrop of distant, or source, stars, researchers from around the world searched for MACHO microlensing events with a special camera developed at Livermore. Scientists monitored millions of stars in the LMC at Mount Stromlo Observatory in Canberra, Australia, from 1992 to 2000. This observatory was chosen because the LMC is only visible from the southern hemisphere.

By observing whether the brightness of any source stars varied over time as a gravitational lens passed between the star and the observatory's detector, the team identified numerous microlensing events toward the Large Magellanic Cloud. Their data to date indicate that between 8 and 50 percent of the Milky Way's mass is in the form of MACHOs.

Using Hubble Space Telescope images to more closely examine the source stars of LMC microlensing events, the team has thus far found that only LMC-5 involved a visible star acting as a lens. All the rest were apparently caused by the gravitational field of a MACHO.

Astronomical research came to a screeching halt at the Mount Stromlo Observatory in January 2003 when a raging bush fire destroyed many buildings, including four telescopes, computers, and a spectrograph being constructed for the 8.2-meter Gemini North telescope in Mauna Kea, Hawaii. The fire destroyed about one-third of Australia's astronomical research program.

source star from Earth, and the motion of the lens across the line of sight of the source star.

With LMC-5, much more information was available, thanks to the image from the Hubble Space Telescope. “If we assume that the red star is the microlens and the other star is the source star, then we have a physical measurement on the sky of the motion of the lens,” says Cook.

The team had already determined the apparent direction and motion across the line of sight of the lens from the distortion in the light curve due to the motion of the Earth. Combining that information with the known distance to the Large Magellanic Cloud, which is very shallow, and the time between the original image and the Hubble image, allowed them to determine the distance the lens had traveled and, hence, its velocity. With the Hubble image—the first ever of a microlens scooting across the heavens—the team had all of the elements needed to determine the distance of the lens and its mass. They found that the mass of the LMC-5 lens was about one-tenth the mass of the Sun.

A Better Way Soon

An even better way to measure the mass of stars will be available in 2009 or so when National Aeronautics and Space Administration launches the Space Interferometry Mission (SIM). SIM will use optical interferometry to measure the tiny, apparent motion of stars, which is caused by microlensing, to determine the masses and distances of stars with much greater accuracy than previously possible. Measuring the mass of individual stars with data from SIM will be a veritable walk in the park.

—Katie Walter

Key Words: gravitational microlensing, massively compact halo objects (MACHOs).

For further information contact Kem Cook (925) 423-4634 (cook12@llnl.gov).

Flexibly Fueled Storage Tank Brings Hydrogen-Powered Cars Closer to Reality

As a Department of Energy national laboratory, Livermore has long been involved in research and development of alternative energy technologies for transportation, including hydrogen fuel. Hydrogen-fueled passenger cars can have significant advantages over today's or tomorrow's gasoline cars. They can eliminate automotive air pollution, reduce our nation's oil dependence, and reduce or eliminate greenhouse gas emissions from transportation, if the hydrogen fuel is produced from nonfossil energy resources.

But as a recent article on the front page of the *Wall Street Journal* (March 7, 2003) makes clear, hydrogen cars may be a long way off. Numerous obstacles must be overcome before passenger cars using hydrogen become a viable alternative to gasoline-powered vehicles. Not the least of these is the development of extremely fuel-efficient passenger cars. Be they fuel-cell vehicles or hybrid vehicles burning hydrogen in an internal combustion engine, these cars must get the equivalent of 60 to 100 miles per gallon (25 to 42 kilometers per liter) and be capable of storing 5 kilograms of hydrogen onboard to achieve a driving range of 300 to 500 miles (480 to 800 kilometers). The world's major automobile manufacturers are addressing this challenge in a variety of hydrogen vehicle development programs.

Meeting the Storage Challenge

Other obstacles to hydrogen cars fall into three large categories: hydrogen production, refueling infrastructure, and hydrogen storage onboard the vehicles. Researchers in Livermore's Energy and Environment Directorate have been addressing these problems for almost a decade. (See *S&TR*, July 1995, pp. 26–27; May 1997, pp. 12–14; December 1999, pp. 4–13.) Recently, a team in Energy and Environment's Energy Technology and Security Program has turned its attention to the challenges of storing hydrogen fuel onboard automobiles. Led by engineer Salvador Aceves, associate program leader for transportation, the group has designed and tested a safe and compact system for on-vehicle storage of hydrogen fuel. The tank, which shows great promise, was featured on the cover of the February 2002 issue of *Mechanical Engineering* and will soon be installed on test vehicles.

The beauty of the Livermore tank, says Aceves, is that it can safely and simultaneously accommodate three forms of hydrogen fuel—conventional high-pressure hydrogen gas, cryogenic compressed gaseous hydrogen, and liquid hydrogen. And it does so while minimizing the storage challenges and maximizing the energy efficiency potential of each.

Three Fuel Forms, One Tank

Similar to compressed natural gas vehicles, prototype hydrogen vehicles use compressed hydrogen, stored onboard at about room temperature and under moderate pressure (25 to 35 megapascals). Unfortunately, these moderate pressures lead to large fuel tanks and/or limited driving range because the energy density of simple hydrogen molecules (H_2) is lower than the energy density of conventional fossil fuels such as gasoline (C_8H_{18}) or natural gas (CH_4), both of which are more complex molecules. One kilogram of hydrogen gas at 25 megapascals occupies nearly 60 liters (16 gallons), but its energy (33.3 kilowatt-hours) is equivalent to just 1 gallon of gasoline. Compressed hydrogen is a simpler, less costly, and more energy-efficient method of storage than other methods and is well suited for the range of the majority of urban drivers in the U.S.: 150 to 200 miles.

Since all gases occupy less volume at colder temperatures, compressed hydrogen can be stored more compactly when cryogenically cooled. At temperatures of 80 kelvins (–193°C), near the boiling point of liquid nitrogen, 60 liters of hydrogen gas at 25 megapascals contains the energy equivalent to more than 3.3 gallons of gasoline, enabling cars using cryogenic hydrogen to greatly extend their driving range.

Liquid hydrogen is even more compact than cryogenic hydrogen, but because hydrogen's boiling point (20 kelvins) is lower than that of any substance except helium, liquefying hydrogen is complicated and not energy efficient. Typically, 11 to 12 kilowatt-hours of electricity are needed to produce 1 kilogram of liquid hydrogen, which contains only 33.3 kilowatt-hours of fuel energy. This high energy penalty is a key factor in the high production cost of liquid hydrogen.

Liquid hydrogen has its advantages, however. It is relatively easy and safe to store and transport in compact, lightweight, low-pressure containers. According to project engineer Gene Berry, a hydrogen car designed to get the equivalent of 60 miles per gallon of gasoline uses 100 liters of liquid hydrogen to travel 420 miles, compared to 240 miles on high-pressure (70 megapascals) compressed hydrogen and 140 miles on moderate-pressure (35 megapascals) compressed hydrogen. Liquid hydrogen is thus ideal for long highway trips. Its advantages help explain why it has become the favorite of BMW's 20-year hydrogen vehicle development program.

The rub is that liquid hydrogen is extremely sensitive to heat, expanding significantly when warmed only a few degrees. When a hydrogen-fueled car is not being driven, heat exchange between the storage tank and the outside environment warms the fuel, causing it to evaporate. As the hydrogen fuel expands, the pressure in the tank increases. The hydrogen must therefore be vented to the atmosphere to prevent the dangerous buildup of excessive pressure.

Cryogenic hydrogen fuel in a standard liquid hydrogen tank typically warms up enough in 3 to 4 days after refueling to require venting. The tank team used computer analysis to determine that when liquid hydrogen is stored in a conventional low-pressure (0.5-megapascal) tank in a car that gets the equivalent of 80 miles per gallon, it would begin to vent and lose fuel if driven (on average) less than about 15 miles daily. Evaporation losses increase sharply if the car is driven less. In a parked car, an entire tank of liquid hydrogen fuel will completely evaporate in just 3 weeks. Eliminating this evaporation is a primary goal of Livermore's tank design.

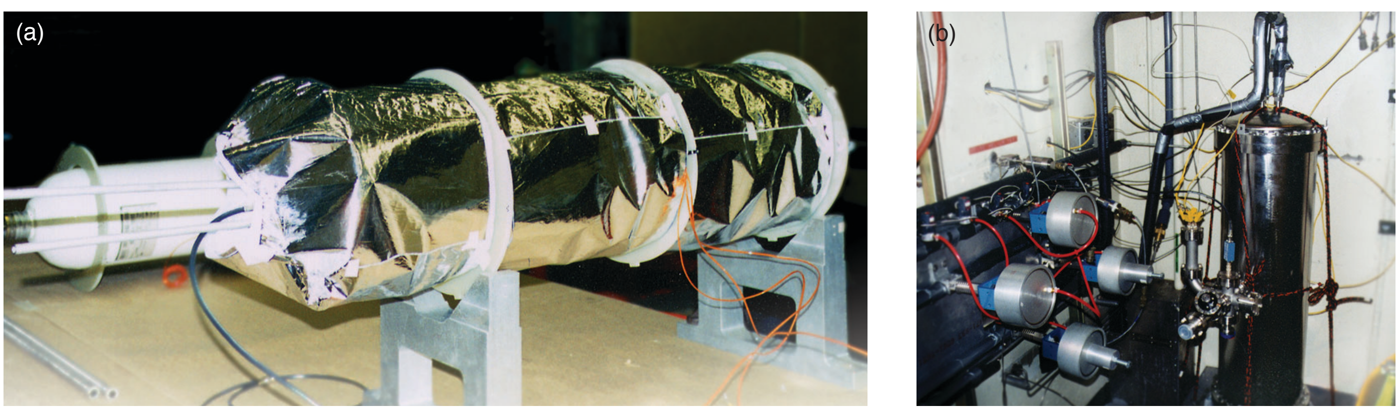
Insulation in a Vacuum to the Rescue

To date, conventional cryogenic hydrogen storage vessels could accommodate only low-pressure liquid hydrogen. By insulating conventional high-pressure vessels, the Laboratory's team designed a tank that successfully combines cryogenics and high pressure to allow three forms of hydrogen to be stored in one tank. Aceves and his team determined that commercially available aluminum-lined pressure vessels coated with composites (Aramid or carbon fiber) identical to those popular for natural gas storage offered the low weight and affordability desired for automotive fuel storage. The researchers coated a standard pressure vessel with 80 layers of highly reflective, metallized Mylar and then enclosed and sealed the insulated inner vessel in a stainless-steel outer tank. A vacuum is then created between the inner and outer tank. "Heat transfer, which is the culprit for evaporation loss, operates through convection, conduction, and radiation," says Aceves. "The vacuum created between the two tanks eliminates the convection and conduction that would otherwise have occurred with a standard tank. The multiple layers of reflective material considerably reduce heat transfer by radiation."

The researchers built openings in the outer jacket for thermocouples, strain gauges, and a capacitive level sensor to measure pressure, temperature, and the fuel level within the test tank. They equipped the tank with safety devices to prevent catastrophic failure in case hydrogen leaked into the vacuum area. Relief valves open if the pressure limits are exceeded, and if the relief valves fail, rupture disks prevent explosive pressure release.

Putting the Tanks to the Test

To determine if the Livermore-designed tank meets rigorous U.S. Department of Transportation and Society of Automotive Engineers safety standards, the researchers constructed tanks to one-fifth scale and subjected them to



The Livermore hydrogen fuel storage tank has two basic parts: (a) a composite-coated interior pressure vessel wrapped with 80 layers of Mylar insulation and (b) an exterior stainless-steel pressure vessel. The vacuum induced between the two vessels minimizes the heat transfer that causes cryogenic hydrogen to evaporate.

Livermore's insulated cryogenic hydrogen tank has undergone 27 different tests to demonstrate its safety and reliability. (a) The tank after being shot with a .30-caliber armor-piercing bullet. The bullet punctured the tank without fragmenting it. (b) The Livermore tank during the bonfire test and (c) following the test. The tank was charred but retained its structural integrity, a key safety consideration.

27 tests of materials, construction, and performance. Many tests involved thousands of repetitions, or cycles. For example, to determine whether the tanks can withstand severe and repeated pressure changes at extremes of internal temperature, the tanks were pressurized from zero to full-service pressure (25 megapascals) and then returned to zero. The cycle was repeated 5,000 times, about 5 times the number of cycles that a typical tank will experience over a 150,000-mile vehicle lifetime. The cycles were first done with an internal tank temperature of 140°F and external ambient air temperatures at 95-percent humidity and then repeated with an internal tank temperature of –60°F and external high-humidity ambient temperatures. The tanks were also subjected to 20 thermal cycles, with tank temperatures ranging from 200°F to –60°F at full-service pressure.

Some of the more dramatic tests included dropping tanks 3 meters onto a hard surface, firing a .30-caliber armor-piercing bullet at a tank from 15 meters, and placing pressurized tanks in bonfires. The tanks survived or suffered acceptable damage. The tank was pierced by the bullet but did not fragment, and it was charred by the fire but retained its structural integrity and did not explode.

The tank design passed all of these tests and met all of the standards. In some instances, the tanks exceeded the testing criteria—and the team's expectations—especially for cryogenic storage. "When the tests showed that the cryogenic tanks were at least as strong as conventional tanks, people sat up and took notice." says Berry. "Suddenly, the Livermore concept was considered a viable option for storing hydrogen on cars of the future."

Now Comes the Real Test

The next step for the Livermore researchers is installing their insulated cryogenic pressure vessels on vehicles for field testing. They are now working on a second-generation tank, which will hold 9 kilograms of liquid hydrogen, energy equivalent to 9 gallons of gasoline. They are working with two partners in getting their tanks on the road: Structural Composites Industries, a leading manufacturer of pressure vessels based in Pomona, California, and Sunline Transit of Thousand Palms, California. Sunline, a mass transit agency serving the Palm Springs area, has agreed to install two second-generation Livermore tanks on pickup trucks. One truck will carry hydrogen, and the other will carry natural gas.

If the second-generation tank is successful, the Livermore team will give the design what many consider the real test: subjecting these tanks to continual, daily use. In these days of high gasoline prices and increasing concerns about air pollution and global warming, on-road testing of the Livermore hydrogen fuel tank is one small step of a long journey.

—Laurie Powers

Acknowledgments: Members of the project team responsible for the work reported in this article are Salvador Aceves, Gene Berry, Francisco Espinosa, Timothy Ford, James Fugina, Joel Martinez, Timothy Ross, and Vernon Switzer.

Key Words: compressed hydrogen, cryogenic compressed hydrogen, hydrogen fuel, liquid hydrogen.

For further information contact Salvador Aceves (925) 422-0864 (aceves6@llnl.gov).

Patents and Awards

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

Process for Direct Integration of a Thin-Film Silicon P-N Junction Diode with a Magnetic Tunnel Junction

Daniel Toet, Thomas W. Sigmon
U.S. Patent 6,541,316 B2
April 1, 2003
A process for direct integration of a thin-film silicon p-n junction diode with a magnetic tunnel junction for use in advanced magnetic random access memory cells of high-performance, nonvolatile memory arrays. The process is based on pulsed laser processing for the fabrication of vertical polycrystalline silicon electronic device structures, in particular p-n junction diodes, on films of metals deposited on low-temperature substrates such as ceramics, dielectrics, glass, or polymers. The process preserves underlayers and structures onto which the devices are typically deposited, such as silicon integrated circuits. The process involves the low-temperature deposition of at least one layer of silicon, either in an amorphous or a polycrystalline phase on a metal layer. Dopants may be introduced in the silicon film during or after deposition. The film is then irradiated with short-pulse laser energy, which is efficiently absorbed in the silicon, resulting in the crystallization of the film and simultaneously in the activation of the dopants by ultrafast melting and solidification. The silicon film can be patterned either before or after crystallization.

System and Method for Characterizing, Synthesizing, and/or Canceling Out Acoustic Signals from Inanimate Sound Sources

John F. Holzrichter, Greg C. Burnett, Lawrence C. Ng
U.S. Patent 6,542, 857 B1
April 1, 2003
A system and method for characterizing, synthesizing, and/or canceling out acoustic signals from inanimate sound sources. Propagating-wave electromagnetic sensors monitor excitation sources in sound-producing systems, such as machines, musical instruments, and various other structures. Acoustical output from these sound-producing systems is also monitored. From such information, a transfer function characterizing the sound-producing system is generated. From the transfer function, acoustical output from the sound-producing system may be synthesized or canceled. These methods enable accurate calculation of matched transfer functions relating specific excitations to specific acoustical outputs. Knowledge of such signals and functions can be used with various applications for sound replication, sound source identification, and sound cancellation.

Method for Measuring and Controlling Beam Current in Ion Beam Processing

Patrick A. Kearney, Scott C. Burkhart
U.S. Patent 6,554,968 B1
April 29, 2003
A method for controlling film thickness of ion-beam sputter-deposition films. Great improvement in film thickness control is accomplished by keeping the total current supplied to both the beam and suppressor grids of a radiofrequency (rf) in beam source constant, not just the current supplied to the beam grid. By controlling both currents with this method, deposition rates are more stable, allowing the deposition of layers with extremely well-controlled thicknesses to about 0.1 percent. The method is carried out by calculating deposition rates based on the total of the suppressor and beam currents and maintaining the total current constant by adjusting rf power, which gives more consistent values.

Surface Contouring by Controlled Application of Processing Fluid Using Marangoni Effect

Michael C. Rushford, Jerald A. Britten
U.S. Patent 6,555,017 B1
April 29, 2003
An apparatus and method for modifying the surface of an object by contracting the surface with a liquid processing solution using the liquid applicator geometry and Marangoni effect (surface-tension-gradient-driven flow) to define and confine the dimensions of the wetted zone on the surface. In particular, the method and apparatus involve contouring or figuring the surface of an object using an etchant solution as the wetting fluid and applying real-time metrology (for example, interferometry) to control the placement and dwell time of the wetted zone locally on the surface of the object, thereby removing material from the surface in a controlled manner. One demonstrated manifestation is in the deterministic optical figuring of thin glass by wet chemical etching using a buffered hydrofluoric acid solution and Marangoni effect.

Awards

Ken Neves, the Laboratory's chief information officer (CIO), and **Mark Seager**, assistant head of Advanced Technology in the Integrated Computing and Communications Department, were named to ***HPCwire***'s list of **Top People and Organizations to Watch in 2003.**

HPCwire is the online magazine for high-performance computing in research laboratories, academia, and industry.

Neves came from Boeing Corporation in 2002 as Livermore's first full-time CIO. *HPCwire* cited Neves's history of innovation: "Being from Boeing, an early adopter of HPC and sophisticated business systems, Ken has a lot of experience in merging and managing business computing and science and technology computing. He has the potential to make a big impact on LLNL."

Seager, who manages the Platforms Program for the Advanced Simulation and Computing Program, was cited for his pioneering work in managing advanced simulation and computing architectures: "Mark has successfully managed partnership architectures, such as ASCI Blue Pacific, White, and Purple and unclassified powerful LLNL Linux cluster. . . . Very high profile projects and position."

At a recent barbeque lunch, about **400 National Ignition Facility (NIF) construction workers** celebrated an outstanding safety record and two **national safety awards of excellence**.

Jacobs Constructors, the NIF construction manager, received a **Construction Industry Safety Excellence Award** for the outstanding safety record achieved by its crew of workers based on the project's duration, worker hours, and number of injuries. The prestigious award was presented by the **Construction Users Roundtable**, an industry group dedicated to promoting cost-effective and safe construction methods.

The **National Safety Council's Perfect Year Award** honored NIF for achieving 1,403,873 employee hours without occupational injury or illness involving days away from work for the year ending December 2002. NIF has received this award for two consecutive years.

Abstracts

Riding the Waves of Supercomputing Technology

For the Advanced Simulation and Computing (ASC) Program and ASCI-type machines, there always seems to be a need for more. More capability to run scientific calculations at large scale. More capacity to process a varied workload from many users simultaneously. To meet these requirements, Livermore has created a computing strategy of straddling and switching to new cost-performance curves of computer technology. Livermore is working off three curves. The first, most mature technology curve is for massively parallel scalable supercomputers, culminating with ASCI Purple in 2004. Purple will fulfill the stockpile stewardship goal to achieve 100 trillion floating point operations per second (teraflops) in the 2004 to 2005 timeframe. To reach multiple petaflops by 2010 requires moving off this curve and on to others. The second curve, a near-term technology based on cluster architecture combined with open-source software, is epitomized by the new Multiprogrammatic Capability Resource system. The third curve involves cell-based supercomputers using system-on-a-chip technology and low-cost, low-power embedded microprocessors. This third technology is embodied in BlueGene/L, designed by IBM and slated for delivery to Livermore in 2004.

Contact:
Michel McCoy (925) 422-4021 (mccoy2@llnl.gov).

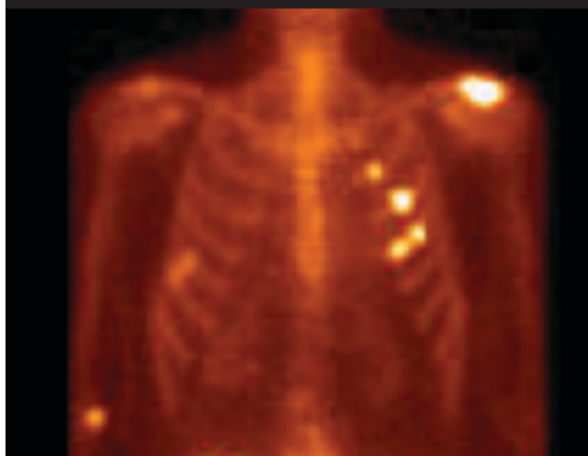
Chromosome 19 and Lawrence Livermore Form a Long-Lasting Bond

Over the past two decades, Livermore researchers have discovered important information about the 1,400 genes belonging to chromosome 19. Livermore scientists mapped the location of hundreds of genes on chromosome 19, discovered the function of many of its genes, and began the task of sequencing the chromosome as part of the Human Genome Project. The final sequencing steps, completed this year by the Joint Genome Institute, filled the gaps in the sequence and increased the overall accuracy to 99.99 percent, or one error per 10,000 bases. Livermore scientists have moved on to the postgenomics era to understand the function of genes and the ensymes or proteins these genes manufacture. They are comparing the human genome to that of other organisms such as the mouse, chicken, and pufferfish. They are also studying the complex mechanisms that govern how some genes regulate the actions of others. Knowledge about chromosome 19 and other chromosomes will improve the understanding of how genes influence disease development, contribute to the discovery of new treatments, illuminate how species evolved, and help scientists form a molecular understanding of life.

Contact:
Lisa Stubbs (925) 422-8473 (stubbs5@llnl.gov).

U.S. Government Printing Office: 2003/583-060-70043

Targeting Radiation Therapy More Precisely



A collaboration between Lawrence Livermore and the University of California at Davis is working to customize the diagnosis and treatment of cancer.

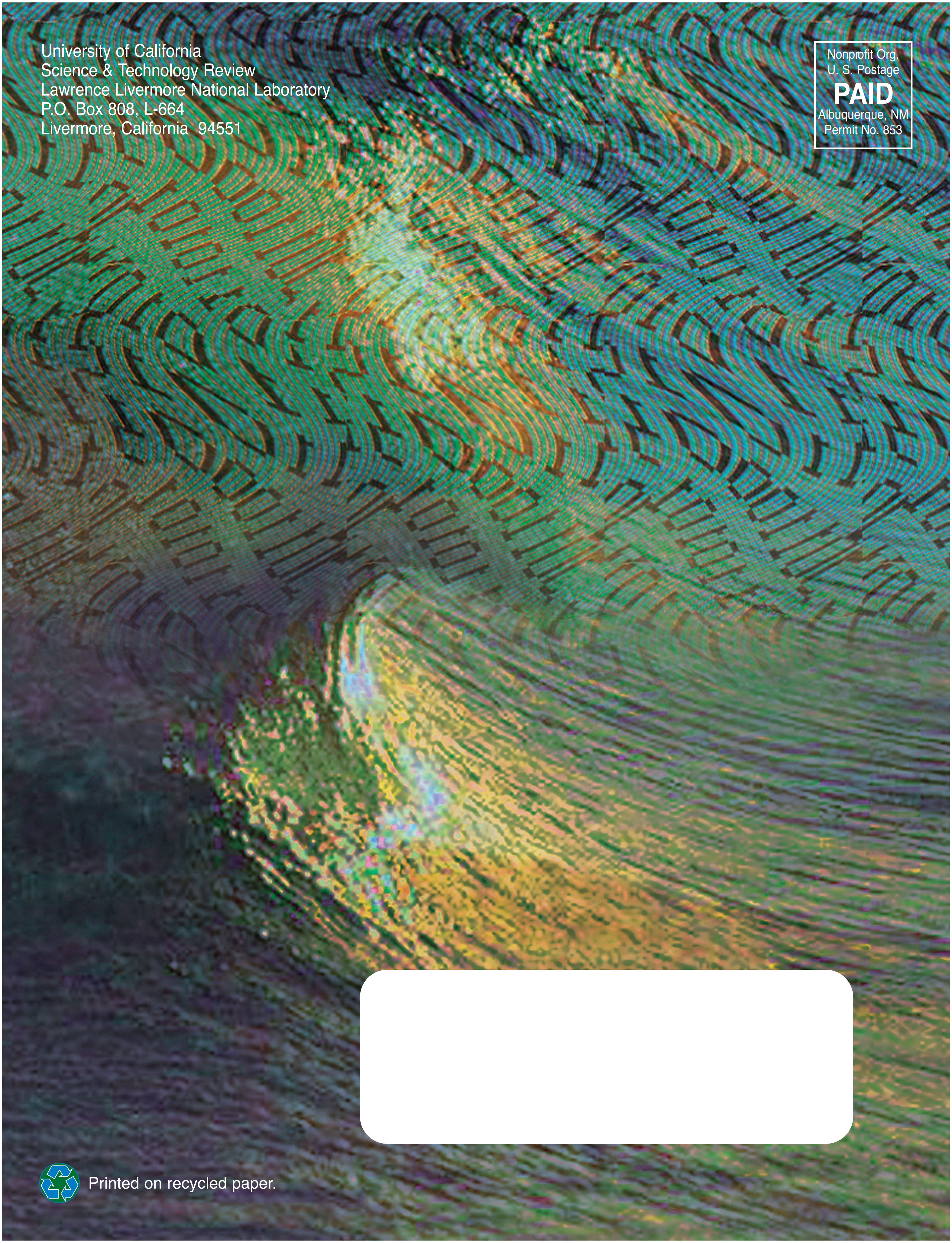
Also in July/August

- ***Cells exposed to low-dose ionizing radiation react differently than those exposed to higher doses of radiation.***

- ***The new Decontamination and Waste Treatment Facility will make it easier for the Laboratory to responsibly handle its hazardous, radioactive, and mixed wastes from "cradle to grave."***

- ***Weapons designers are developing munitions that better direct their destructive power to the intended target.***

Coming Next Month



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