

Oak Ridge Leadership Computing Facility
Annual Report 2010–2011

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On the cover:

Leadership-class molecular dynamics simulation of the plant components lignin and cellulose. This 3.3 million-atom simulation was performed on 30,000 cores of the Jaguar XT5 supercomputer and investigated lignin precipitation on cellulose fibrils, a process that poses a significant obstacle to economically viable bioethanol production. Simulation by Jeremy Smith, ORNL. Visualization by Mike Matheson, ORNL.

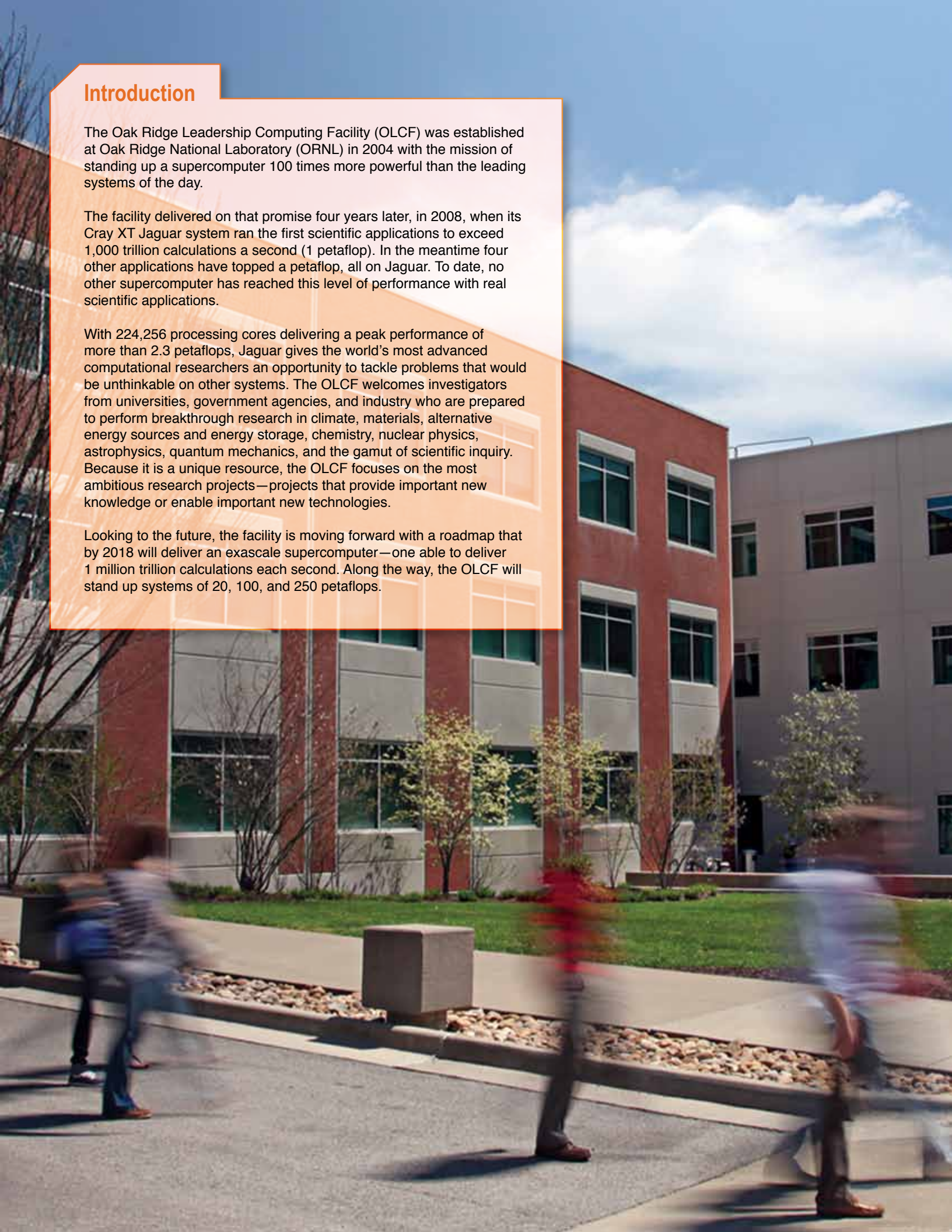
Introduction

The Oak Ridge Leadership Computing Facility (OLCF) was established at Oak Ridge National Laboratory (ORNL) in 2004 with the mission of standing up a supercomputer 100 times more powerful than the leading systems of the day.

The facility delivered on that promise four years later, in 2008, when its Cray XT Jaguar system ran the first scientific applications to exceed 1,000 trillion calculations a second (1 petaflop). In the meantime four other applications have topped a petaflop, all on Jaguar. To date, no other supercomputer has reached this level of performance with real scientific applications.

With 224,256 processing cores delivering a peak performance of more than 2.3 petaflops, Jaguar gives the world's most advanced computational researchers an opportunity to tackle problems that would be unthinkable on other systems. The OLCF welcomes investigators from universities, government agencies, and industry who are prepared to perform breakthrough research in climate, materials, alternative energy sources and energy storage, chemistry, nuclear physics, astrophysics, quantum mechanics, and the gamut of scientific inquiry. Because it is a unique resource, the OLCF focuses on the most ambitious research projects—projects that provide important new knowledge or enable important new technologies.

Looking to the future, the facility is moving forward with a roadmap that by 2018 will deliver an exascale supercomputer—one able to deliver 1 million trillion calculations each second. Along the way, the OLCF will stand up systems of 20, 100, and 250 petaflops.



Best at the Petascale, First to the Exascale



Jeff Nichols, Associate Laboratory Director
for Computing and Computational Sciences

The Oak Ridge Leadership Computing Facility exists to push the boundaries of computational science, tackling and overcoming challenges that could not otherwise be attempted.

Created seven years ago, its mission was to stand up a system 100 times more powerful than the leading supercomputers of the day. It succeeded with Jaguar, which is now capable of 2.3 petaflops.

Jaguar has been among the world's top three supercomputers through six iterations of the semiannual Top500 List of the world's most powerful systems. It spent a year at the top of the list in 2009 and 2010, and it is still the most powerful supercomputer in the United States. This is a very good run in a world as volatile as high-performance computing, but it doesn't begin to tell the story. The value of a scientific supercomputer is not in its ranking, but in the work it can accomplish. Jaguar sets itself apart because it has brought real, working scientific applications into the petascale age.

Consider two measures of Jaguar's success as a scientific workhorse: petaflop applications and the Gordon Bell Prize.

Faster simulations gather more data and, thereby, provide greater detail of the physical systems they describe. As a result, the hazy, general picture of earlier simulations becomes clearer and more detailed. To date, five scientific applications have topped 1 petaflop, all on Jaguar. Thomas Schulthess—head of the Swiss National Supercomputing Centre—and colleagues had the first with DCA++, which models high-temperature superconductors. Another team, led by Markus Eisenbach of ORNL, holds the record to date with WL-LSMS, an application that analyzes magnetic systems and, in particular, the effect of temperature on these systems. This application reached 1.84 petaflops on Jaguar.

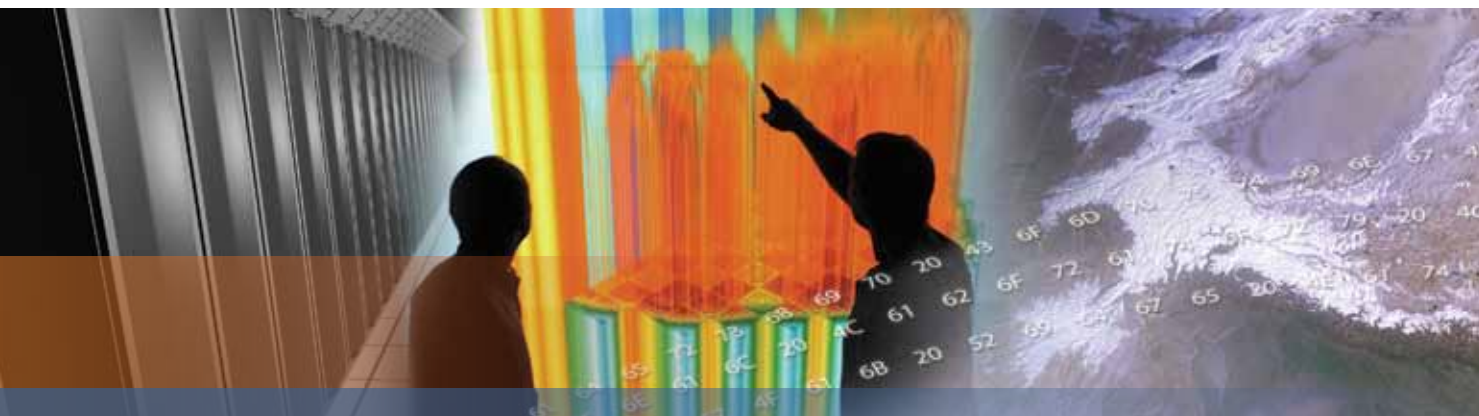
The Gordon Bell Prize comes from the Association of Computing Machinery each year to recognize the world's pre-eminent application. Prizewinners for the past three years ran on Jaguar, including Schulthess in 2008 and Eisenbach in 2009. The winning application in 2010 simulated 200 million realistic red blood cells and their interaction with plasma in the circulatory system. This effort came from a team led by George Biros of Georgia Tech.

We are proud to have led the way into the petascale age. We are even more excited to be pushing toward the next major milestone: a supercomputer able to perform a million trillion calculations each second, otherwise known as an exaflop. That is a one followed by 18 zeroes.

We expect to achieve the exascale by 2018. Our next system, called Titan, should be up and running next year and will be as much as 10 times more powerful than Jaguar, able to reach from 10 to 20 petaflops. Titan will represent a major change from Jaguar in configuration as well as speed, and this change will bring challenges for our users as well as for us.

Jaguar reached the petascale by connecting hundreds of thousands of central processing units, or CPUs. These are the same chips that run home computers, but while a home computer may have two processing cores, Jaguar has 224,000.

This approach, however, has its limits; high among them are space and power requirements. An exascale supercomputer relying on the same design as Jaguar would contain 500 times as many processing cores—more than 100 million. It would require 500 times as much space. And it would require 500 times as much power. The current Jaguar system draws about 7 megawatts of electricity; 500 times that amount would be 3½ gigawatts, or about three times the power output of the nearby Watts Bar nuclear power plant.



To overcome these obvious obstacles, Titan will use a combination of traditional CPUs and graphics processing units (GPUs), developed a decade ago to improve graphics rendering for computer displays. GPUs more recently have been used very effectively to speed high-performance computers, taking the parallel approach inherent in a system like Jaguar and pushing it to a new level. While a traditional processor may have two, four, or eight computing cores, a graphics processor can have hundreds, giving it the ability to divide simple calculations and process them with blistering speed.

We are proud to have led the way into the petascale age. We are even more excited to be pushing toward the next major milestone: a supercomputer able to perform a million trillion calculations each second, otherwise known as an exaflop.

The challenge for us is that we must continue to revolutionize the supporting hardware and software that takes the theoretical potential of a new system and makes it a practical reality. The challenge for our users will be in the fact that they must rewrite many of their applications to take advantage of this new level of parallelism. As a result, we will be working with researchers to rewrite their code in order to exploit the most parallelism possible.

The good news is that their efforts will be applicable in systems well beyond Titan. The world's most powerful supercomputers will use GPUs and other accelerators for the foreseeable future, not just at

ORNL but around the world. Researchers who want to push the limits of their fields will have to adapt their codes to this new level of parallelism, but once they do, their efforts will pay off for years to come.

We envision two systems beyond Titan to achieve exascale performance by about 2018. The first will be an order of magnitude more powerful than Titan, in the range of 200 petaflops. This system will be an exascale prototype, incorporating many of the hardware approaches that will be incorporated at the exascale. We hope to scale this solution up to the exascale.

ORNL will not be alone in pushing the boundaries of high-performance computing. The top two spots on the Top500 List now belong to supercomputers in Japan and China. In fact, there are four countries represented in the top 10 spots and seven in the top 20.

Nevertheless, the OLCF and ORNL will maintain leadership in this very competitive field for years to come. ORNL has become known as a lab for computing, and with good reason. In addition to Jaguar, we house and support the National Science Foundation's most powerful supercomputer, the University of Tennessee's Kraken system, which is also the most powerful academic supercomputer in the country. We also house and support the National Oceanic and Atmospheric Administration's most powerful supercomputer, Gaea.

Wherever the forefront of scientific supercomputing goes, we will be there.

In a League of Its Own

When it comes to real science, Jaguar has no peer

Jaguar has had an impressive run among the world's most powerful supercomputers.

It has spent the last three years ranked among the world's three most powerful systems, which is impressive when you consider the brutal competition at the pinnacle of supercomputing. In fact, you need to go back to June 2006 in order to find a Top500 List in which Jaguar is not in the top 10.

But the Top500 List does not tell the whole story.

Because it relies on the benchmarking High Performance Linpack test, the list does not evaluate applications that produce scientific results. In fact, if you focus on performance in the service of serious research, Jaguar is in a league of its own. No other system in the world has anything comparable to Jaguar's record of scientific productivity.

"Jaguar remains a unique resource," noted Bronson Messer, acting director of science at the Oak Ridge Leadership Computing Facility. "Though it feels like computing on any modern computer—for example a workstation or a departmental cluster—the machine is really more like the Large Hadron Collider in Europe or the Hubble Space Telescope; it's a unique scientific instrument."

Jaguar's prominence at the forefront of scientific computing can be best illustrated with two measures. The first is the annual Gordon Bell Prize, which recognizes the world's foremost scientific application. The second is the roster of scientific applications that have broken the petaflop barrier.

Five applications have sustained performance of greater than 1 petaflop; all of them were running on Jaguar. Gordon Bell Prize winners for the past three years also ran on Jaguar, as did many finalists for the prize, all of which broke new ground in fields from seismology to biology to electronics.

"For most of the history of computational science, simulation has been a way to confirm physical intuition," Messer noted. "But now, with applications that can run at sustained petaflop speeds, you're able to run a numerical experiment.

"As you increase resolution you see the development of physical phenomena that you know happen but were unable to see in simulations before now. And, because you are doing it via simulation, you control that universe. You can change various parameters and you can see how this particular phenomenon actually reacts."

Gordon Bell Prize 2008: High-temperature superconductors

An application that simulates superconducting copper-oxide materials brought in the 2008 Gordon Bell Prize for a team led by Thomas Schultness of ORNL and the Swiss National Supercomputing Centre. DCA++, as the application is known, was the first scientific application to break the petaflop barrier, reaching 1.35 petaflops on a Jaguar system that, at the time, had 180,000-plus processor cores and a peak performance of 1.64 petaflops.

Superconducting materials are both immensely useful—being indispensable in applications ranging from magnetic resonance imaging

machines to the Large Hadron Collider to magnetic levitation transportation systems—and immensely challenging, because they must be kept very cold. Copper-oxide materials known as cuprates are the most advanced superconductors discovered so far, yet they must still be kept well below minus 200 degrees Fahrenheit to be superconducting. DCA++ simulates cuprate materials atom by atom in order to better uncover the secrets of high-temperature superconductivity and, possibly, design new superconducting materials that need not be kept so cold.



A team led by Thomas Schulthess of the Swiss National Supercomputing Centre, center, was awarded the 2008 Gordon Bell Prize for its simulations of high-temperature superconductors.

Two other 2008 finalists took advantage of Jaguar. A team led by Lin-Wang Wang of Lawrence Berkeley National Laboratory won a special Gordon Bell Prize for algorithmic innovation with an application that conducts first-principles calculations of electronic structure. A team led by Laura Carrington of the San Diego Supercomputing Center used the system to shatter its own record in modeling seismic waves traveling through the earth. The experience of these leading computational scientists bodes well for groundbreaking science in the years to come.

“It’s amazing that a code this complex could be ported to such a large system with so little effort,” noted Carrington. “This was a landmark calculation on the ORNL petaflop system that enables a powerful new tool for seismic wave simulation.”

Gordon Bell Prize 2009: Magnetic systems

The 2009 prize went to ORNL’s Markus Eisenbach and colleagues, who used 223,000 processors to reach 1.84 petaflops on a Jaguar system that had been upgraded to 224,000 processors and a peak performance of 2.33 petaflops.

Their application—WL-LSMS—analyzes magnetic systems and, in particular, the effect of temperature on those systems. By accurately revealing the magnetic properties of specific materials—even materials that have not yet been produced—the application is useful in the search for stronger, more stable magnets.

Another ORNL-led team was a finalist for the 2009 prize. Edoardo Aprà and colleagues achieved 1.39 petaflops on Jaguar in a first-principles, quantum-mechanical exploration of the energy contained

in clusters of water molecules. The team used a computational chemistry application known as NWChem, which was developed at Pacific Northwest National Laboratory.

The application used 223,200 processing cores to accurately study the electronic structure of water by means of a quantum chemistry technique known as coupled cluster. The team will make its results available to other researchers, who will be able to use these highly accurate data as inputs to their own simulations.



A team led by ORNL's Markus Eisenbach, left, won the 2009 Gordon Bell Prize for its work on Jaguar using WL-LSMS, a materials code useful in analyzing magnetic systems.

Gordon Bell Prize 2010: Red blood cells in plasma

Jaguar was prominent again for the 2010 prize, hosting four of six finalists, including the winner. Georgia Tech's George Biros and colleagues took the prize with MoBo, a fluid dynamics application that simulates blood flow. The team used 196,000 processors to run at 700 trillion calculations a second, or 700 teraflops, simulating 200 million red blood cells and their interaction with plasma in the circulatory system.

The team's work was a leap forward not only because of the number of blood cells being simulated, but also because of the realism of those cells. While earlier simulations were of spherical red blood cells, MoBo simulated cells that wiggle and change shape, like a water balloon. In addition, it included the long-distance communication that red blood cells have through plasma.

An honorable mention in the 2010 competition went to Schulthess and Anton Kozhevnikov of ETH Zurich and Adolfo G. Eguiluz of the University of Tennessee–Knoxville. The team reached 1.3 petaflops and scaled to the full Jaguar system in a method that solves the Schrödinger equation from first principles for electronic systems while minimizing approximations or simplifying assumptions.

A third finalist was a team led by Thomas Jordan, director of the Southern California Earthquake Center (SCEC), which used Jaguar to perform the world's most advanced earthquake simulation to date, focusing on the state's San Andreas Fault. The team used nearly all of Jaguar's processing cores to simulate a magnitude 8 quake shaking a 125,000-square-mile swath across Southern California. Known as M8, the simulation reached 220 teraflops, more than twice the speed of any previous large-scale seismic simulation.

The team used an earthquake wave propagation application program called AWP-ODC, for Anelastic Wave Propagation–Olsen–Day–Cui, based on a numerical method for calculating earthquake waves originally developed by team member and San Diego State University geophysics professor Kim Olsen. The application calculates both the rupture as it travels along the fault and the earthquake waves and resultant shaking as they spread through the region.

The SCEC team simulated a 340-mile rupture that began in Central California and continued nearly to the Mexican border. The simulation went on to assess the shaking produced by this rupture on a chunk of the earth's crust 500 miles long, 250 miles wide, and 50 miles deep.

The simulation needed the power of Jaguar for two principal reasons, according to SCEC information technology architect Philip Maechling. First was the size of the region being studied, which the simulation divided into 436 billion 40-cubic-meter cells. Second was the frequency of the seismic waves, which the simulation was able to calculate up to 2 hertz, or 2 cycles per second, without resorting to approximation.

No previous earthquake simulation of this scale has been able to directly calculate earthquake waves above 1 hertz. According to team member Yifeng Cui, a computational scientist at the University of California–San Diego's San Diego Supercomputing Center, each doubling in wave frequency requires a 16-fold increase in computational resources. On the other hand, building engineers who analyze structural responses to strong ground motions use waves up to 10 hertz in their analyses, so M8 represents a milestone toward the larger goal of similar simulations at even higher frequencies.

Finally, researchers from the University of Texas–Austin (UT), the California Institute of Technology, and Rice University used Jaguar to advance an innovative collection of algorithms that selectively focuses a supercomputer's power.

The team has been conducting groundbreaking simulations of convective flows within the earth's mantle, the multimillion-year rising and falling of hot, viscous rock that is a main driver for the motion of tectonic plates. Its work on the Texas Advanced Computing Center's Ranger system earned it a spot on the cover of the August 27 *Science* magazine. On Jaguar the team scaled the algorithms to the entire system and reached 175 teraflops.

The algorithms advance a technique known as adaptive mesh refinement, or AMR, which focuses a computer's power on the most important and dynamic areas of a simulation. In particular, they improve the simulation's ability to reallocate computing tasks among processors, allowing the simulation to run on hundreds of thousands of processors without getting bogged down.



In 2010, a team led by Georgia Tech's George Biros, third from left, won the Gordon Bell Prize for its work on Jaguar simulating blood flow.

While AMR is not a new approach, researchers have had great difficulty scaling the technique for large supercomputers. Different regions become more or less active during the course of a simulation, meaning the cells in those regions become larger and smaller and work must, therefore, be reallocated among the processors. As a result, simulations run the risk of using progressively more of a system's power to reallocate resources and progressively less to do the actual calculations.

The team was able to overcome this obstacle, with the simulations on Jaguar using only 0.05 percent of the system's resources specifically on the AMR.

"Algorithms in the past have had difficulty scaling to even 10,000 cores," noted UT computational geoscientist Omar Ghattas, "so the fact that we ran to over 200,000 cores with very high parallel efficiency, we believe that's a big accomplishment. We have on the order of a 5,000- to 10,000-fold reduction in the number of cells. This is almost a four-orders-of-magnitude reduction in the problem size."

At the petascale: Modeling the journey of electrons

Four of the applications that have broken the petaflop barrier have been either winners or finalists in the Gordon Bell competition: Schulthess's teams' prize-winning simulation of high-temperature superconductors and solution to the Schrödinger equation for electronic systems, Eisenbach's team's prize-winning analysis of magnetic systems, and Aprá's team's simulation of water molecules.

A fifth petaflop application came from a team led by Gerhard Klimeck of Purdue University. Klimeck and Purdue's Mathieu Luisier used more than 220,000 processor cores and reached 1.03 petaflops to model the journey of electrons as they travel through electronic devices at the smallest possible scale.

The team is pursuing this work on Jaguar with two applications, known as Nanoelectric Modeling (NEMO) 3D and OMEN (a more recent effort whose name is an anagram of NEMO). The team calculates the most important particles in the system—valence electrons located on atoms' outermost shells—from their fundamental properties. These are the electrons that flow in and out of the system. On the other hand, the applications approximate the behavior of less critical particles—the atomic nuclei and electrons on the inner shells.—by *Leo Williams*

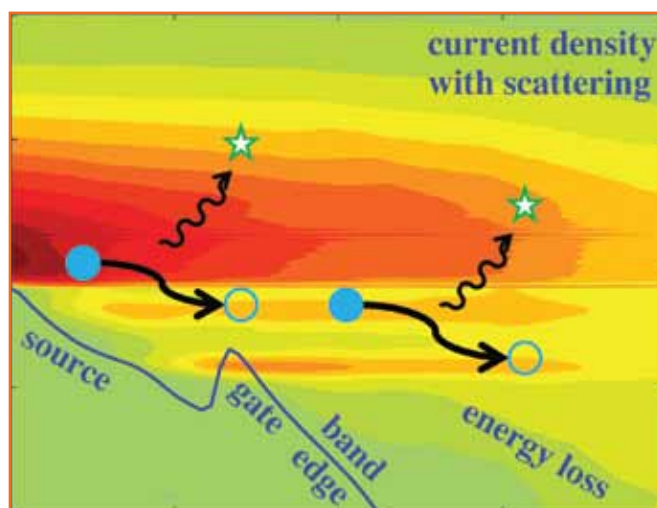


Illustration of electron-phonon scattering in a nanowire transistor. The current is plotted as a function of position (horizontal) and energy (vertical). Electrons (filled blue circles) lose energy by emitting phonons or crystal vibrations (green stars) as they move from the source to the drain of the transistor. Image courtesy Gerhard Klimeck, Purdue University.

4.5 BILLION HOURS AND COUNTING



INCITE gives researchers unprecedented computing power

Computational researchers are an ambitious bunch, hunting for new knowledge at the limits of the universe, the nooks and crannies of the nanoscale, and everywhere in between.

Groundbreaking computational research, however, relies on groundbreaking computing power. Scientists use all the computing resources they can get, but they could often use more—sometimes much more. That’s where the Innovative and Novel Computational Impact on Theory and Experiment program comes in.

Through INCITE, as it is more commonly known, the world’s most advanced computational researchers receive substantial time on some of the world’s most powerful supercomputers. The only requirement is that they make the most of these unique resources.

The resources are provided by the Department of Energy’s (DOE’s) Office of Science, the United States’ largest supporter of research in the physical sciences. INCITE researchers work on two world-class Office of Science systems, the OLCF’s Jaguar, currently ranked number three in the world, and the Argonne Leadership Computing Facility’s Intrepid, ranked number 15.

Jaguar has a peak performance of 2.33 petaflops, while Intrepid can reach as much as 557 teraflops. Together they have roughly the computing power of 135,000 dual-core laptops.

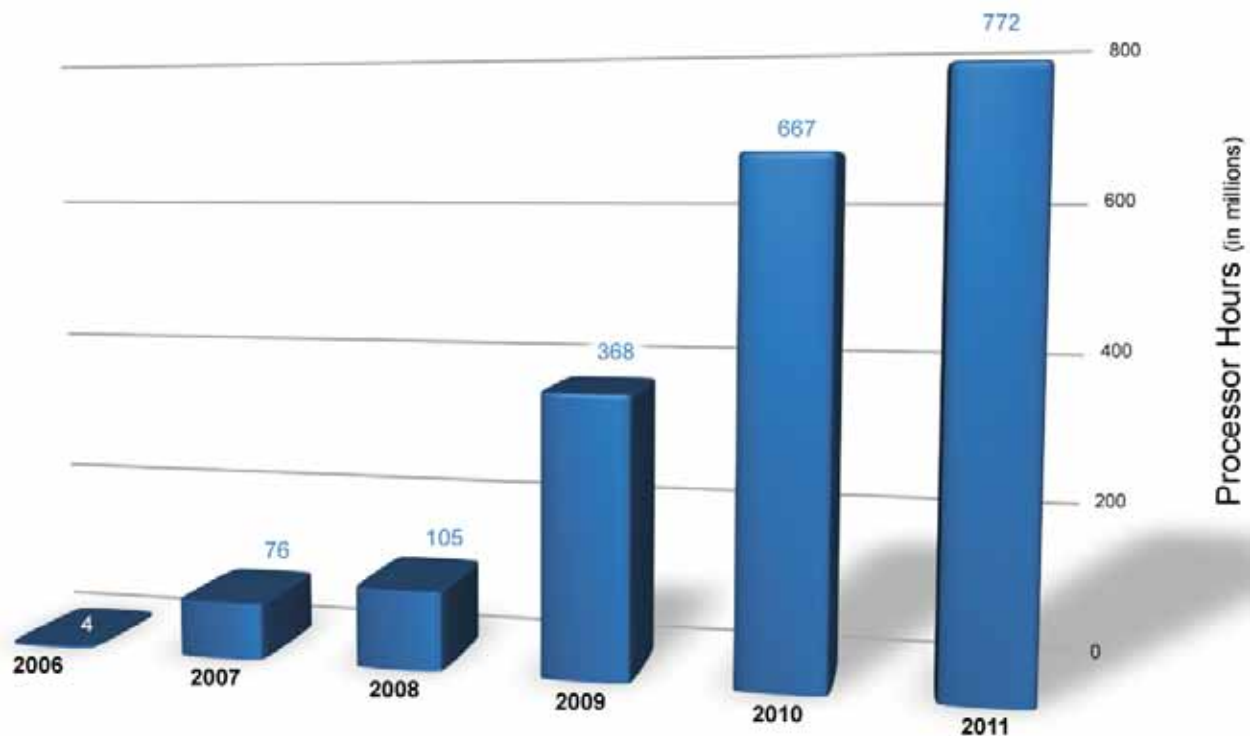
Now managed by the two computing facilities, the INCITE program was created in 2003 by Raymond Orbach, then DOE’s undersecretary for science. Orbach explained the reasoning behind INCITE in a 2007 talk to the Council on Competitiveness.

“It is often said that science is based on two pillars,” he said, “namely experiment and theory. In fact, high-end computation, especially through simulation, is the third pillar of science. It is actually a staple support as well. It gives us the ability to simulate things which cannot be done either experimentally or for which no theory exists—simulations of complex systems which are simply too hard or so far are not amenable to analytic approaches.”

INCITE at the petascale

The OLCF is deeply committed to the INCITE program, supporting it with America’s most powerful supercomputer, the Cray XT5 Jaguar system, as well as world-class support systems and a staff of highly skilled supercomputer experts and computational scientists. OLCF liaisons are experts in their fields—chemistry, physics, astrophysics, mathematics, numerical analysis, computer science—but they are also experts in designing code and optimizing it for Jaguar. A large project may ask its liaison to join the research team as a full-fledged member, or it may choose instead to consult with its liaison only on specific challenges.

INCITE Hours Allocated to OLCF



This support helps ensure that the world's most ambitious computational research scientists get the tools and help they need.

Jaguar, created to be at the vanguard of supercomputing, hosted each of the five applications reported to have broken the petaflop barrier. This speed is critically important to researchers needing to improve knowledge and advance technology.

"Applications that can run at sustained petaflop speeds are able to do huge computations," said Bronson Messer, acting director of science at the OLCF. "This means they're able to run a numerical experiment—very highly resolved with really good physical models. You get numbers out that you would have confidence comparing to an experimental or theoretical result.

"That's a new thing, to some extent—to be able to make quantitative predictions with simulations. We've had examples of that for a long time, but now we have a wave of applications."

"As you increase resolution you see the development of physical phenomena that you know are there but weren't present in earlier simulations," he said. "A good example are the recent, very-high-resolution regional climate models where you get hurricanes. They don't get born if you're not able to resolve the shear layer in the atmosphere that forms."

Researchers interested in doing work on the INCITE supercomputers participate in an annual call for proposals, with proposals reviewed by experts from national laboratories, universities, and industry. Winners

are picked both for their ability to make the most of the supercomputers and their potential to advance science and technology. In general, INCITE projects are expected to use 20 percent or more of the INCITE systems—about 45,000 processing cores in Jaguar's case.

The INCITE program allocates computing resources by the processor hour. Many of the world's most powerful systems, including Jaguar, use processors much like those found on home computers. But while your laptop may have two or even four processing cores, supercomputers have tens to hundreds of thousands.

A processor hour, then, is a single hour on one processing core. A single hour using all of Jaguar's 224,000 processing cores, in turn, would be 224,000 processor hours. For a dual-core laptop to reach 224,000 processor hours it would have to run day and night for 12 ½ years.

INCITE started off modestly by today's standards. In its first year, 2004, three projects received just under 5 million processor hours total from Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center. In contrast, the 57 awardees in 2011 received a total of 1.7 billion processor hours. Those allocations averaged 27 million hours, with one receiving more than 110 million hours.

The OLCF does its part

By the time 2011 wraps up, researchers from academia, industry, and government laboratories will have been allotted more than 4.5 billion processor hours from INCITE over the years.

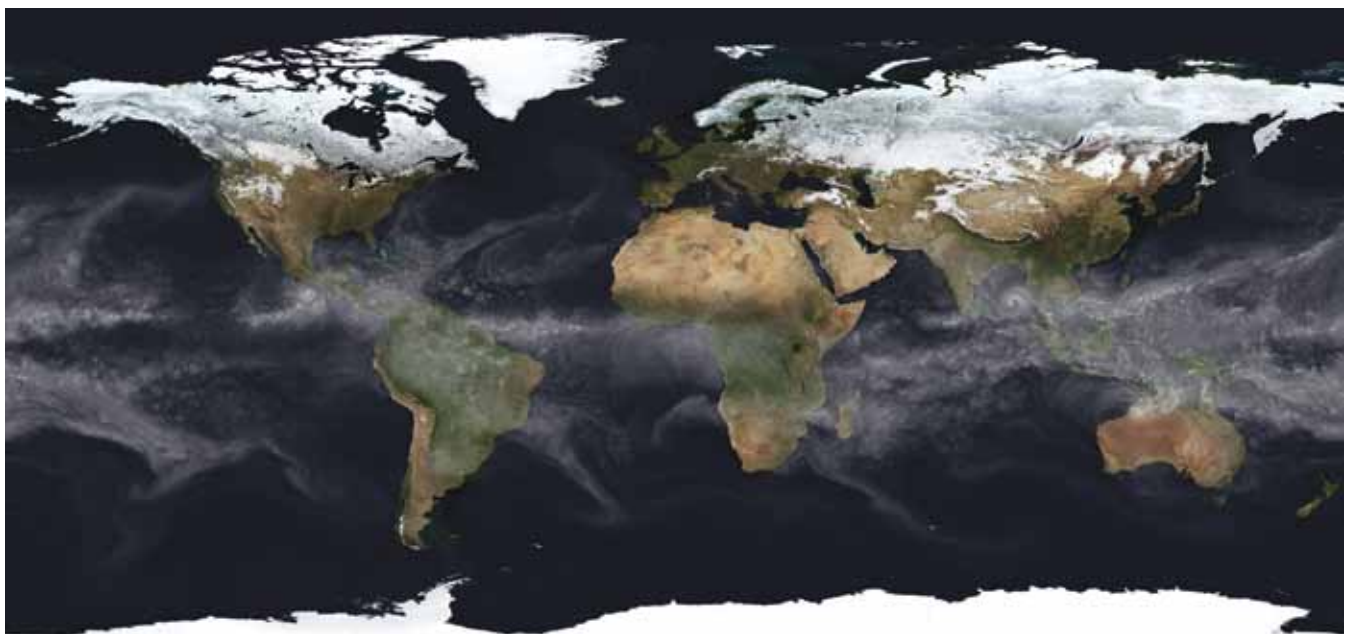
Most of those hours will have come from the OLCF. The facility first joined the program in 2006, providing 3.5 million processor hours to five projects. By 2010 the OLCF was hosting 45 projects with allocations totaling 950 million processor hours. All told, the OLCF has contributed 178 yearly allocations totaling 2.5 billion processor hours.

Those projects run the gamut of energy, technology, and basic science research:

- **Engineering** researchers have modeled the design of aircraft. They have simulated the design and operation of nuclear reactors. And they have simulated the safety of transporting and storing commercial explosives.
- **Chemists** have simulated radically more powerful car batteries. They have worked to understand the process of combustion in internal combustion engines. They have simulated gasifier technology for the production of relatively clean energy from coal. And they have taken a close look at the chemical catalysts that are immensely important to many industrial processes.
- **Biologists** have simulated the production of ethanol from woody plants such as switchgrass and poplar trees. They have looked at the replication of genetic material and techniques for sequencing DNA. They have looked at the role of proteins in membrane fusion. And they have looked at the role of proteins in biological membranes.
- **Materials** scientists have examined electronics and technology at the scale of atoms and molecules. They have modeled the quantum mechanical forces at work in electronic devices and the quantum mechanical states of charge carriers. They have modeled high-temperature superconductors and solar cells at the nanoscale. And they have simulated the binding of molecules on surfaces to better understand catalysis, corrosion, crystal growth, and many other phenomena.
- **Fusion** researchers have simulated ITER, which, when built, will be the world's largest fusion reactor and is set to begin operation by the end of the decade. These researchers have focused on plasma turbulence at the scale of ions and at the much smaller scale of electrons. They have simulated energy loss caused by plasma turbulence. They have examined the edge of the plasma with an eye to confinement of the fusion reaction. And they have looked at radio wave heating of the plasma.
- **Astrophysicists** have used INCITE to explore the universe at fantastic scales. They have simulated the explosion of stars eight or more times the mass of the sun. They have run 13 billion-plus-year simulations of nearly undetectable dark matter gathering to determine the size and shape of the galaxy. And they have examined the behavior of astrophysical plasmas around the solar system.
- **Earth and climate** scientists have developed ever-more refined and predictive models for climate in the future and into the far past. They have simulated hurricanes in order to improve forecasting. They have simulated earthquakes in order to improve building safety and emergency preparedness. And they have examined contaminant migration in groundwater and the feasibility of storing carbon dioxide deep underground.

This is, of course, a woefully incomplete list. Another INCITE project was promising enough to get a callout from President Obama in the 2011 State of the Union Address.

The proper simulation of water vapor distribution in the climate system is essential to an accurate treatment of the hydrological cycle and the planetary radiation budget. This image shows the simulated monthly-averaged distribution of the total column water vapor from a high-resolution configuration of the CCSM Community Atmospheric Model. Visualization courtesy Jamison Daniel, ORNL.



Nuclear simulation gets attention

“At Oak Ridge National Laboratory,” the president said, “they’re using supercomputers to get a lot more power out of our nuclear facilities.” “They,” in this context, is the Consortium for Advanced Simulation of Light Water Reactors, an ORNL-led collaboration of national laboratories, universities, private industry, and other organizations.

The application they’re using is called Denovo, created by ORNL physicist Thomas Evans. It solves the Boltzmann equation, which describes the statistical distribution of individual particles in a fluid, to simulate any radiation that does not interact strongly with the radiation’s source, whether it be photons, electrons, or the neutrons responsible for nuclear fission.

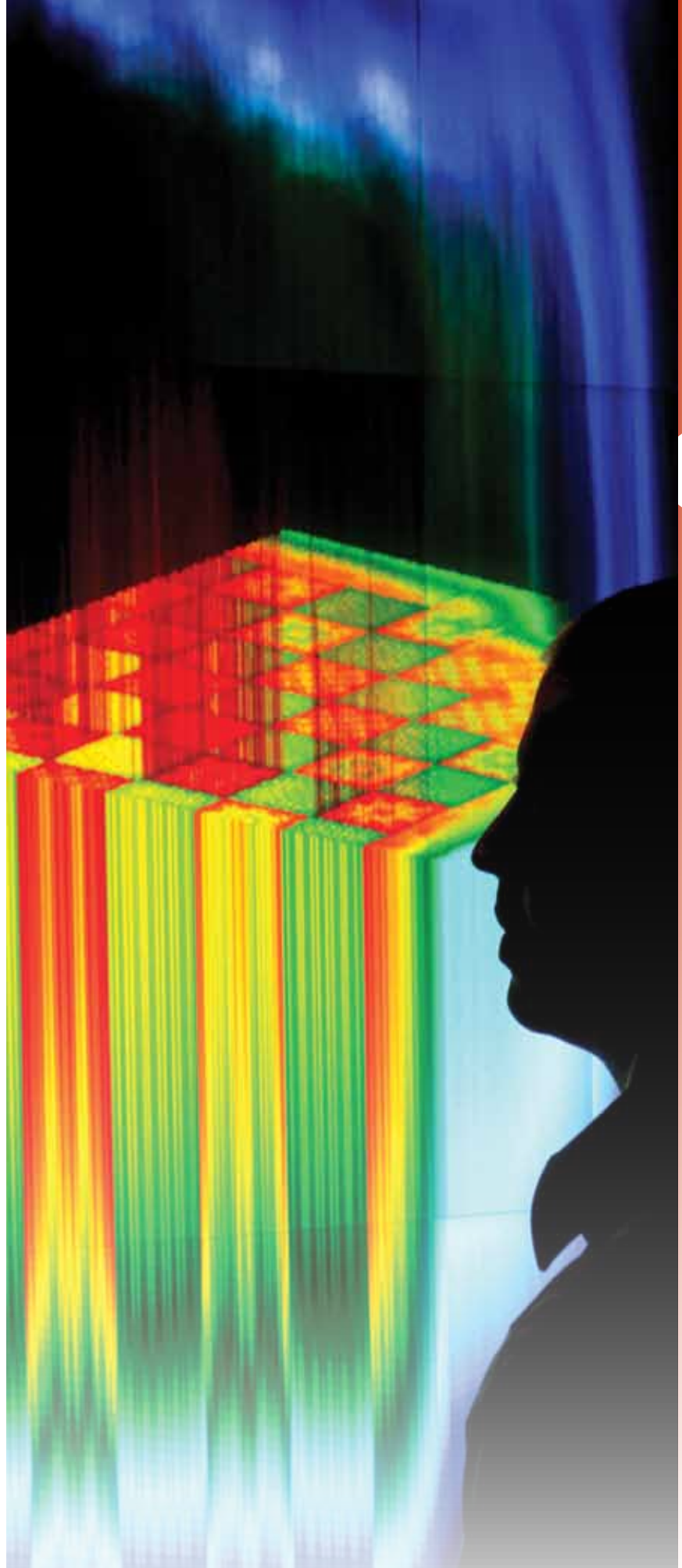
INCITE gives Evans and colleagues the resources to perform simulations of unprecedented detail on Jaguar with allocations of 8 million processor hours in 2010 and another 18 million in 2011.

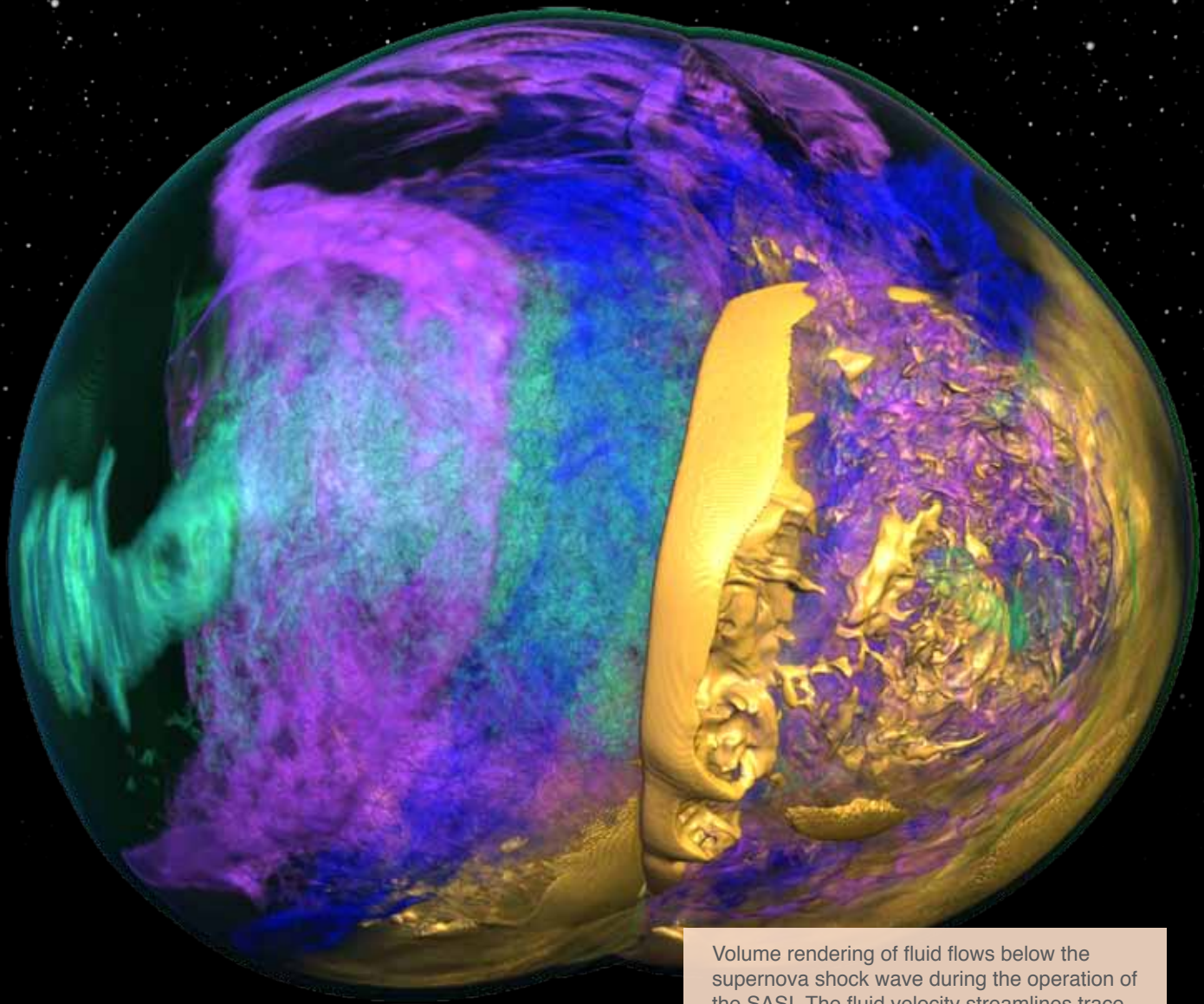
ORNL will be able to contribute progressively more to the program as it moves beyond the petascale toward an exascale system 500 times more powerful than Jaguar by the end of the decade.

These resources will arrive none too soon for a computational science community that already understands what it will be able to do with such systems.

- When chemists are able to perform accurate, first-principles, nanoscale simulations of the enzymatic breakdown of switchgrass into its component sugars at the nanoscale, they will have taken a large step toward producing low-cost ethanol that helps wean us from our reliance on foreign oil.
- When astrophysicists have worked out the precise manner in which collapsing iron cores blow massive stars into space, they will have uncovered the secrets of the universe’s most productive element factories.
- When chemists are able to design new materials maximized for strength, resilience, chemical reactions, electrical properties, or any combination of attributes, few industries will remain unaffected.

Researchers in these fields and many others look forward to getting access to the next generation of scientific supercomputers. INCITE will be there to make sure they do.—*by Leo Williams*





Volume rendering of fluid flows below the supernova shock wave during the operation of the SASI. The fluid velocity streamlines trace out complex flow patterns in the simulation. Image courtesy Kwan-Liu Ma, University of California–Davis.

Exploring the Magnetic Personalities of Stars

Massive stars are inherently violent creatures—they burn, they churn, they turn, all the while creating and held hostage by constantly changing magnetic fields of almost unfathomable strength.

And, eventually, they explode, littering the universe with the elements of life as we know it: hydrogen, oxygen, carbon, etc. Everything including ourselves is the result of some star's violent demise. "We are stardust, we are golden, we are billion-year-old carbon" goes the song "Woodstock" by Crosby, Stills, Nash, and Young. Even the hippies know it.

And no stars do it better than those that will one day become core-collapse supernovas (CCSNs), or stars greater than 8 solar masses. The evolution and nature of these elemental fountains is still a mystery, one of the greatest unsolved problems in astrophysics. But perhaps

not unsolved for long. A team led by ORNL's Tony Mezzacappa is getting closer to explaining the origins of CCSN explosions with the help of Jaguar.

Essentially, said Eirik Endeve, lead author of the team's latest paper, researchers want to know how these magnetic fields are created and how they impact the explosions of these massive stars. A recent suite of simulations allowed the team to address some of the most fundamental questions surrounding the magnetic fields of CCSNs. Its findings were published in the April 20, 2010, issue of *The Astrophysical Journal*.

In untangling the mystery surrounding the stars' powerful magnetic fields, researchers could ultimately explain a great deal as to why these stellar giants evolve into elemental firecrackers.

In an effort to locate the source of the magnetic fields, the team simulated a supernova progenitor, or a star in its pre-supernova phase, using tens of millions of hours on Jaguar, the United States' fastest supercomputer. The process revealed that we still have much to learn when it comes to how these stellar marvels operate.

Rotation isn't everything

Collapsed supernova remnants are commonly known as pulsars, and when it comes to magnetic fields, pulsars are the top players in the stellar community. These highly magnetized, rapidly rotating neutron stars get their name from the seemingly pulsing beam of radiation emitted by a pulsar, similar to the varying brightness produced by lighthouses as they rotate. This rotation is thought to be a big factor in determining the strength of a pulsar's magnetic field—the faster a star rotates the stronger its magnetic fields.

Supernova progenitors tend to be slower-rotating stars. Nevertheless, the simulations of these progenitors revealed a robust magnetic-field-generation mechanism, contradicting accepted theory that rotation could be a primary driver.

Simulations of these progenitors revealed a robust magnetic-field-generation mechanism, contradicting accepted theory that rotation could be a primary driver.

Interestingly, this finding builds on the team's previous work, which together with the latest simulations reveals that the culprit behind pulsar spins is likewise responsible for their magnetic fields. The earlier simulations, the results of which were published in "Pulsar spins from an instability in the accretion shock of supernovae" in the January 2007 edition of *Nature*, demonstrated that a phenomenon known as the spiral mode occurs when the shock wave expanding from a supernova's core stalls in a phase known as the standing accretion shock instability (SASI). As the expanding shockwave driving the supernova explosion comes to a halt, matter outside the shockwave boundary enters the interior, creating vortices that not only start the star spinning, but also yank and stretch its magnetic fields as well.

This new revelation means two things to astronomers: first, that any rotation that serves as a key driver behind a supernova's magnetism is created via the spiral mode, and second, that not only can the spiral mode drive rotation, it can also determine the strength of a pulsar's magnetic fields.

Another major finding of the team's simulations is that shear flow from the SASI, when counter-rotating layers of the star rub against one another during the SASI event, is highly susceptible to turbulence, which can also stretch and strengthen the progenitor's magnetic fields, similar to the expansion of a spring.

These two findings taken together show that CCSN magnetic fields can be efficiently generated by a somewhat unexpected source: shear flow-induced turbulence roiling the inner core of the star. "We found that starting with a magnetic field similar to what we think is in a supernova progenitor, this turbulent mechanism is capable of magnifying the magnetic field to pulsar strengths," said Endeve.

The GenASiS of magnetic fields

The team used the General Astrophysical Simulation System (GenASiS) to study the evolution of the progenitor's magnetic fields. GenASiS, under development by Christian Cardall, Eirik Endeve, Reuben Budiardja, and Tony Mezzacappa at ORNL and Pedro Marronetti at Florida Atlantic University, features a novel approach to neutrino transport and gravity and makes fewer approximations than its earlier counterpart, which assumed CCSNs were perfectly spherical.

The simulations essentially solved a series of magnetohydrodynamic equations, or equations that describe the properties of electrically conductive fluids. After setting the initial conditions, the team ran several models at low and high resolutions, with the highest-resolution models taking more than a month to complete. Initially, said Endeve, they were run at lower resolutions, but very little significant activity occurred. However, as they ramped up the resolution, things got interesting.

The model starts at 4,000 processing cores, said Endeve, but as the star becomes more chaotic with turbulence and other factors, the simulations are scaled up to 64,000 cores, giving the team a more realistic picture of the magnetic activity in a CCSN. He added that the fact that the time to solution for these hugely varying job sizes is the same due to Jaguar's queue scheduling policy is a "great advantage."

"The facilities here [OLCF] are excellent," said Endeve, adding that the center's High Performance Storage System is very important to the team's research, as one model produces hundreds of terabytes of data. "We have also received a lot of help from the visualization team, especially Ross Toedte, and the group's liaison to the OLCF, Bronson Messer," he said.

The team will next incorporate sophisticated neutrino transport and relativistic gravity, which will give it an even more realistic picture of CCSNs. However, to make such a powerful code economical, said Endeve, it will need to employ an adaptive mesh. And it will no doubt require Jaguar's unprecedented computing power.

This latest discovery is just one more step toward unraveling the mysteries of CCSNs. As GenASiS continues to evolve, the team will be able to investigate these important stellar cataclysms at unprecedented levels, bringing science one step closer to a fundamental understanding of our universe.—by Gregory Scott Jones



EARTHQUAKE SIMULATION ROCKS SOUTHERN CALIFORNIA

California takes earthquakes very seriously. The state straddles two major tectonic plates and is subject to relatively frequent, often major, potentially devastating quakes.

It should come as no surprise, then, that the most advanced simulation of an earthquake ever performed on a supercomputer focuses on California and its San Andreas Fault. A team led by Southern California Earthquake Center (SCEC) director Thomas Jordan used Jaguar to simulate a magnitude-8 quake shaking a 125,000-square-mile area of Southern California and assess its impact on the region. The simulation earned the team a slot as one of six finalists for the 2010 Gordon Bell Prize, awarded to the world's most advanced scientific computing application.

Known as M8, the SCEC project simulated a 6-minute earthquake half again as powerful as the temblor that destroyed San Francisco in 1906—or 30 times as powerful as the quake that devastated Haiti last year.

According to SCEC information technology architect Philip Maechling, the center chose magnitude 8 because it is one of the largest quakes that could plausibly hit Southern California.

“Some of these investigations, especially the one we just did on Jaguar, go back to a change from emergency management organizations after Hurricane Katrina,” Maechling noted. “Before Katrina they were asking, ‘What’s likely to happen? Give us the most probable scenarios that we’re going to have to face.’ But after Katrina they changed the question and said, ‘Tell us what’s the worst that could happen.’ My understanding is that they were changing the question because they want to be ready for not only the most likely, but also the worst case.”

The San Andreas Fault forms the boundary between the Pacific and North American tectonic plates. The Pacific Plate includes a sliver of California and Baja California, as well as Hawaii and most of the Pacific Ocean, while the North American Plate includes the remainder of the United States, Greenland, and a hefty chunk of eastern Russia.

The SCEC team simulated a 340-mile rupture that began on the San Andreas Fault near Cholame—an unincorporated community in San Luis Obispo County best known for its proximity to James Dean’s fatal car accident—and continued southeast to Bombay Beach—a desert community on the eastern shore of the Salton Sea, 225 feet below sea level. The simulation went on to assess the shaking produced by this rupture on a chunk of the earth’s crust 500 miles long, 250 miles wide, and 50 miles deep.

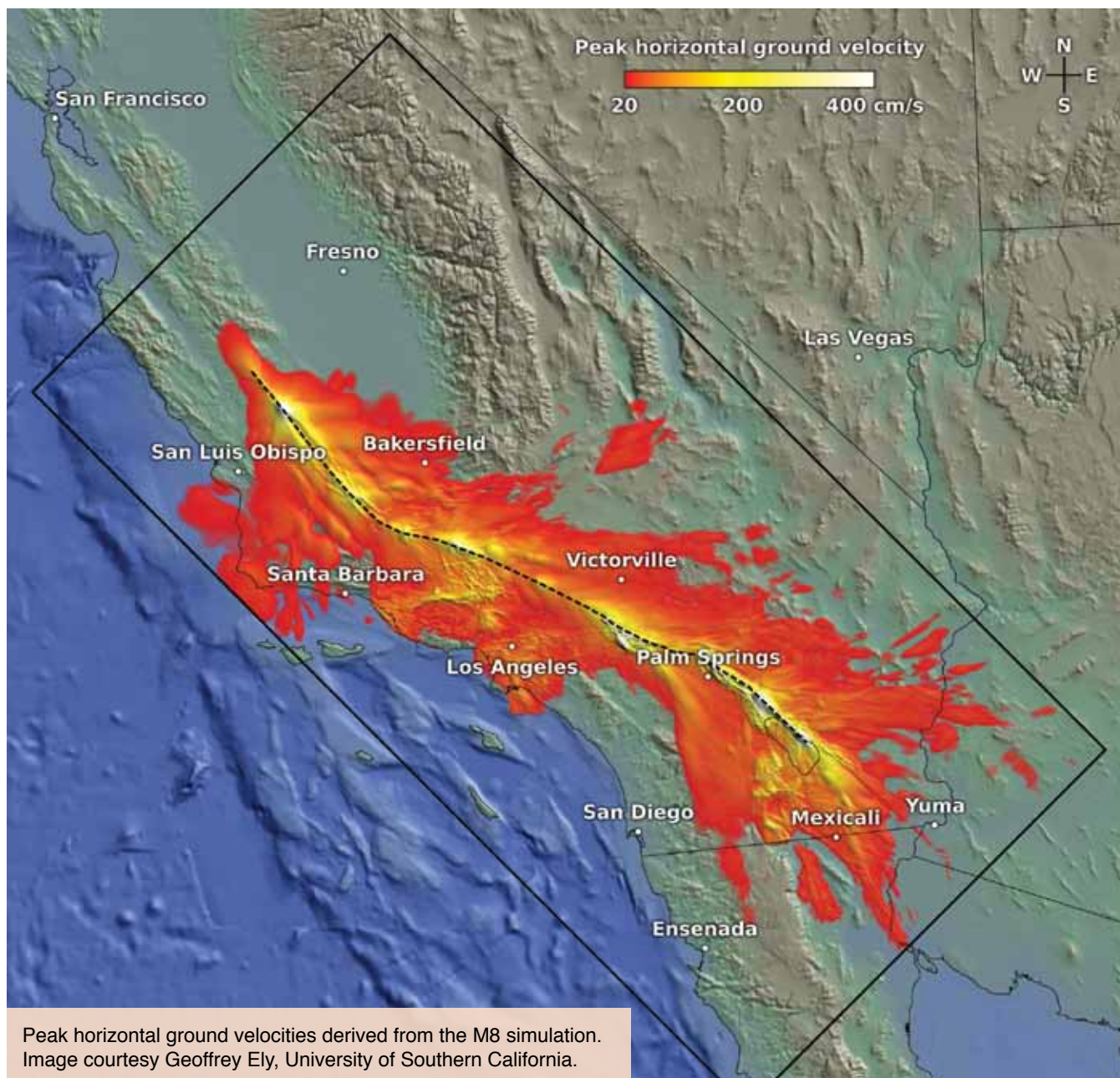
That chunk is home to 20 million people—about one in 15 Americans. As a result, information provided by the M8 project will be valuable not only to seismologists, but also to building designers and emergency planners working to minimize the devastation brought on by Southern California’s inevitable next big shakeup.

The M8 simulation required Jaguar for two reasons, Maechling noted. First was the size of the region being studied, which the simulation divided into 435 billion 40-cubic-meter cells. Second was the frequency of the seismic waves, which the simulation was able to calculate up to 2 hertz, or 2 cycles per second, without resorting to approximation.

No earthquake simulation of this scale has been able to directly calculate earthquake waves above 1 hertz. According to computational scientist Yifeng Cui of the San Diego Supercomputing Center at the University of California—San Diego, each doubling in wave frequency requires a 16-fold increase in computational resources. On the other hand, building engineers analyzing structural responses to strong ground motions use waves up to 10 hertz in their analyses, so M8 represents a milestone toward the larger goal of similar simulations at even higher frequencies.

Imagine a bathtub full of water. If you kick the bathtub, the water will start sloshing back and forth in the tub. That’s an analogy to what happens to seismic waves in a sedimentary basin.

“Going to these higher frequencies will allow us to capture a lot more parameters of the waves,” noted SDSU geophysics professor Kim Olsen. “For example, you can characterize the waves by the displacement from side to side at a point, or the velocity of the point from side to side or up and down, or the acceleration of the point. With the low frequency we might be able to capture the displacement or even the velocities, but the acceleration of the point or the ground location is really a higher-frequency concept. We won’t be able to capture that acceleration unless we go to higher frequencies—2 hertz or preferably even higher. And that acceleration is really needed for a lot of purposes, especially in structural engineering and building design.”



The project conducted its first Jaguar simulation in April 2010, running for 24 hours and taking advantage of nearly all of Jaguar's 224,000-plus processing cores. The simulation reached 220 teraflops, more than twice the speed of any previously completed large-scale seismic simulation. It used an earthquake wave propagation application program called AWP-ODC—for Anelastic Wave Propagation—Olsen-Day-Cui—based on a numerical method for calculating earthquake waves originally developed by Olsen. Solving a coupled system of partial difference equations defined on a staggered grid, the application calculated the rupture as it traveled along the fault, and the earthquake waves and resultant shaking as they spread through the region.

One reason the M8 simulation produced accurate ground motions for all locations within the simulation region is that it used an accurate three-dimensional (3D) model of Southern California's complex geology. Decades of oil exploration mean that the geology of the area

has been thoroughly analyzed, and accurate 3D geological models are available for the region.

Earthquake experts have discovered that the nature of the geology makes a profound difference in the way an earthquake plays out. Unfortunately, the layers of sediment that fill valleys and underlie most populated areas have the habit of shaking longer and harder than other forms of geology.

"The waves are generally stronger in promulgating through sedimentary basins such as those below Los Angeles, San Fernando, and San Bernardino," Olsen explained, "and the thickness of relatively loose sediments in these basins can exceed a kilometer. In those areas the waves tend to get amplified, and the duration of the waves tends to get extended."

In fact, he said, these geologically unconsolidated and often highly populated regions tend to trap earthquake waves, which then bounce back and forth rather than moving on.

“Imagine a bathtub full of water,” he said. “If you kick the bathtub, the water will start sloshing back and forth in the tub. That’s an analogy to what happens to seismic waves in a sedimentary basin.”

The team has compared results from the M8 simulation with data averaged from many real earthquakes and is generally pleased. In particular, the average shaking seen in the M8 simulation on rock sites (i.e., areas other than sedimentary basins) matches very well with the available data. The ground motion in sedimentary basins such as Los Angeles and Ventura (northwest of Los Angeles) was generally larger than predicted by the average data records, noted Olsen, but that discrepancy is readily explained by the fact that averaged records do not reflect effects caused by complex source propagation and 3D basin amplification in a specific earthquake. In particular, he noted, the simulation includes long stretches in which the ground ruptures faster than the speed of a particular wave known as the shear wave. This “supershear” rupture creates a wave effect analogous to a sonic boom and may account for the especially strong ground shaking in the basins. Additional M8 rupture scenarios planned within SCEC will attempt to address this important scientific question.

In time these simulations will contribute significantly to the information used by the state’s building designers and emergency agencies to prepare for future earthquakes.

“Basically, we combine different realizations of the same earthquake on the same stretch of the fault into what we call an ensemble of ground motions,” explained Olsen. “We take the average ground motions for all of the points of these different realizations, including different epicentral locations and slip on the fault, and find the variation around the mean. I think that’s a lot more valuable for engineers. That will give them an idea of how uncertain the ground motion is.”

According to Maechling, this knowledge will ultimately be useful to scientists and other experts looking at earthquake-prone regions across the globe, not just in California.

“If you’re studying earthquakes, Southern California is a good spot,” he said. “We’ve got a big plate boundary. The geology—a lot of it’s in the desert—is well exposed. There’s a lot of instrumentation in the region, ground motion sensors and GPS and strain meters. Plus there are a lot of people at risk.

“We’re doing simulations in order to develop and validate predictive models of earthquake processes and then to use these models to better understand the seismic hazard in Southern California. The things we learn about earthquakes here should be applicable to earthquakes around the world.”—by *Leo Williams*

OLCF Vis Team Helps Simulate Japanese Crisis

Soon after the earthquake and tsunami crippled Japan’s Fukushima Dai-Ichi nuclear plant in March of 2011, ORNL began simulating the crisis, employing the laboratory’s unique mix of talented nuclear specialists and computational scientists in an effort to provide the Japanese government with information.

In order to give the ORNL team a view of exactly what is occurring in and around the plant, two OLCF visualization specialists, Jamison Daniel and David Pugmire, are simulating various aspects of the plant site, from fly-bys of the reactor building itself to the behavior of the spent fuel rods within.

According to Pugmire, one of the major issues being studied is the decay rate of different fuel rod bundles in the spent fuel pool. Because the bundles are put into the pool at different times, knowing which bundles are where is critical to mitigating the consequences.

The effort is a mix of computer-aided design and data gleaned from the OLCF’s simulations, which have used a variety of codes, including those developed by the ORNL-led Consortium for Advanced Simulation of Light Water Reactors.

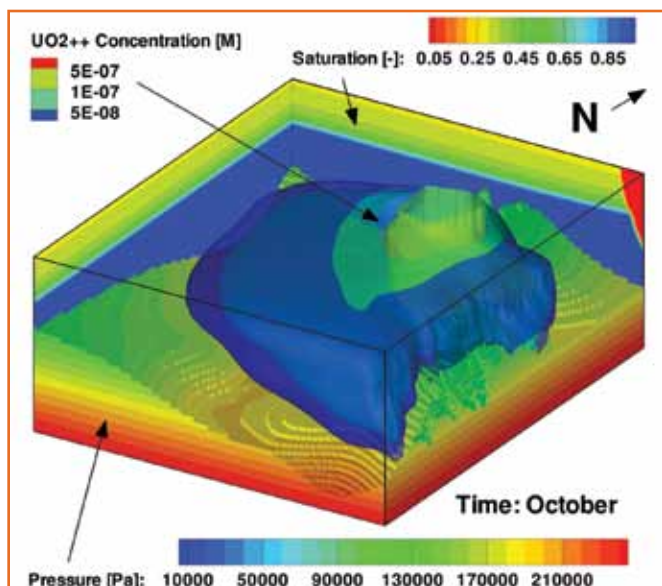
The results are forwarded to ORNL Director Thom Mason, who then sends them up the chain of command to Energy Secretary Steven Chu. From there it can be provided to Japanese scientists and officials.

And while the simulations are currently being done on smaller ORNL computing resources, that may not be the case for long. “We’re working up to do some large-scale simulations (on some of the bigger machines),” said Jeff Nichols, ORNL’s associate lab director for scientific computing. —by *Gregory Scott Jones*



Rendering of the Fukushima reactor building spent fuel rod pool from above. The spent fuel rods are placed into one of three racks. The rods are colored by the date they are placed into the spent fuel pool.

SUPERCOMPUTERS ASSIST CLEANUP OF DECADES-OLD NUCLEAR WASTE



Peter Lichtner and colleagues run the PFLOTRAN code on Jaguar to model the distribution of uranium at the Hanford Site's 300 Area. Image courtesy Peter C. Lichtner, LANL.

The Hanford Site in Washington state—which produced fuel slugs for nuclear weapons, acted as a waste storage facility for nearly five decades, and was one of three primary locations for the Manhattan Project—is among the most contaminated nuclear waste grounds in the country. A research team led by Peter C. Lichtner of Los Alamos National Laboratory (LANL) is using Jaguar to build a three-dimensional model of an underground uranium waste plume at the Hanford Site's 300 Area. A better understanding of the underground migration properties of uranium, which has infiltrated the Columbia River, may aid stakeholders in weighing options for contaminant remediation.

“The project's results could certainly help one decide how to go about remediating the site, if it's even feasible,” said Lichtner, whose project receives funding from the DOE offices of Biological and Environmental Research and Advanced Scientific Computing Research. “The results could apply to other sites along the Columbia River that are contaminated too. And what we learn from this site we should be able to apply to other sites as well, not only at Hanford, but also around the country— at Oak Ridge and other areas dealing with contamination.”

The Hanford plume has been polluting groundwater and the nearby Columbia River for decades. Waste from nuclear weapons production has been stored at Hanford since the early 1940s, mostly in underground tanks. But the uranium now penetrating the groundwater and river had simply been discharged to ponds and trenches, Lichtner said.

This research, among the latest in cleanup efforts at the Hanford Site, stems from a 1989 Tri-Party Agreement involving the Washington Department of Ecology, the Environmental Protection Agency (EPA), and DOE.

Lichtner's collaborators include Glenn Hammond of Pacific Northwest National Laboratory, Bobby Philip and Richard Mills of ORNL; Barry Smith of Argonne National Laboratory, Dave Moulton and Daniil Svystskiy of LANL, and Al Valocchi of the University of Illinois, Urbana-Champaign.

Uncovering the unseen

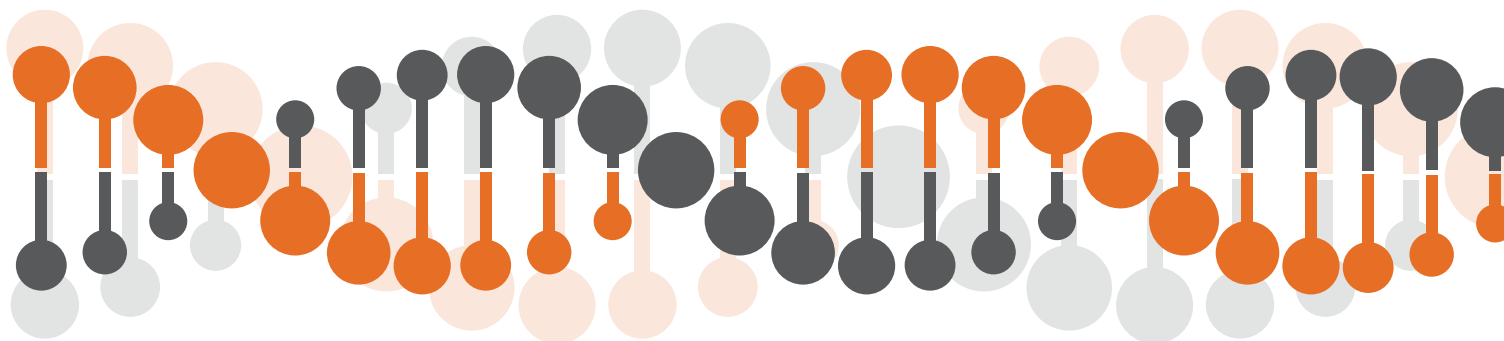
The Hanford Site covers 586 square miles of land. Contaminants of several types and quantities are spread throughout the site, including uranium, copper, and sodium aluminate. The uranium plume is in Hanford's 300 Area, a roughly 1.5 square mile site approximately 100 yards west of the Columbia River.

As uranium decays it emits alpha particles. Because skin blocks alpha particles, external exposure is not deemed a risk. In fact, uranium is classified as a heavy-metal hazard rather than a radiation one. Ingestion in high doses can cause bone or liver cancer or kidney damage. The EPA has set a contaminant limit of 30 micrograms per liter. The uranium contaminating Hanford's 300 Area exceeds this limit by four times, according to field tests.

A challenge for Lichtner's team is to predict the loss of uranium from the plume into the river. Initial simulation results coupled with field tests indicate that from 55 to 110 pounds of uranium leach into the Columbia River each year from the estimated 55 to 83 tons of source uranium. Yet until further research is conducted, these numbers remain very uncertain, said Lichtner, whose goal is to decrease this uncertainty.

The team performed massively parallel simulations of depleted uranium flow through soil using PFLOTRAN, a code developed under a project called SciDAC-2, which aims to advance computing at the petascale. The code has been run on more than 130,000 processors of Jaguar to describe the flow of fluid through porous media, in this case the movement of soluble depleted uranium through a soil mixture of sand, gravel, and fine-grained silts. The plume measures $984 \times 1,422 \times 22$ yards and was simulated using nearly 2 million control volumes, or grid cells, of $5.5 \times 5.5 \times 0.5$ cubic meters each. The team calculated the uranium loss from the plume and the flux into the Columbia River at 1 hour intervals, which allowed construction of realistic models of the river's interaction with the migrating plume.

The chemical properties of uranium and additional compounds composing the plume require the model to account for more than 28 million degrees of freedom—the number of actions these compounds might take as the plume migrates. The team simulated 1 year in only 11 hours by using more than 4,000 processors. Such speed is crucial to Hanford's timely remediation. —by Wes Wade



Supercomputers Simulate the Molecular Machines That Replicate and Repair DNA

Imagine you are an astronaut. A piece of space junk has cut a gash into the side of the space station, and you have been tasked with repairing the damage. Your spacesuit is equipped with a clamp, which you open, slide onto a tether connecting you to the space station, and close. Then you move to the far end of the gash and begin applying composite material to fill the holes. You glide along the gash making repairs until you are done.

DNA replication, modification, and repair happen in a similar way. That's what groundbreaking biochemical simulations run on one of the world's fastest supercomputers have revealed. Ivaylo Ivanov of Georgia State University, John Tainer of the Scripps Research Institute, and J. Andrew McCammon of the University of California–San Diego used Jaguar to elucidate the mechanism by which accessory proteins, called sliding clamps, are loaded onto DNA strands and coordinate enzymes that enable gene repair or replication. Their findings, published in the May 10, 2010, issue of the *Journal of the American Chemical Society*, inspire a new approach for attacking diverse diseases.

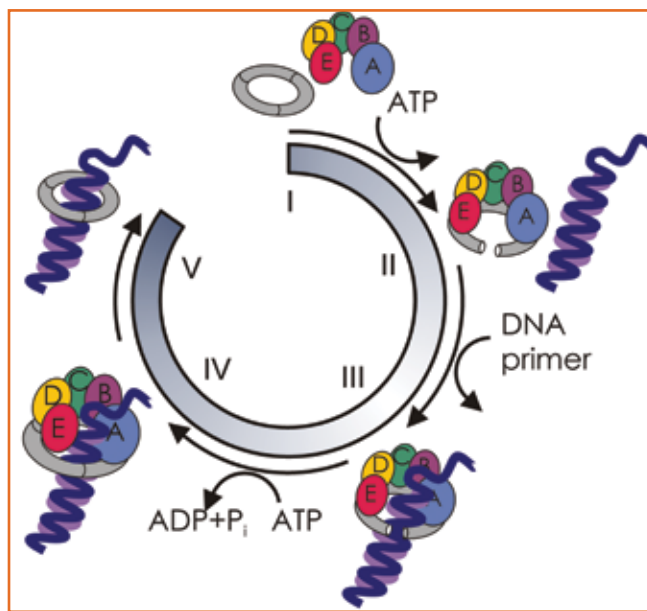
“This research has direct bearing on understanding the molecular basis of genetic integrity and the loss of this integrity in cancer and degenerative diseases,” said Ivanov, whose investigation was supported by the Howard Hughes Medical Institute and the National Science Foundation’s Center for Theoretical Biological Physics. The project focused on the clamp-loading cycle in eukaryotes—or plants, animals, and other organisms whose genetic material is enclosed in a nuclear membrane. Prokaryotes, such as bacteria, whose genes are not compartmentalized, also have a molecular machine to load clamps, but it works a little differently. Viruses, on the other hand, do not have their own clamp loaders but instead co-opt the replication machinery of their hosts.

So how does the molecular machine work in a eukaryote? The researchers revealed that a clamp loader (replication factor C) places a doughnut-shaped sliding clamp (proliferating cell nuclear antigen, or PCNA) onto DNA. The clamp loader first binds to the clamp to activate its opening with energy from adenosine triphosphate (ATP). Protein secondary structures, or beta sheets, at the junctures of the clamp’s three subunits, separate at one juncture. A complex made up of the open clamp and the clamp loader then encircles primer-template

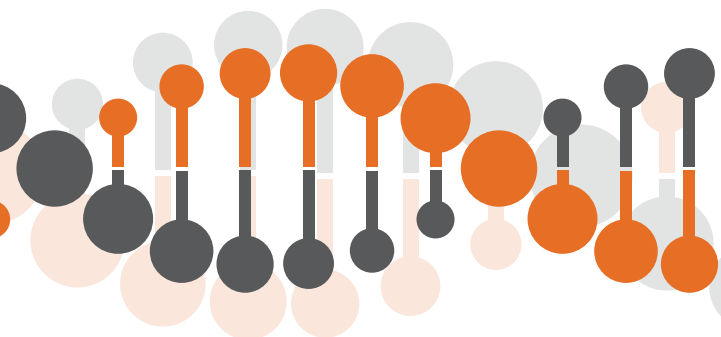
DNA, which is double-stranded in one region and single-stranded in another. Again activated by ATP, the clamp closes and is now free to slide along the DNA strand and coordinate enzymes needed for replication and repair.

These sliding clamps and clamp loaders are part of the replisome—the molecular machinery responsible for the faithful duplication of the genetic material during cell division. “The replisome is very complex and dynamic, with interchanging parts. It’s an incredibly challenging system to understand,” explained Ivanov. “Simulating just a few of its constituent parts—the clamp/clamp loader assembly—required a system of more than 300,000 atoms. To make progress simulating the system in a reasonable amount of time, we needed access to large-scale computing.”

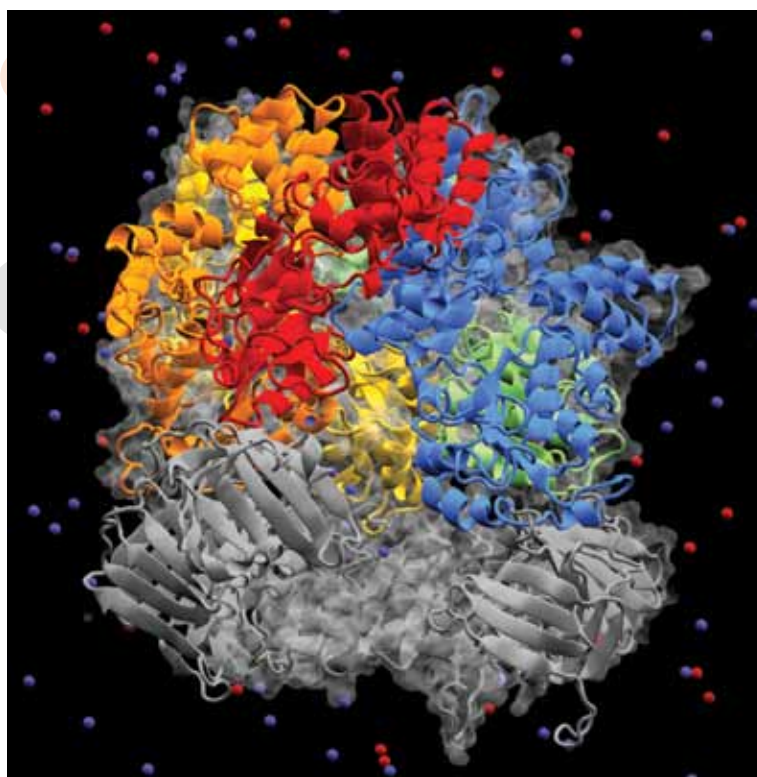
An allocation of supercomputing time through the INCITE program allowed the researchers to run NAMD, a molecular dynamics code.



The clamp-loading cycle. Image courtesy Ivaylo Ivanov, Georgia State University.



OLCF supercomputers illuminate the workings of the molecular machinery that opens and loads sliding clamps onto DNA. Sliding clamps play vital roles in both DNA replication and repair. Here the clamp loader (with its subunits shown in blue, green, yellow, orange, and red) is depicted in complex with a ring-open sliding clamp (shown in gray) and counterions (spheres). Image courtesy Ivaylo Ivanov, Georgia State University, and Mike Matheson, ORNL.



The work consumed more than 2 million processor hours on the Jaguar XT4 and XT5 components in 2009 and 2010, taking a few months of total computing time. Using the kind of machine on which NAMD is usually run, a single simulation continuously running would have taken years.

Master coordinator

In DNA replication the clamp slides along a strand of genetic material made of building blocks called nucleotides. Nucleotides differ only in the type of base they carry, so bases are what determine the genetic message. Enzymes called polymerases catalyze the formation of a new DNA strand from an existing DNA template. The association of the sliding clamps with polymerases significantly increases the efficiency of strand replication, as it prevents polymerases from falling off the DNA and makes sure replication continues uninterrupted. Polymerases iteratively add one of four bases to DNA strands until they have strung together thousands of them.

In DNA repair, the sliding clamp serves as the master coordinator of the cellular response to genetic damage. A number of proteins, such as cell cycle checkpoint inhibitors or DNA repair enzymes, attach themselves to the clamp to perform their functions. In this capacity the role of the clamp is to orchestrate a variety of DNA modification processes by recruiting crucial players to the replication fork, a structure in which double-stranded DNA gives rise to single-stranded prongs that act as templates for making new DNA.

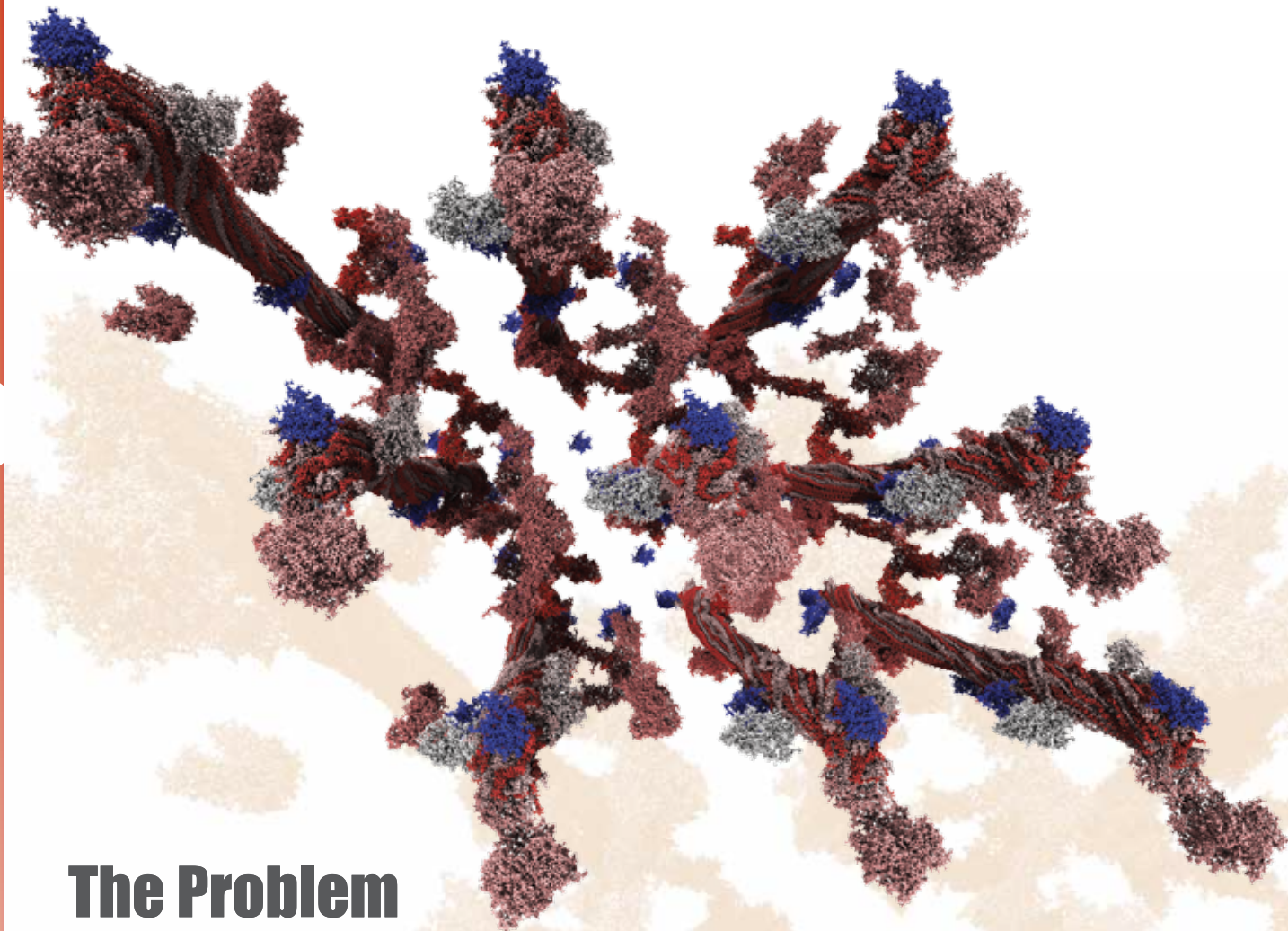
Given the dual function of PCNA in replication and repair, it is not surprising that this clamp has been implicated in diseases accompanied by excessive replication and unchecked cell growth, such as cancer. PCNA modifications are key in determining the fate of the replication

fork and, ultimately, both tumor progression and treatment outcome. Therefore, PCNA has been used as a diagnostic and prognostic tool (biomarker) for cancer.

Most studies of DNA replication have focused on polymerases. Gaining a better understanding of the replisome, however, may shift the spotlight. “Instead of just focusing on polymerase, we can interfere with many different components within this complex machinery,” Ivanov said. “That may allow new drug targets to be developed for hyperproliferative diseases such as cancer.”

Improved understanding of the replisome may make it possible to exploit differences among organisms as diverse as viruses, bacteria, plants, and animals. Although clamp loaders from different kingdoms of life share many architectural features, significant mechanistic differences exist, specifically in the ways ATP is used. Drugs targeted to the clamp loader could selectively inhibit replication of viral DNA in diseases such as chickenpox, herpes, and AIDS without interfering with DNA replication in normal human cells. Similarly, in processes with increased DNA replication, such as cancer, inhibiting clamp loading might produce therapeutic effects without unwanted side effects.

In the future Ivanov and his colleagues will study mechanisms of alternative clamps such as a PCNA-related protein complex that signals the cell to arrest division upon detection of DNA damage. Ultimately, the researchers, fueled by enthusiasm at the therapeutic prospects, want to demystify the entire clamp-loading cycle.—*by Dawn Levy*



The Problem with Cellulosic Ethanol

Simulation provides a close-up look at the molecule that complicates next-generation biofuels

Lignin is very handy in many ways. In your diet it provides much of the fiber that keeps you happy and healthy. In a plant it helps keep the stalk and branches standing and strong. And in the future it may become the carbon fiber that makes cars and trucks lighter and more fuel efficient.

But for those who distill cellulosic ethanol, it's just a bother.

A team led by ORNL's Jeremy Smith has taken a substantial step in the quest for cheaper biofuels by revealing the surface structure of lignin clumps down to 1 angstrom (equal to a 10 billionth of a meter, or smaller than the width of a carbon atom). The team's conclusion, that the surface of these clumps is rough and folded, even magnified to the scale of individual molecules, was published June 15, 2011, in the journal *Physical Review E*.

Smith's team employed two of ORNL's signature strengths—simulation on Jaguar and neutron scattering—to resolve lignin's structure at scales ranging from 1 to 1,000 angstroms. Its results are important because

lignin is a major impediment to the production of cellulosic ethanol, preventing enzymes from breaking down cellulose molecules into the sugars that will eventually be fermented.

Lignin itself is a very large, very complex molecule made up of hydrogen, oxygen, and carbon. In the wild its ability to protect cellulose from attack helps hardy plants such as switchgrass live in a wide range of environments. When these plants are used in biofuels, however, lignin is so effective that even expensive pretreatments fail to neutralize it.

The value of switchgrass

Switchgrass has many virtues as a source of ethanol, the primary renewable substitute for gasoline. It already grows wild throughout the country, it thrives in nearly any soil, and it appears to be happy in regions both wet and dry. Unlike traditional biofuel crops such as corn, switchgrass does not require constant care and attention, and it does not take up land and resources that would otherwise go toward producing food.

Yet the hardiness that allows switchgrass to thrive in inhospitable environments makes it stubbornly resistant to breakdown and fermentation.

“Nature has evolved a very sophisticated mechanism to protect plants against enzymatic attack,” explained team member Loukas Petridis, a computational physicist at ORNL, “so it is not easy to make the fuels. What we’re trying to do is understand the physical basis of biomass recalcitrance—resistance of the plants against enzymatic degradation.”

Switchgrass contains four major components: cellulose, lignin, hemicellulose, and pectin. The most important of these is cellulose, another large molecule, which is made up of hundreds to thousands of glucose sugar molecules strung together. In order for these sugars to be fermented, they must first be broken down in a process known as hydrolysis, in which enzymes move along and snip off the glucose molecules one by one.

Lignin blocks hydrolysis in two ways. First, it gets between the enzymes and the cellulose, forming a physical barrier. Second, it binds to passing enzymes, essentially taking them out of the game. Lignin does this job so well that ground-up switchgrass must be pretreated before it is hydrolyzed. After it is ground into small pieces, the switchgrass is heated above 300 degrees Fahrenheit in a dilute acid to make the cellulose more accessible to the enzymes.

Even then the lignin refuses to cooperate. While hemicellulose and pectin wash away with the pretreatment, the lignin re-forms into aggregates on the cellulose, droplets that can capture up to half the enzymes that are added to the mixture. These aggregates are the focus of Smith’s team’s study. The better that scientists are able to understand the aggregates, the better able they will be to design a more effective pretreatment process and find more successful enzymes.

According to Petridis, the team used neutron scattering with ORNL’s High Flux Isotope Reactor to resolve the lignin structure from 1,000 down to 10 angstroms. A molecular dynamics application called NAMD (for Not just Another Molecular Dynamics program) used Jaguar to resolve the structure from 100 angstroms down to 1. The overlap from 10 to 100 angstroms allowed the team to validate results between methods.

NAMD uses Newton’s law of motion to calculate the motion of a system of atoms—here lignin and water—typically in time steps of a femtosecond, or 1 thousand trillionth of a second. The two methods—neutrons and supercomputing—confirmed that the surface of lignin aggregates is highly folded, with a surface fractal dimension of about 2.6. The surface fractal dimension is a measure of the roughness or irregularity of a surface and ranges from 2 (very smooth) to 3 (very folded). The value of 2.6 is similar to that of broccoli. This roughness gives enzymes far more opportunity to get caught up in the lignin than a smooth surface would. In fact, a lignin droplet has about 3½ times as much surface area as it would if it were smooth.

Smith’s project is the first to apply both molecular dynamics supercomputer simulations and neutron scattering to the structure of biomass. In fact, said Petridis, the two methods reinforce one another very well. On the one hand, neutron scattering could not reveal the

structure at the smallest scales. On the other hand, simulation could not cover the full range of scales even on Jaguar, the United States’ most powerful supercomputer.

“When you look at the combination of neutrons and simulation, first of all it has not been done on lignins before. The combination of techniques gives you a multiscale picture of lignin. Neutron scattering can probe length scales, for example, from 10 angstroms all the way up to 1,000 angstroms.

“On the other hand, molecular dynamics simulations can go to smaller length scales—from 1 angstrom or even subangstrom all the way to 10 or even 100 angstroms. This is why we have been able to study the structure of the lignin droplets over various length scales. Not only was the finding new, but these techniques were used for the first time to study lignocellulose.”

While this research is an important step toward developing efficient, economically viable cellulosic ethanol production, much work remains. For example, this project focused only on lignin and included neither the cellulose nor the enzymes; in other words, it can tell us where the enzymes might fit on the lignin, but it has not yet told us whether the enzymes and lignin are likely to attract each other and attach.

Moving forward, the team is pursuing even larger simulations that include both lignin and cellulose. The latest simulations, on a 3.3 million-atom system, are being done with another molecular dynamics application called GROMACS (for Groningen Machine for Chemical Simulation).

This research and similar projects have the potential to make bioethanol production more efficient and less expensive in a variety of ways, Petridis noted. For example, earlier experiments showed that some enzymes are more likely to bind to lignin than others. The understanding of lignins provided by this latest research opens the door to further investigation into why that’s the case and how these differences can be exploited.

“To understand how this happens, you need an atomic-level or molecular-level description of both the enzymes, which we have already, and the lignin droplets, which we didn’t have until now. One thing we’d like to look at in the future is the interactions between the enzyme and the lignin. Of course, that would be a lot of work and require a lot of computer time.”

The research promises to be very enlightening, Petridis said, especially because it delves into areas that could not be fully explored before.

“Not knowing the structure of the droplets that play such an important role in biomass recalcitrance shows you that the field of biomass research has a lot of interesting questions to answer.” —*by Leo Williams*

Industrial Partnerships *Driving Development*

A 3-mile-per-gallon improvement in fuel efficiency may not sound like a big leap, but applied to large, Class 8 trucks it may lower the country's energy bill by \$5 billion. With this goal in mind, BMI Corporation is working to make shipping more affordable and efficient, and with the help of OLCF computing resources it is able to go from concept to product in half the time of traditional research and development.

And the company is not alone.

In an increasingly competitive international economy that presents increasingly complex problems, high-performance computing (HPC) has become an essential ingredient for industrial success. For the last two years, the OLCF has opened its doors to American companies through ORNL's Industrial High-Performance Computing Partnership Program, giving them the resources to drive innovation at blazing speed.

The program is bringing together some of the brightest researchers in American industry. The partnership helps industry create cutting-edge technologies that may not have been possible otherwise—pushing forward in areas ranging from security to energy efficiency. In addition, collaboration between industry and government works to answer the questions arising from the fast-paced world—continually presenting never-before-seen challenges—that is HPC. Supercomputing has grown exponentially, and the development curve is pointed exponentially upward.

General Motors (GM) is working to boost automobile fuel efficiency by incorporating thermoelectric materials into cars' exhaust systems, allowing them to capture energy in the form of waste heat that would otherwise be lost. The Boeing Company is employing computational fluid dynamics to model the most efficient airplanes possible. General Electric (GE) is promoting renewable energy by working on the next generation of turbines to power machines in both air and water. And Ramgen Power Systems is designing a product to bury carbon dioxide (CO₂) underground, keeping it out of the atmosphere.

With help from the OLCF, these companies are creating a fleet of next-generation American technologies. HPC has been called a game-changing technology, and with the Industrial HPC Partnership Program, more and more companies will be able to change the game in their own fields.

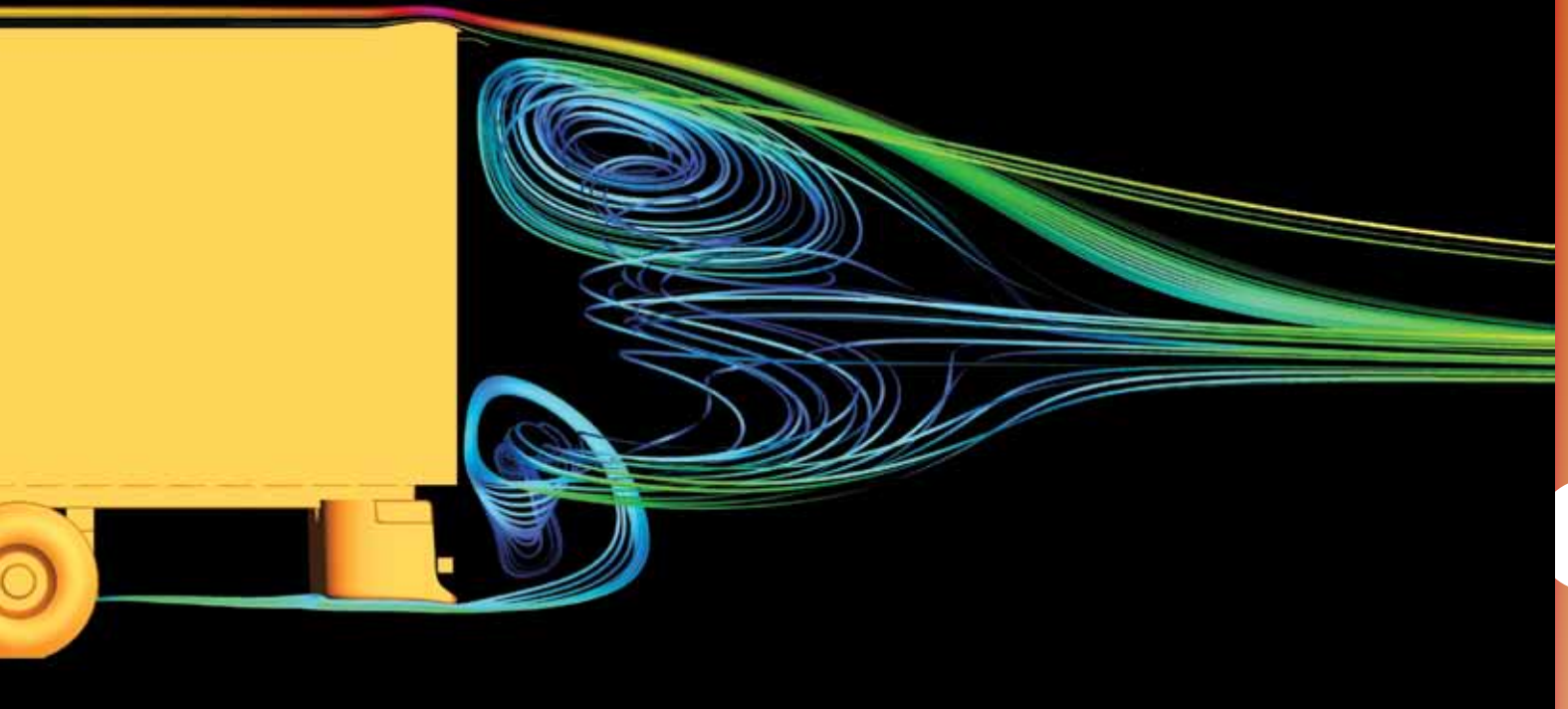
Shaping the shipping industry

The world is realizing the importance of sustainable energy. As limited resources sustain a continually growing population, innovation in many industries is becoming imperative.

Take transportation, for example. Engineering services company BMI Corporation, based in Greenville, South Carolina, collaborated with its sister company SmartTruck and with researchers from ORNL, the National Aeronautics and Space Administration, and the Boeing Company to improve the efficiency of the country's biggest gas guzzlers.



A trailer equipped with BMI Corp. SmartTruck UnderTray components.



BMI's goal in working with the transportation industry has always been to improve aerodynamics and efficiency, be it on the race track, in the air, or on the interstate. The company collaborated with the Aeron Corporation to design the first supersonic business jet, ran simulations to improve the cruising abilities of the MD80 commercial jet liner, worked with NASCAR on the Sprint Series vehicles' aerodynamic profiles, and helped Ford Motor Company improve aerodynamics for its hydrogen concept cars.

For the last two years, though, BMI has focused on America's massive fleet of Class 8 tractor-trailers. These 18-wheel monsters deliver roughly 75 percent of consumer products in the United States every year; some traverse more than 150,000 miles in a year. Unfortunately, they also emit millions of pounds of CO₂ in the process.

"There has not been much investigation into how to make trucks aerodynamic. But we've shown we can make big systems very aerodynamic—just look at planes. You can do the same with trucks if you do it right," said BMI founder and CEO Mike Henderson.

In an effort to reduce tractor-trailer emissions, BMI set out to design a practical add-on to improve efficiency. The company's SmartTruck UnderTray system is the first phase of a project BMI hopes will change freight transport.

The company needed the power of a supercomputer to do the job, as it learned early on when it ran aerodynamic simulations on a computer cluster with 96 processing cores. With that system BMI was unable to simulate the more complex fluid dynamic models being generated. With Jaguar, however, BMI suddenly had access to 224,000 cores, making previously impossible calculations a reality.

The company's R&D efforts were an eclectic affair, incorporating supercomputer simulation on Jaguar, aerodynamics testing in collaboration with Boeing and with NASA's Kennedy Space Center, and closed-track fuel-efficiency runs. The resulting UnderTray system is a collection of polycarbonate forms strategically placed underneath

and on the sides of Class 8 truck trailers. BMI believes it is close to getting trucks over the 9 mile-per-gallon mark—a 33 percent increase in efficiency from today's most advanced trailers.

Considering that Class 8 trucks travel over 130 billion miles per year, UnderTray technology could lead to a reduction of 16.4 million tons of CO₂ in the atmosphere (about half of China's total emissions in 2007). It could also cut annual fuel costs by about \$13,500 per truck by reducing each truck's yearly fuel intake by 4,500 gallons.

BMI used the FUN3D fluid dynamics code developed by NASA to simulate wind resistance on trucks, modeling half the truck and trailer using over 100 million grid points. The research team looked for realistic add-ons that could be installed by purchasers on site, giving the more than 1.3 million Class 8 trucks roving from coast to coast technology they could implement in a reasonable time and at a reasonable cost.

"Our first goal was to design add-on parts for existing trucks and trailers to make them more aerodynamic," Henderson said. "By reducing drag we boost fuel efficiency and cut the amount of carbon that's being dumped into the environment."

Researchers had anticipated it would take 3 ½ years of rigorous testing and verification before a product was ready for manufacture. With the help of Jaguar, however, they were able to put the first SmartTruck UnderTray systems on the production lines in 18 months.

Heavy Duty Trucking magazine cited the UnderTray system as one of 2010's top 20 new products, and BMI has already begun outfitting trucks for PepsiCo, Frito-Lay, Con-way, and Swift Transportation.

Henderson hopes this is only the beginning and SmartTruck can look to new vehicles designed for improved efficiency and performance. "We hope to soon turn our attention to creating a brand-new, highly aerodynamic vehicle with optimum fuel efficiency," he said. The eventual goal of the project would be to make trailer trucks more aerodynamic than a car.

In 2009, the California Air Resources Board began requiring all Class 8 vehicles to add aerodynamic elements to improve their fuel efficiency by 5 percent. Tests of the current UnderTray system have already shown increases of 7 to 12 percent, easily meeting the state's requirements for freight vehicles. In addition, the EPA partnered with the freight industry and recently began the SmartWay program, an effort to reduce greenhouse gas emissions by certifying and recognizing companies that are taking steps to decrease their carbon footprint.

Partnerships for progress

HPC's ability to produce results quickly has piqued the interest of many businesses. Some have achieved groundbreaking results on Jaguar.

Such is the case with Ramgen Power Systems, a Seattle-based company focusing on shockwave compression, technology that may one day capture and bury CO₂ to help in the fight against global warming. The company's supersonic shock compression technology would not only spare the atmosphere millions of pounds of CO₂ over time but also make carbon compression affordable. Shawn Lawlor, Ramgen's founder and chief technology officer, said that the design of its rotor-disk compressor could also be applied in flight propulsion and gas turbine design.

Like BMI, GM aims to improve the efficiency of transportation through research, but on a smaller scale.

A typical car loses 60 percent of the energy generated by its engine to waste heat, but a team led by GM researcher Jihui Yang is using Jaguar to perform nanoscale simulations of materials that may convert some of that heat energy directly into electricity. The electricity, in turn, can power systems such as the electric water pump, lights, radio, and global positioning system, functions that would no longer drain the vehicle's primary power source. Yang's group is focusing on LAST, a thermoelectric material containing lead, antimony, silver, and tellurium. Ultimately, it hopes further research will allow it to design thermoelectric materials via simulation, so only the most promising materials are manufactured for actual testing.

Improved flight efficiency in the commercial aviation industry could also translate into gigantic savings, and the Boeing Company is using Jaguar to help find where those improvements may be.

As Boeing researchers simulate thrust reversers—which slow down airplanes—and try to predict where, when, and to what degree drag affects flight, they are also improving computational fluid dynamics codes, supporting advancement in the greater HPC community as well as in Boeing's next-generation aircraft. The team is working to scale up these codes to achieve faster, more detailed, more physically accurate results, ultimately giving the scientific community more simulations with more information from which to learn.

Work on fluid dynamics helps propeller blades and wings become more efficient for planes in the air, and the same principle can be applied to wind turbines on the ground.

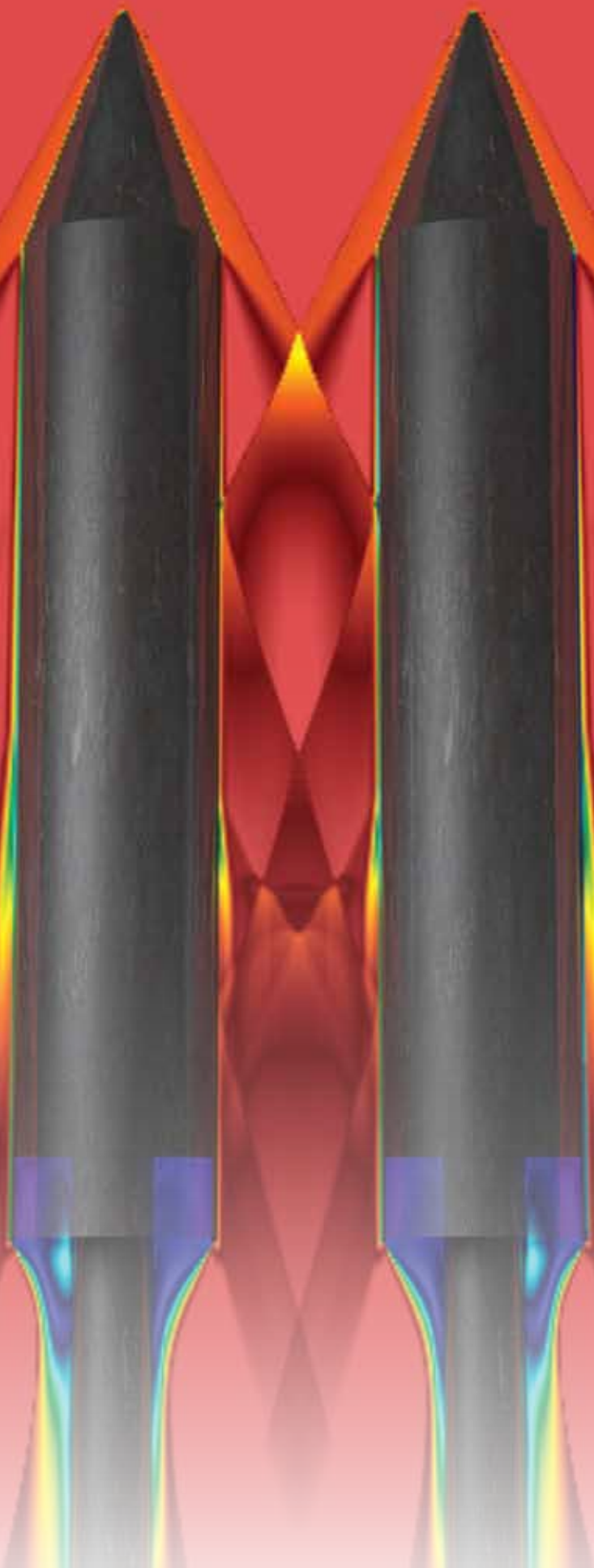
GE, one of the largest multinational corporations in the world, is using its Global Research arm to turn conceptual energy sources into realities, create new technologies, and improve upon traditional ways to generate power. Via Jaguar, GE has been able to take turbine simulations from looking at portions of a turbine at a time to full system-level simulations, allowing researchers to make design decisions that would have been pure guesswork without computation. Simulations for next-generation wind turbines are capable of giving researchers data on not only the aerodynamic efficiency of turbine blades, but also the associated noise stemming from wind turbines.

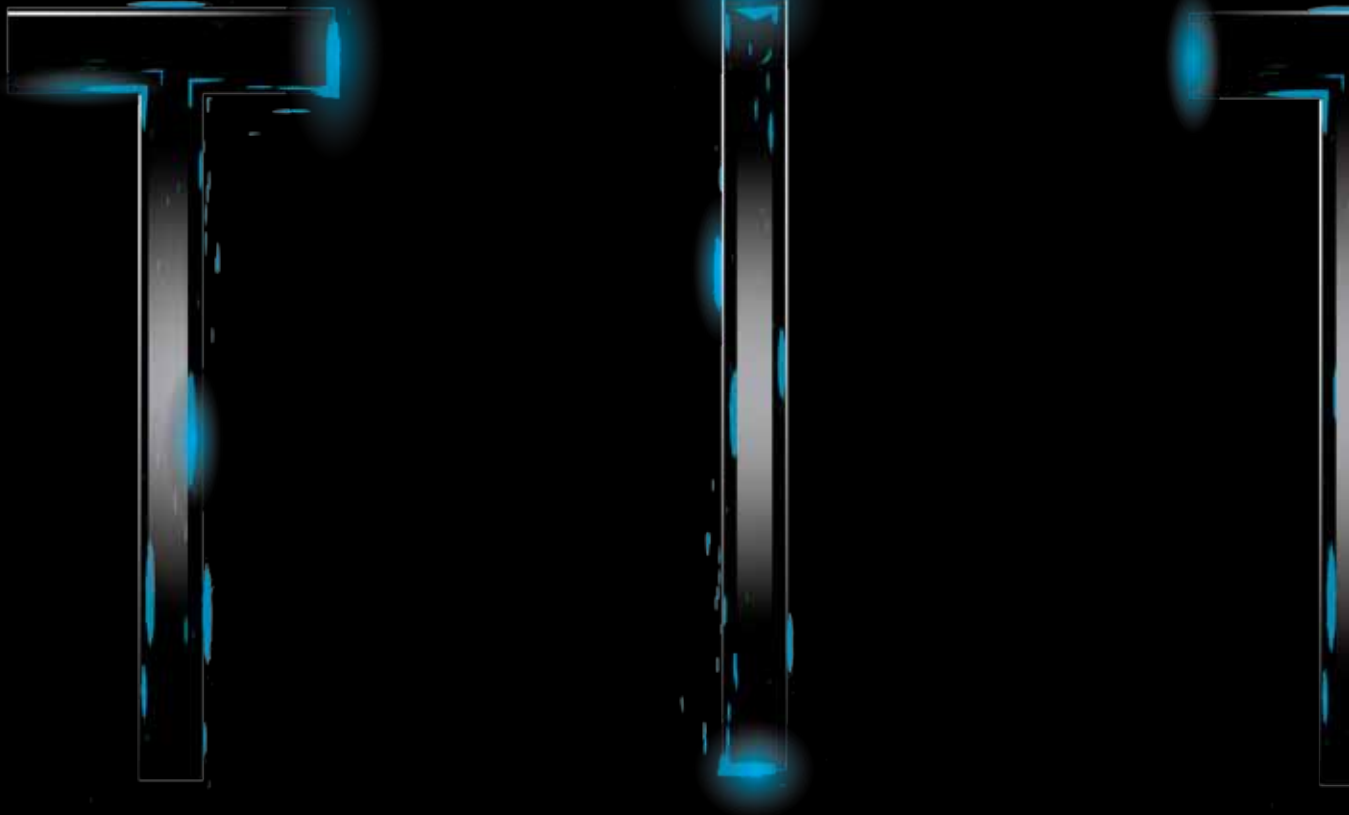
“We are able to optimize an entire turbine from nozzle to exhaust dock,” said Mike Idelchik, vice-president of GE Global Research's Advanced Technologies. This allows researchers to see their design as a big picture and refine aspects before producing prototypes and running experiments. Their current work focuses on accurately simulating improved-efficiency, low-pressure turbines.

These projects all share the goal of improving American energy security. By slowing down our consumption of fossil fuels and working toward alternative means of powering our lives, they make everything from daily commutes to turning on the television less reliant upon imported fossil fuels. Many of these research projects are just scratching the surface and include plans for fine-tuning their products or developing new ones.

These companies were the first generation of industrial partners collaborating with the OLCF to advance their fields and improve energy consumption and efficiency. The OLCF is poised to partner with any company working to aid the country's energy mission and advance the field of computation in the process.—*by Eric Gedenk*

Ramgen Power Systems is using Jaguar to simulate equipment that will achieve carbon sequestration at a significantly lower cost than that offered by conventional equipment. This image is the high-resolution result of a billion-cell two-body simulation showing the complex reflected structures colored by mach number. Visualization by Mike Matheson, ORNL.





OLCF's next-generation system to light the way to exascale

On the road to exascale systems (i.e., systems able to reach 1,000 petaflops), the OLCF will be walking in uncharted territory. As on any great journey, the familiar will have to be left behind.

For more than 50 years computers have roughly doubled in speed every 2 to 2½ years, regularly increasing the performance of electronic devices and giving hardware and software designers a comfortable knowledge of what's ahead and how best to prepare for it.

Well, those days are over. Conventional processing architectures are quickly reaching their maximum potential, and if computers are to continue to increase in power and speed, a revolutionary change in strategy is necessary. Introducing Titan.

It's recently become clear that America's best chance of achieving exascale computing power rests with an architecture that utilizes more powerful nodes than today's systems. This will be achieved via a marked increase in the number and, likely, the types of processing cores.

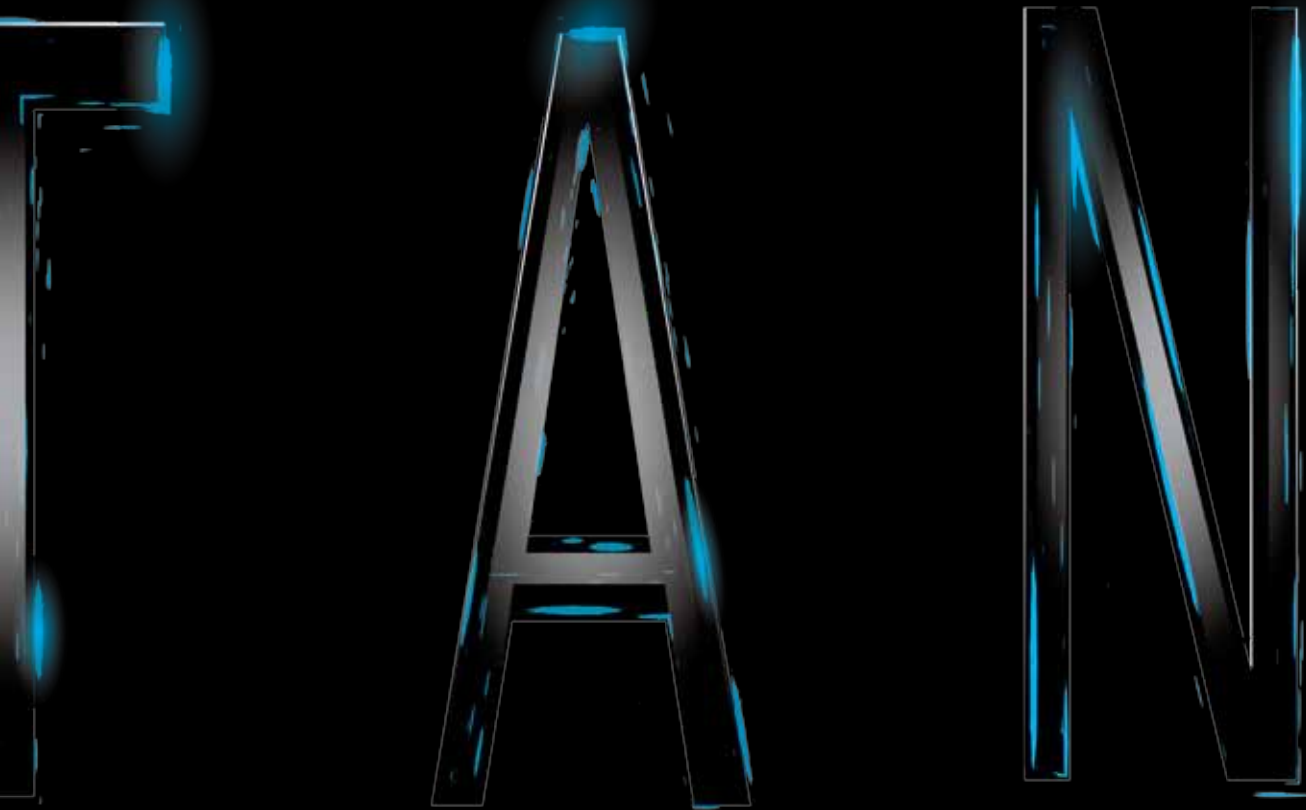
Whereas recent gains have been achieved by adding more homogenous cores, essentially just ramping up the number of CPUs, Titan's heterogeneous architecture will couple different types of processors, allowing each to do what it does best, thus increasing the power and efficiency of the overall machine. Specifically, Titan will feature the familiar AMD Opteron CPUs alongside general-purpose GPUs, a more energy-efficient technology for crunching numbers.

The arguments for Titan's heterogeneous, multi-core architecture are twofold: (1) it seems to be the most straightforward way of increasing computational power, and (2) it accomplishes an exponential increase in computing power with only a slight increase in power consumption, a major expense when you're dealing with the most powerful machines in the world.

The ultimate goal of exascale computing is to achieve a thousandfold increase in delivered performance but within a power envelope that's roughly twice what Jaguar uses now, a 500-fold increase in power efficiency. Titan is the first step toward achieving this landmark metric.

But it's not all about the hardware. To achieve the required power savings, software designers and computational scientists are going to have to change the way they program. Specifically, the applications of the future need to minimize communication between processors, the most computationally expensive aspect of large-scale computational science. The codes that best take advantage of Titan's enormous computing power will be those that maximize data locality.

Nothing about Titan will be easy, but the effort will be necessary if America is to continue to lead the way in HPC, increasingly recognized as a vital part of a successful, competitive technological future. "We believe that we are taking the concrete first step towards a viable exascale architecture," said the OLCF's acting director of science, Bronson Messer.



The aim of Titan is to achieve 20 petaflops, or a peak speed just under 10 times faster than Jaguar, while performing groundbreaking science. That will most likely make Titan the fastest machine in the world. While Titan will retain the same overall cooling and power infrastructure, just about everything else will have to change. It starts with the hardware.

Hardware

Despite its revolutionary promise, Titan is in many ways evolved from Jaguar's existing XT architecture. This heritage is a great advantage for a system that must be rapidly and efficiently deployed. "The cabinets will look the same, but the guts will be somewhat different," said Messer.

The main game changer is the introduction of the GPUs. These application accelerators, spawned from the video game industry, will afford an enormous increase in floating-point performance, which means simulations that would take weeks or months on Jaguar might run in days on Titan. When it comes to productive computational science, time is vital, and the introduction of Titan's GPUs will allow researchers to achieve faster breakthroughs via more simulations over time.

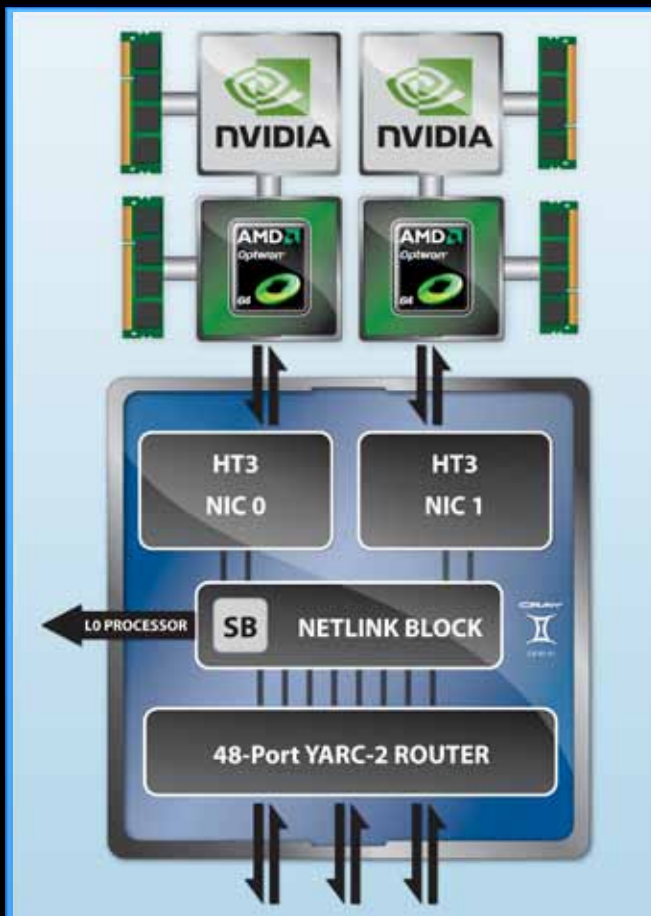
The beauty of GPUs lies in their massively parallel nature. Unlike conventional CPUs, which perform operations serially, or one-by-one, GPUs are capable of performing many different operations at once. In Titan, they will be soldiers, and the CPUs the generals. In other words, the GPUs will be marshaled to perform the most intensive

calculations because of their ability to rapidly crunch numbers, while the AMD Opterons will be responsible for "command and control" in various scientific applications.

Specifically, Titan and Jaguar will differ as follows: Each compute node on the current Jaguar XT architecture has two Opteron CPUs, and every node is connected via Cray's Seastar custom router chips. Titan will remove one Opteron from each node and replace it with a GPU, and the Seastar chips will be replaced by a new interconnect chip dubbed Gemini.

Gemini is Titan's second major breakthrough. Essentially, Gemini increases the computer's ability to do one-sided communication, allowing one processor to share data with another processor without the need for time-consuming "handshaking." This improvement is key, as communication between nodes is one of the most expensive elements of HPC.

As Titan is deployed, there will also be some changes in the computational ecosystem, or the attendant hardware and software surrounding the machine. Perhaps first and foremost among these is the Spider file system. In order to play ball with Titan, the OLCF will add hundreds of gigabytes per second of bandwidth and tens of petabytes of storage to Spider. Because Titan will be capable of producing more data at any given moment than Jaguar, the new system will have to keep up in terms of storage and file input/output.



Titan's architecture represents the latest in adaptive hybrid computing. The node above combines AMD's 16-core Opteron™ 6200 Series processor and NVIDIA's Tesla X2090 many-core accelerator. The result is a hybrid unit with the intranode scalability, power-efficiency of acceleration, and flexibility to run applications with either scalar or accelerator components. This compute unit, combined with the Gemini interconnect's excellent internode scalability, will enable Titan's users to answer next-generation computing challenges.

These changes, though incremental, represent an enormous leap when taken together. As Titan is deployed there will no doubt be trials and tribulations, but in the end the machine will most likely represent the future of, and will once again place the nation as the leader in, HPC.

But the hardware is just one dimension of the challenge to come. No matter how powerful Titan becomes, it's only as good as the programs it runs.

Software

The primary software challenge on Titan is to uncover and exploit three levels of parallelism: distributed, in which a task or physical domain is divided among a number of nodes; thread level, in which each task from the distributed workload is divided into discrete threads of execution on local processors; and vector level, in which the threads are further divided and sent to the GPUs for increased performance.

Currently, the software on Jaguar does a great job of distributed parallelism. Tools like the Message Passing Interface (MPI) and Global Arrays allow various applications to communicate between processors efficiently. These same tools also allow application writers to distribute work over lots of processors, one of Jaguar's best assets.

Further, Jaguar allows ways to expose the thread level of parallelism via shared memory processing in the form of methods like OpenMP and Pthreads, standards for creating parallel threads in a shared memory environment.

The most immediate software challenges reside in the third layer of parallelism, i.e., the vector. Ultimately, Titan's potential lies in optimizing the use of the GPUs through effective vector-level programming, where the real power and speed of the GPUs is found.

Take climate simulation, for instance. These complex exercises rely heavily on distributed parallelism, essentially dividing the surface of the Earth into grid cells, with each living cell on an individual processor. At each of these grid points, however, there is a lot going on; for instance, each contains numerous variables to describe various components of the Earth system, e.g., the atmosphere, the ocean, and the Sun's radiation, adding up to plenty of physics at individual grid points. On current systems these calculations are usually done serially, one-by-one, at each grid point.

However, they can also be tackled at the thread level by exploiting the fact that at each grid point you have multiple layers of parallelism for each calculation. Tapping this unrealized parallelism can increase the fidelity of the simulations, speeding them up and allowing the use of more sophisticated approximations, resulting in greater overall accuracy.

On Titan, the additional availability of vector-like parallelism via the GPUs means even more optimized simulations. For example, a researcher might use an atmospheric chemistry package on Jaguar that had previously been out of reach because it took months to run, said Messer, adding that researchers at ORNL are already reducing months-long wallclock times on Jaguar to a handful of days with GPUs.

"Ultimately we hope the applications on Titan will be full-scale simulations where every layer of parallelism available is exploited," he said.

After much trial and error, the supercomputing community is now discovering ways to do just that. The current champ is CUDA, a language extension from GPU-maker NVIDIA. The fact that it's simply a language extension, and not a new language, is a very good thing for programmers and scientists alike.

That they don't have to learn an entirely new language and can simply plug CUDA into their existing codes is an enormous convenience, particularly with codes that have evolved over years. Unfortunately, effective use of CUDA requires an in-depth knowledge of the physical structure of the GPUs and the surrounding hardware. Few programmers possess this kind of knowledge, and because GPUs are relatively new it could be a while before the community absorbs a sound understanding of their architecture. Programming that demands hardware knowledge is known as low-level programming, and the OLCF is doing its best to avoid this model. CUDA is almost there, said Messer, hovering between

high-level, in which less knowledge of a machine's hardware is required, and low-level.

“We need a higher-level description of doing this,” said Messer, adding that several of the OLCF's partners, including Cray, The Portland Group (PGI), and CAPS, a leading provider of multi-core software tools, are looking at a compiler-based approach to this kind of software. The joint product will in all likelihood be another language extension but one that operates at a higher level, i.e., one that doesn't require as much hardware knowledge. In essence, this new extension will tell the computer what the user wants to happen and the computer will decide how best to accomplish the task during runtime.

The great benefit of a higher-level extension, besides not requiring as much low-level programming, is that the code will work on any platform if the directives, or instructions in the compiler (a computer program that transforms a programming language such as Fortran into another computer language such as binary), are done right. In other words, the GPUs will be ignored on a machine without them, thus allowing users to run their codes on a variety of platforms and in the long run benefitting HPC across the field.

Of course, directives present challenges as well, said Messer. Because the compiler is making the decisions, the user isn't necessarily guaranteed the highest performance from an application. Compilers, it turns out, are not optimal decision makers. The brunt of the work on the new partnership language extension involves making this penalty as small as possible. Currently, Cray, PGI, and CAPS are working on new compiler technologies that will allow the compiler to make better decisions and help researchers get the most from their codes and their time on Titan.

As a testament to this work, Cray's compiler on S3D, a combustion code developed at Sandia National Laboratories (SNL) that is improving the efficiency of internal combustion engines and boilers, has gotten performance numbers that are equivalent to hand-coded CUDA. This is an enormous breakthrough for one simple reason: Programmers may no longer need to learn the minutiae of GPU architecture to reach their maximum potential on Titan.

A hallmark of scientific software is that it is constantly under development, said Messer. The cutting-edge applications running on leadership-class platforms like Jaguar are necessarily always changing, becoming more efficient and realistic. This constant development leads to a consistent barrage of problems and bugs that must be solved before the software can be used to perform numerical experiments. Because Titan will be a new platform with complex hardware, it will be difficult to know what broke and exactly where it broke.

That's where the next challenge lies: tools.

Tools

When it comes to Titan, two types of tools will be critical for success: debuggers and performance analysis tools.

Software is never simple, and when it comes to world-class supercomputers with mission-critical programs, it's at its most complex. Finding errors is essential to ensuring that simulation results are as accurate as possible.

The OLCF is working closely with Allinea to extend its DDT debugging product, a leading tool for debugging parallel MPI and Open MP programs, to include GPU debugging. Because GPUs are so new, figuring out how to program a debugger to accommodate their presence is a monumental task, and one that is being met head-on by the OLCF/Allinea partnership.

On the performance analysis front, the OLCF is also working with Technical University Dresden on its Vampir package, a modeling tool used to measure performance and discover bottlenecks. By helping to identify inefficient sections of code and allowing researchers to view the applications in progress, Vampir lets programmers and researchers optimize their applications and get the most performance from Titan's heterogeneous architecture.

If Titan is to be the monster machine envisioned, debugging and performance analysis will be absolutely crucial to realizing its potential and implementing the OLCF's future program plan and philosophy.

“Titan is the first step towards ensuring America's exascale future. With Titan, the OLCF will embark on a new era in simulation, one sure to contribute immensely to science and America's competitive technological future,” said OLCF Director Buddy Bland.

Application Readiness

The first thousand nodes of Titan are scheduled for installation in late 2011, but the OLCF began preparing for the arrival of its next leadership resource long before the hardware was purchased. Titan's novel architecture alone is no HPC game-changer without applications capable of utilizing its innovative computing environment.

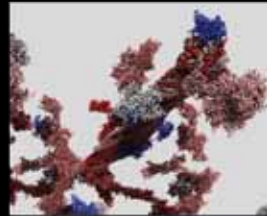
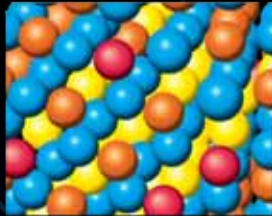
In 2009 the OLCF began compiling a list of candidate applications that were to be the vanguards of Titan—the first codes that would be adapted to take full advantage of its mixed architecture. This list was gleaned from research done for the 2009 OLCF report *Preparing for Exascale: OLCF Application Requirements and Strategy* as well as from responses from current and former INCITE awardees. Initially 50 applications were considered, but this list was eventually pared down to a set of six critical codes from various domain sciences:

- S3D, developed by Jacqueline Chen of SNL, is a direct numerical simulation code that models combustion. In 2009, a team led by Chen used Jaguar to create the world's first fully resolved simulation of small lifted autoigniting hydrocarbon jet flames, allowing for representation of some of the fine-grained physics relevant to stabilization in a direct-injection diesel engine.
- WL-LSMS calculates the interactions between electrons and atoms in magnetic materials—such as those found in computer hard disks and the permanent magnets found in electric motors. It uses two methods. The first is locally self-consistent multiple scattering, which describes the journeys of scattered electrons at the lowest possible temperature by applying density functional theory to solve the Dirac equation, a relativistic wave equation for electron behavior. The second is the Monte Carlo Wang-Landau method, which guides calculations to explore system behavior at all temperatures, not just absolute zero. The two methods were combined in 2008 by Markus Eisenbach of ORNL to calculate

Preparing for Exascale: Six Critical Codes

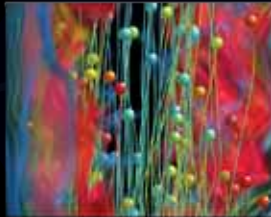
WL-LSMS

Role of material disorder, statistics, and fluctuations in nanoscale materials and systems.



LAMMPS

Simulated time evolution of the atmospheric CO₂ concentration originating from the land's surface.

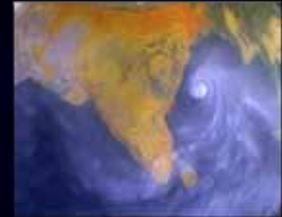


S3D

How will the next generation of diesel/bio fuels burn more efficiently?

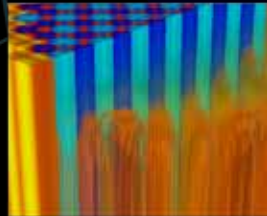
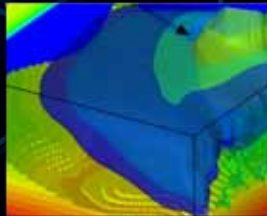
CAM-SE

Answers questions about specific climate-change-adaptation and -mitigation scenarios.



PFLOTRAN

Stability and viability of large-scale CO₂ sequestration; predictive containment groundwater transport.



Denovo

High-fidelity radiation transport calculations that can be used in a variety of nuclear energy and technology applications.

magnetic materials at a finite temperature without adjustable parameters. The combined code was one of the first codes to break the petascale barrier on Jaguar.

- PFLOTRAN, developed by Peter C. Lichtner of Los Alamos National Laboratory, simulates groundwater contamination flows.
- Developed by ORNL's Tom Evans, Denovo allows fully consistent multi-step approaches to high-fidelity nuclear reactor simulations.
- Cam-SE represents two models that work in conjunction to simulate global atmospheric conditions. CAM (Community Atmosphere Model) is a global atmosphere model for weather and climate research. HOMME, the High Order Method Modeling Environment, is an atmospheric dynamical core, which solves fluid and thermodynamic equations on resolved scales. In order for HOMME to be a useful tool for atmospheric scientists, it is necessary to couple this core to physics packages—such as CAM—regularly employed by the climate modeling community.
- LAMMPS, the Large-scale Atomic/Molecular Massively Parallel Simulator, was developed by a group of researchers at SNL. It is a classical molecular dynamics code that can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scales.

Once the applications were chosen, teams of experts were assembled to work on each. These teams included one liaison from the OLCF's Scientific Computing Group who is familiar with the code; a number of people from the applications' development teams; one or more representatives from hardware developer Cray; and one or more individuals from NVIDIA, which will be supplying the GPUs to be used in Titan.

“The main goal is to get these six codes ready so that when Titan hits the floor, researchers can start doing real science,” said Messer. Using a single problem from varying domains, the teams have worked to identify parts of each code that are capable of being accelerated via GPUs.

Guiding principles

Before work began on these six codes, the development teams acknowledged some fundamental principles intended to optimize their adaptations. First, because these applications are current INCITE codes, they are under constant development and will continue to be after Titan is in production—any changes made must be flexible. Second, and perhaps most important, these applications are used by research teams the world over on various platforms.

“We had to make sure we made changes to the codes that won't just die on the vine,” said Messer, adding, “we had to ensure that our changes

at the very least do no harm while they are running on other, non-GPU platforms.” The teams discovered that some of their modifications not only made the codes functional on hybrid systems, but actually helped performance on non-GPU architectures. A prime example is Denovo, which has experienced a twofold increase in performance speed on traditional CPU-structured systems since being adapted.

“We’ve made changes that we’re sure are going to remain within the ‘production trunk’ of all these codes—there won’t be one version that runs on Titan and another version for traditional architectures,” said Messer. It’s essential for developers to be able to check a code out of a repository that can be compiled on any architecture; otherwise, the work done by these teams won’t survive time.

The development teams have learned plenty from their work thus far. First, application adaptation for GPU architectures changes data structures (the way information is stored and organized in a computer so that it can be used efficiently), a fact that is creating the most difficult work for the teams. GPUs have to be fed information correctly, like voracious animals—they can’t be sated with little “bites” of information, but require huge amounts of data at once. Developers have carefully examined the codes line by line to identify large chunks of data that can be “fed” to these ravenous GPUs.

“Titan is the first step towards ensuring America’s exascale future. With Titan, the OLCF will embark on a new era in simulation, one sure to contribute immensely to science and America’s competitive technological future,”
—OLCF Director Buddy Bland.

Second, the teams have learned how to marshal data for the GPUs. This requires the developers to know a lot about the hardware of the GPU to effectively code with CUDA, which works with a variety of programming languages such as C, C++, and Fortran.

These two discoveries are the key to enabling strong scaling of applications at the exascale. “What we’ve discovered at the petascale is that research teams have run out of weak scaling,” said Messer, referring to the label associated with increasing the size of the problem to be solved. Users have reached the point where they can make quantitative predictions with their codes and don’t have to increase the problem size, or they’ve simply reached the limit of where the code base can take them.

“It’s now become a question of strong scaling—producing a greater number of sophisticated simulations in a shorter amount of time,” Messer explained. “We expect this at the exascale.”

As HPC adopts hybrid architectures and moves closer to the exascale, code development teams will work toward a directives-based approach for code adaptation. Commands will be placed in applications that order the compiler to figure out how to execute complex portions of the code via GPUs. If a code with directives runs on a machine without GPUs, the code will have commands that tell the machine to simply skip the directives. OLCF code development teams are working with the OLCF’s Application Performance Tools Group on tools and compilers and also with Cray directly to adapt Cray, PGI, and CAPS compilers for use with directives-based codes.

Ultimately, said Messer, all of the applications running on Titan will be able to exploit the GPUs to achieve a level of simulation virtually unthinkable just a few years ago. Simply put, standing up and operating Titan will be America’s first step toward the exascale and will cement its reputation as the world leader in supercomputing. With Titan, America can continue to solve the world’s greatest scientific challenges one simulation at a time.—*by Gregory Scott Jones and Caitlin Rockett*

OLCF

RESOURCES

PAVE THE WAY



In 2008, the OLCF started building the world's most powerful computer for science. The machine, dubbed Jaguar, sprang up and quickly became one of the most powerful supercomputers in the world.

Today, as the OLCF looks to new horizons in the world of supercomputing, Jaguar remains the most productive scientific computing machine in the world, tackling previously impossible problems, from the smallest building blocks of matter to the vast expanses of space.

Jaguar revs up

Jaguar has grown from an initial peak speed of 119 teraflops to its current incarnation, capable of 2.33 petaflops.

The Jaguar XT5 spreads out over 5,000 square feet, with 200 cabinets housing 18,688 compute nodes. Each node has 16 gigabytes of memory, giving the entire system 300 terabytes of memory. Information can travel in and out of Jaguar at 240 gigabytes per second, with data being directed by 256 service and input/output (I/O) nodes.

Each node runs Cray's version of the SuSE Linux operating system. The modified Linux platform removes unnecessary processes from

each node and minimizes interruptions. This Linux environment connects Jaguar's system services, networking software, communications, I/O, mathematical libraries, compilers, debuggers, and other performance tools.

All of these processes give Jaguar a peak power density of 1,750 watts per square foot, necessitating a liquid cooling system to dissipate heat. Cray designed the ECOphlex cooling technology. Using R-134a, a high-temperature refrigerant used in automobile air conditioners, ECOphlex conditions air as it is drawn into the machine while removing heat as the air enters and exits. This efficient cooling system saves 2.5 million kilowatt hours annually.

And not only is Jaguar efficient, it is also reliable. In fact, the expected scheduled availability of Jaguar was exceeded by 10 percent in 2010. This additional availability meant that users had more time to compute, analyze, and manage their projects.



Cray Jaguar XT5 supercomputer

2010 OLCF User Survey Highlights

- Overall ratings for the OLCF were positive, as 90% reported being “satisfied” or “very satisfied” with the OLCF overall. On the scale of 1 = Very Dissatisfied to 5 = Very Satisfied, the mean rating was 4.31, a slight increase from 4.28 in 2009.
- Overall satisfaction with the OLCF has seen a year-to-year increase in the mean of the responses on a scale of 1 = Very Dissatisfied to 5 = Very Satisfied. The results were 3.7 in 2006, 4.1 in 2007, 4.2 in 2008, 4.28 in 2009, and 4.31 in 2010.
- User feedback:

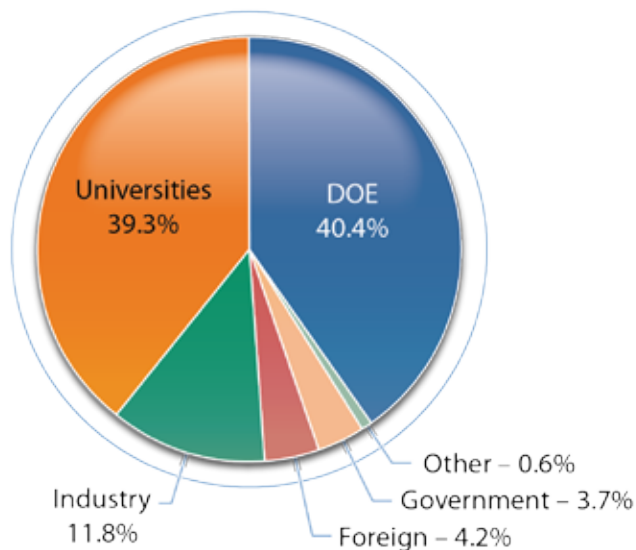
“The help services provided by the OLCF are the best I have ever experienced in over a decade of interaction with multiple supercomputer centers.”

“Project staff experiences when contacting OLCF support have been very positive. Support staff seems to be very customer oriented and works hard to maximize the customer experience. I appreciate the comments provided by subject matter experts and the proactive approach of reaching out to users via telephone conference calls and on-site meetings.”

“At the human (support) and technical (software, admin) level, OLCF is a first-rate institution.”

User queries were answered in less than three days 87 percent of the time, with an average response time of 31 minutes. In the OLCF annual user survey conducted to gauge users’ experiences, the OLCF averaged a grade of 4.3 out of 5, with no one ranking the facility below 3.5.

2010 OLCF User Community by Sponsor

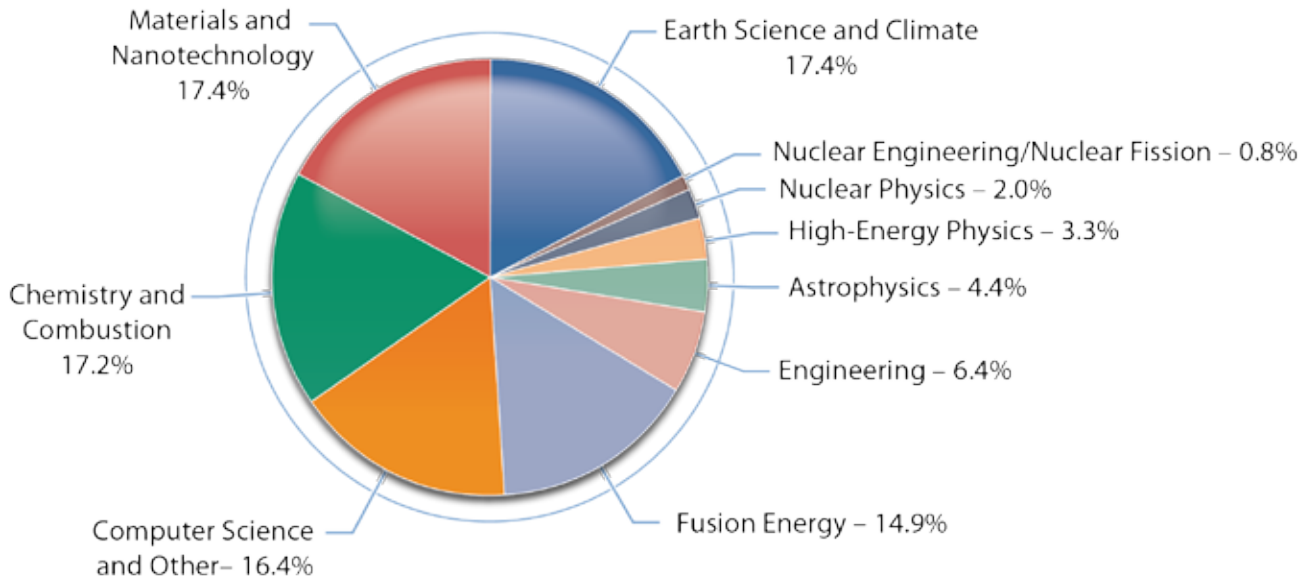


The OLCF user community

Over 1,000 users from 58 countries currently use Jaguar. The OLCF provides this diverse set of users not only with world-class computational resources, but also with a network of skilled professionals who help research teams glean the most from their simulations. The OLCF comprises five groups that provide high-performance computer users with specialized help throughout their allocation—from code optimization before simulation runs to data visualization and analysis once runs have been completed.

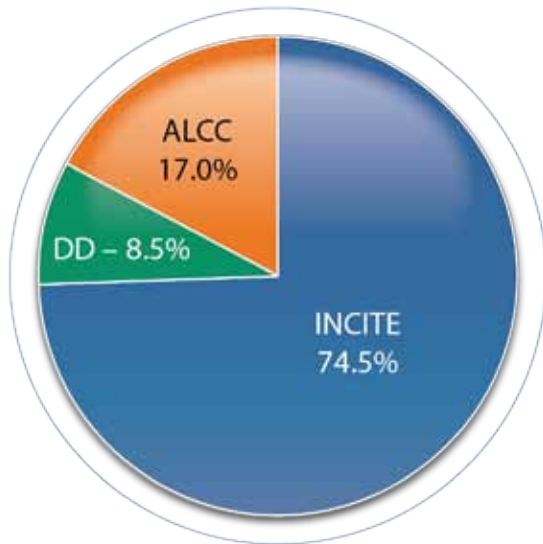
Each research team with substantial time on Jaguar is assigned a liaison from the Scientific Computing Group who is familiar with the field of research. Liaisons help their assigned groups design and optimize code and workflow, as well as address any computational issues that arise. The User Assistance and Outreach Group represents the front line of support for OLCF users, creating accounts for new users, providing technical support to research teams, and generating documentation on OLCF systems access, policies, and procedures. The Technology Integration Group ensures that users have up-to-date networks, file systems, and archival storage infrastructure. The High Performance Computing Operations Group monitors the high-performance systems 24 hours a day, 7 days a week, providing administration, configuration, and cybersecurity. Finally, the Application Performance Tools Group provides users with new modeling tools, languages, middleware, and performance-characterization tools that help research teams access and improve the performance of their applications on current and emerging OLCF computing systems.

2010 INCITE Allocation Hours on Jaguar XT5 by Discipline



Access to Jaguar is available through three programs: INCITE, the DOE Office of Advanced Scientific Computing Research Leadership Computing Challenge (ALCC), and Director's Discretionary.

2010 Allocation Hours on Jaguar XT5

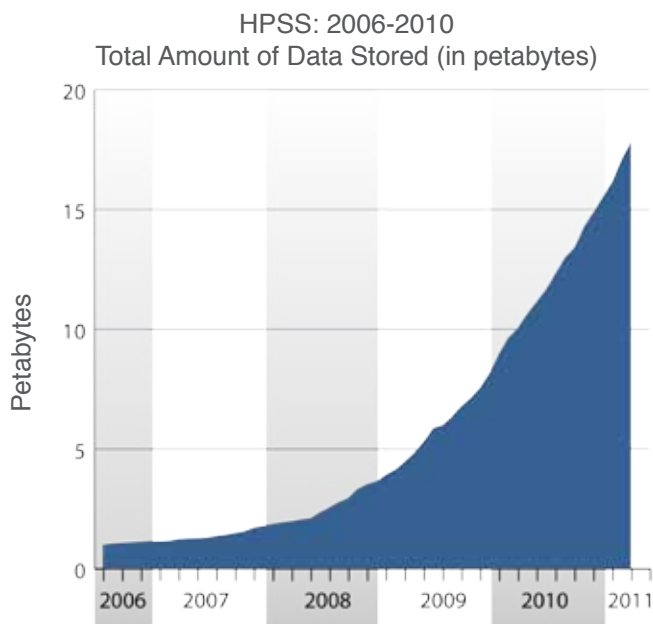


Most projects receive time on Jaguar through INCITE, which distributes approximately 60 percent of the available time. The program facilitates high-impact, grand-challenge research that would otherwise be impossible without leadership-class systems. To secure an INCITE allocation, a project must demonstrate effective use of a leadership-class machine for production simulations, typically using at least 20 percent (approximately 45,000 cores on Jaguar) of the resource for single

production runs. INCITE issues annual calls for proposals and examines projects for both the team's computational readiness and the research's potential for impact. The potential for impact is the predominant factor in award decisions, so it is essential for researchers to express how the proposed work may enable scientific discovery or facilitate technological breakthroughs. Awards vary from project to project, but an average project receives more than 20 million processor hours. Allocations in 2011, which average 27 million processor hours per project and include one allocation topping 110 million processor hours, are the largest awards ever made under the INCITE program.

The ALCC, managed by DOE, allocates up to 30 percent of the available time on Jaguar. ALCC seeks projects of special interest to DOE, with particular emphasis on high-risk, high-payoff simulations in fields directly related to the department's energy mission in areas such as clean energy alternatives or climate simulation. ALCC allocations are also awarded to projects that extend the community of possible leadership-machine users. The ALCC program awarded over 368 million processor hours on Jaguar in 2011.

The final 10 percent of time available on the leadership-class machines is allocated through the Director's Discretionary program. This program provides a way for teams to request access to leadership systems in order to get started with leadership computing and other development work, typically in preparation for a future INCITE submittal. Researchers can also request time to carry out benchmarking, since INCITE proposals must include data from benchmarking carried out on one of the leadership machines or a system of similar architecture. Director's Discretionary awards are typically on the order of 1 million processor hours. As with the INCITE and ALCC programs, researchers from around the world are eligible to apply for Director's Discretionary time.



Data management

OLCF users require high-speed storage and retrieval for the large collections of data generated during research. To help users keep track of their data securely, the OLCF maintains one of the largest archival storage systems in the world. After the High Performance Storage System (HPSS) writes data onto disks by high-speed data movers, the data is gradually transferred to tapes. The OLCF has changed the HPSS server and switched the platform to Linux, improving performance and redundancy. Staff members are constantly adding more disk and tape resources to handle the ever-growing mountain of data produced on the center's resources—HPSS grew from 1,000 terabytes in 2006 to nearly 18,000 terabytes in 2010.

In 2007 the OLCF adopted InfiniBand fabric center-wide. InfiniBand is a switched-fabric, high-performance communication system in which individual nodes are connected to multiple network switches. The system is the industry standard for high-performance networking and enables users to move large amounts of data throughout the center's many platforms, including the visualization cluster for analysis, the Lustre file system, and storage. The OLCF was the first institution to incorporate InfiniBand networking on a Cray XT system. This upgrade was essential to achieving petaflop computing.

Another major challenge is the need to move large amounts of data from one location to another quickly and efficiently. Many OLCF teams are spread around the world, meaning that accurate, high-speed data delivery is imperative. High-speed data transfer is needed not only around the center, but also between the OLCF and other research institutions.

The Lustre-based file system, Spider, lies at the center of the OLCF's technological integration. Spider organizes data from the multiple computing platforms into a unified file system. The project began in 2005, and now Spider is the main operational file system connecting the XT5 partition of Jaguar, the LENS visualization cluster, the Smoky development cluster, and the center's dedicated GridFTP servers—at a blazing-fast bandwidth of 240 gigabytes per second.

The center uses two 10-gigabit-per-second connectors to ESNet, the DOE community's primary internet network. This gives the OLCF high-speed access to other DOE research facilities and other networks. The center has partnered with the Advanced Networking Initiative—funded by the American Recovery and Reinvestment Act—to build a prototype network for connecting DOE Office of Science centers, namely the OLCF, Argonne Leadership Computing Facility, and National Energy Research Scientific Computing Center. This network is poised to become a backbone network for the ESNet network by next year.

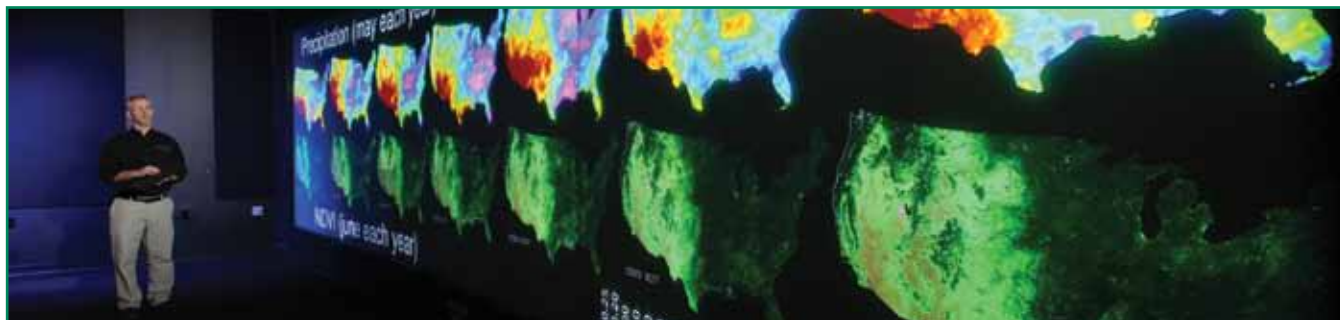
Data analysis

Visualization

The Exploratory Visualization Environment for Research in Science and Technology (EVEREST), with its 30-foot-wide, 10-foot-tall visualization screen, is one of the most important data analysis tools at the OLCF. The visualization facility gives researchers a sharp, detailed view of simulations.

Researchers using OLCF facilities automatically receive access to EVEREST and the LENS cluster supporting the facility. LENS is a 32-node cluster, with each node containing four quad-core, 2.3 gigahertz AMD Opteron processors with 64 gigabytes of memory, one NVIDIA GeForce 8800 GTX graphics processing unit (GPU) with 768 megabytes of memory, and one NVIDIA Tesla GPU with 4 gigabytes of memory. Its purpose is to channel data generated on Jaguar into visual results, fostering scientific discovery.

The 27-projector Powerwall displays images at 11,520-by-3,072 pixels—a total of 35 million pixels. The 15-node everest cluster has its own dedicated Lustre file system, and each node houses two dual-core AMD Opteron processors and two NVIDIA 8800 GTX GPUs.



OLCF visualization staff are versed in a variety of software, including VisIt, EnSight, POV-Ray, AVS/Express, ParaView, and IDL, which work in partnership with Chromium to deliver OpenGL and DMX to the Powerwall. The team assists users in anything from writing visualization software so users may see their data to helping users get their images on the wall.

eSiMon simulation tool

Computational scientists have a new weapon at their disposal.

Researchers from the OLCF have recently released the Electronic Simulation Monitoring (eSiMon) Dashboard version 1.0 to the public, allowing scientists to monitor and analyze their simulations in real-time.

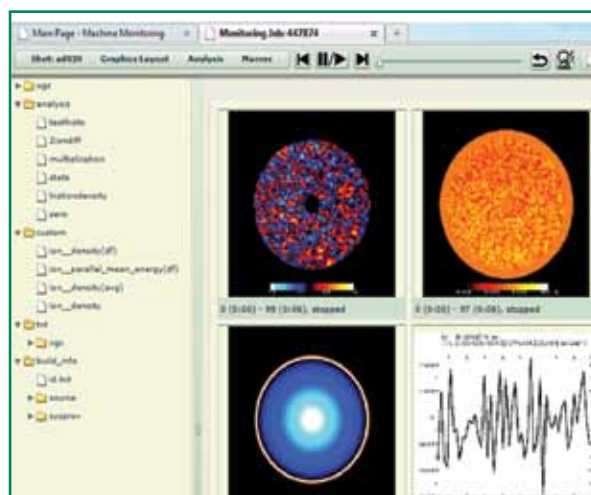
Developed by the Scientific Computing and Imaging Institute at the University of Utah, North Carolina State University, and ORNL, this “window” into running simulations shows results almost as they occur, displaying data just a minute or two behind the simulations themselves. Ultimately, the Dashboard allows the scientists to worry about the “science” being simulated, rather than learn the intricacies of HPC such as file systems and directories, an increasingly complex area as leadership systems continue to generate petabytes of data.

The package offers three major benefits for computational scientists. First, it allows monitoring of the simulation via the web. It is the only single tool available that provides access and insight into the status of a simulation from any computer on any browser. Second, it hides the low-level technical details from the users, allowing the users to ponder variables and analysis instead of computational elements. And finally, it allows collaboration between simulation scientists from different areas and degrees of expertise. In other words, researchers separated geographically can see the same data simultaneously and collaborate on the spot.

Furthermore, via easy clicking and dragging, researchers can generate and retrieve publication-quality images and video. Hiding the complexity of the system creates a lighter and more accessible web portal and a more inclusive and diverse user base.

Researchers can also take electronic notes on the simulation as well as annotate movies. Other features include vector graphics with zoom/pan capabilities, data lineage viewing, and downloading of processed and raw data onto local machines. Future versions will include hooks into external software and user-customized analysis and visualization tools.

“We are currently working on integrating the eSiMon application programming interface into an ADIOS method so that ADIOS users automatically get the benefit of monitoring their running simulation,” said the OLCF’s Scott Klasky, a leading developer of ADIOS, an open-source I/O performance library.



The eSiMon Dashboard.

Say Hello to ADIOS 1.2

The year 2010 saw the release of ADIOS 1.2, the latest incarnation of one of computational science’s most effective I/O tools.

Developed by a partnership led by the OLCF’s Scott Klasky, ADIOS has helped researchers make huge strides in fusion, astrophysics, and combustion. The new version features some interesting improvements that will doubtless aid researchers in taking full advantage of leading supercomputing platforms.

For instance, users can now use the application programming interface (API) directly to interactively construct new variables during run time. ADIOS also features a custom I/O method that writes data to subfiles and aggregates it into larger pieces for maximum performance on leadership-class systems. And now, users who run on large systems can switch from running on P-processors and writing to P-files—or one file or M-files, transparently. Version 1.2 also features further support for self-describing data in the output. For example, users can automatically retrieve the average value, minimum, maximum, and

standard deviation for all arrays at negligible computational cost. And finally, version 1.2 features some new asynchronous transport methods, allowing even faster I/O.

“The focus for this release is broader compatibility and user convenience. The introduction of the API calls to replace the XML file addresses long-standing requests from a small, but vocal, part of our user community,” said team member Jay Lofstead. “The AMR-focused enhancements broaden the classes of application that can use ADIOS while maintaining 100 percent backward compatibility. Some additional changes smooth the user experience.”

Taken separately, all of ADIOS’s individual improvements represent significant advances toward more efficient simulations. Taken together, they embody a major innovation in the way computational science will be conducted.—by Gregory Scott Jones

Providing power

The road to exascale computing is beset with obstacles—engineering specialized hardware, developing innovative software, and designing resourceful tools are just some of the challenges that must be met. Just as roads, water supplies, and power grids enable human civilization, HPC has its own infrastructure needs that make leadership-class computational science possible.

With computing, the most fundamental question is how to efficiently power bigger, faster machines, especially machines that are expected to compute one quintillion calculations per second and store tens of petabytes of data. Bringing in new hardware often means it's time for old hardware to go; this is the case with the Cray XT4 located on the second floor of ORNL's Computational Sciences Building. An 84-cabinet XT4 belonging to the OLCF was decommissioned on March 1, 2011. The removal of this machine frees up an electrical switchboard that redirects electricity from a transformer that carries 2.5 mVA (million volt amperes), or 2 million watts.

According to Jim Rogers, OLCF director of operations, this switchboard will be reconfigured using a series of power distribution units and remote distribution units, which take high voltage and current and convert them to smaller, usable power levels. The electricity will sustain the new 32-cabinet file system, which will store up to 10 petabytes of data for the first landmark in OLCF's road to the exascale—a Cray EX6 called Titan, a machine expected to reach a peak speed of 10–20 quadrillion calculations per second.

Titan's first steps

Titan's story actually begins with the OLCF's current leadership machine, Jaguar, the Cray XT5 that currently holds the number three spot on the Top500 List of the world's most powerful supercomputers. Late this year, OLCF plans to replace each of the node boards in Jaguar with Cray's newest XK6 nodes. Each node will increase from 12 to 16 cores, with the memory per node increasing from 16 to 32 gigabytes. Jaguar's

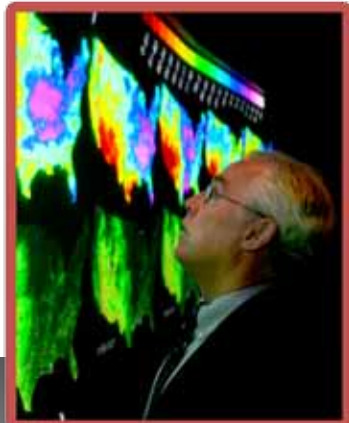
Seastar interconnect, which allows each of the system's nodes to communicate with one another, will be replaced with Cray's latest Gemini network, increasing bandwidth, decreasing latency, and providing for one-sided communications and atomic memory operations.

Jaguar's new configuration will provide more node hours for computation, double available memory for larger problems, and present a more stable, fault-tolerant network. Ultimately this 1,000-node system will serve as a test partition for users to optimize their applications for Titan—the OLCF's first hybrid architecture system, exploiting both traditional CPUs and GPUs.

Titan's initial configuration will build on upgrades to Jaguar by adding NVIDIA application accelerators to the 1,000-node system in late 2012. Titan's peak performance speed is expected to clock in between 10 and 20 petaflops, which is five to ten times faster than Jaguar's current peak speed. After staggered upgrades and acceptance tests, Titan's fully upgraded system is projected to be accessible to all users by 2013.
—by Caitlin Rockett



WORLD-CLASS SYSTEMS DESERVE WORLD-CLASS PEOPLE



OLCF staff ensure that our systems are indeed high-performance

The OLCF exists to ensure that our world-class systems reach their full potential and deliver regular scientific breakthroughs. From the day-to-day challenges involved in running unique simulations on unique resources to the long-term planning needed to ensure that scientific advances continue unabated, the OLCF works tirelessly to guarantee the quality of both current and future research.

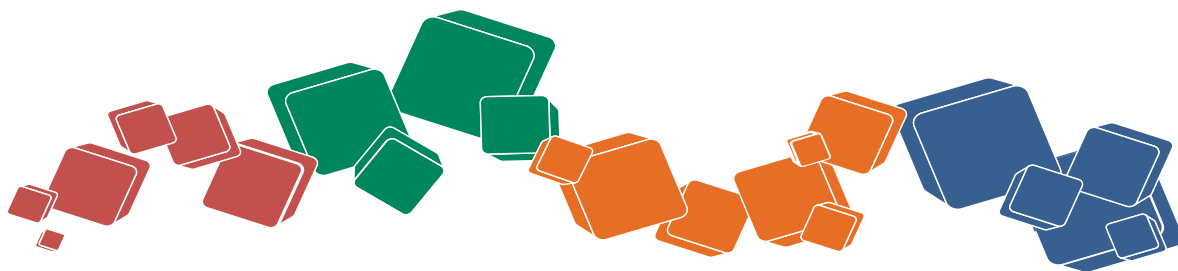
The process is guided by our management team. Director Jim Hack manages the overall vision of the center, while Project Director Buddy Bland supervises installation and upgrades of the OLCF supercomputers. They are aided by Deputy Director Kathlyn Boudwin. Acting Director of Science Bronson Messer guides the research teams that use the computing systems. And Director of Operations Jim Rogers manages day-to-day

operations and planning for future systems and infrastructure.

Our scientific researchers may have their closest working relationship with liaisons in the Scientific Computing Group, or SciComp. The liaisons are experts in their fields—chemistry, physics, astrophysics, mathematics, numerical analysis, computer science—but they are also experts in designing code and optimizing it for the OLCF systems. A large project may ask its liaison to join the research team as a full-fledged member, or it may choose instead to consult with its liaison only on specific challenges. SciComp is also where researchers will find visualization and workflow experts to help them deepen their insights and streamline their work. Contact group leader Ricky A. Kendall for more information at kendallra@ornl.gov.

The User Assistance and Outreach Group provides professional consultation to our users and communicates OLCF goals and accomplishments to our sponsors and the public. Our user assistance professionals provide day-to-day support to researchers, helping them through a wide range of high-performance computing challenges that include debugging, optimization, and compiling of codes, and access and file system issues. The group also provides documentation and relates important information to the user community through weekly email notifications. User Assistance also offers training and education opportunities to facilitate efficient use of computing resources.

Our outreach staff communicate the facility's goals and accomplishments through the OLCF website, regular newsletters and reports, and articles in outside publications. They create



highlights and other articles focused on scientific research and on OLCF systems and facilities. They also create posters, videos, slideshows, and other materials for public display at the OLCF and other venues. For information concerning the User Assistance and Outreach Group, contact Ashley D. Barker, group leader, at ashley@ornl.gov.

The High Performance Computing Operations Group keeps the OLCF leadership systems running, working with the infrastructure systems as well as with Jaguar and other OLCF supercomputers. Group members monitor systems 24 hours a day, seven days a week, 365 days a year and are responsible for administration, configuration management, and cybersecurity. The group also tests systems when they are installed and upgraded and uses diagnostic tools to continually monitor them. Group members anticipate problems before

those problems arise, and they identify components that are near failure. The group also ensures that all systems conform to ORNL cybersecurity policy. For more information, contact Ann Baker at bakerae@ornl.gov.

The Technology Integration Group (TechInt) is responsible for updating and integrating the networks, file systems, and archival storage infrastructure into the OLCF computing systems. The group researches and evaluates emerging technologies and provides system programming to seamlessly integrate new technologies and tools into the infrastructure as they are adopted. TechInt co-developed the OLCF's HPSS storage system and is constantly working to increase the speed of data transfer and implement cybersecurity measures for the OLCF's area-wide network. As OLCF computing resources continue to scale up, TechInt works to develop tools such as

compilers, debuggers, and performance-analysis tools that allow users to take full advantage of the leadership-class systems. Contact Galen Shipman, group leader, for more information at gshipman@ornl.gov.

The Application Performance Tools Group researches, tracks, and purchases a wide range of software tools that help researchers access and improve the performance of their applications on current and emerging OLCF computing systems. The group also manages contacts with vendors for the purchase of new modeling tools, languages, middleware, and performance-characterization tools. The group focuses primarily on issues that arise for research applications when they are run on very large-scale systems, such as Jaguar. For more information, contact Rich Graham, group leader, at rlgraham@ornl.gov.



Education, Outreach, and Training

Education and Outreach

The OLCF seeks to strengthen the scientific community not only through its superlative resources and skilled staff, but also through the education of future researchers and computational scientists.

Bobby Whitten of the OLCF User Assistance and Outreach Group explains that the move toward exascale computing means that training and education for current and potential users is more important than ever. “In the past our resources were easily programmable homogenous systems,” he explained. “GPUs are changing the way we do business—therefore we have to change the way we think about both the hardware and the applications we use to do science.” The short-term goal is to educate users about how to employ GPUs to expose new levels of parallelism within their codes, while the long-term goal is to prepare users to harness billion-way parallelism with their codes.



In addition to teaching users how to employ the center’s leadership resources, Whitten also helps educate future users. Whitten co-teaches a series of online HPC classes for Morehouse College students. In its second year, the course gives students a broad overview of current HPC topics including parallel programming models, visualization of data, and an introduction to astrophysics and molecular dynamics computer models.

The year 2010 marked the third year of the OLCF’s partnership with the Appalachian Regional Commission (ARC), a body of educators and business people whose goal is to support the educational development of the Appalachian region by offering college and career options to underprivileged and minority high school students. Ten students participated in the two-week ARC program in 2010, where they were given the opportunity to collaboratively build a supercomputer, test its speed via the High-Performance Linpack code (which is used to rank computers on the Top500 List), and determine when their cluster would have been ranked fastest in the world.

The OLCF also offered several seminars in 2010 covering HPC topics, with an emphasis on petascale computing and the future of exascale computing. The center tries to schedule at least one seminar each month, bringing in principal investigators and domain specialists who interact and collaborate with OLCF staff and/or use OLCF resources. The series is a great way for ORNL researchers to interact with colleagues from around the world and a vehicle for researchers to present scientific results from use of the OLCF facilities.

The OLCF also acts as a liaison between its user community and the community at large. Through user meetings, public tours (more than 950 in 2010), and speeches to outside groups through the ORNL Speakers Bureau, the facility supports a strong connection with the public that ultimately supports and benefits from the science conducted.

The Research Alliance in Math and Science

Twenty four students from eighteen colleges and universities across the continent and Puerto Rico took advantage of the unique opportunities and facilities at the Oak Ridge National Laboratory through a summer internship in the Research Alliance in Math and Science (RAMS) program. From freshmen at the University of Tennessee to post graduate students from the University of California, Berkeley, students were engaged in leading-edge research projects with mentors primarily from the Computing and Computational Sciences (CCS) Directorate. Projects ranged from climate research to performance

tuning to data analytics to sensors to robotics to applied mathematics and other on-going research areas. Several students participated in the LCF-led workshop “Crash Course in Supercomputing,” while a few participated in the 2010 Scientific Discovery through Advanced Computing conference. The RAMS program aims to identify and mentor underrepresented populations in science, technology, engineering, and mathematics disciplines through hands-on research projects and encouragement to seek advanced degrees with the long-term goal of increasing workforce diversity. The RAMS program is sponsored by the Office of Advanced Scientific Computing Research and is administered through the CCS Directorate Office.

Workshops

Lustre Scalability Workshop

May 19 and 20, 2010

As HPC moves closer to exascale capabilities, storage systems must concurrently expand to handle increasing amounts of data provided at increasing speed. To meet future data needs, the OLCF collaborated with Sun Microsystems and Cray to host this two-day workshop on the design of next-generation Lustre-based storage systems.

This workshop brought together key Lustre developers and engineers to identify scalability issues and develop a realistic roadmap to deliver a system capable of multiple terabytes per second of bandwidth. Participants were given the opportunity to review the proposed Lustre architecture to meet High Productivity Computing Systems performance and scalability requirements, and also developed a plan for a system capable of managing exabytes of storage by 2015.

Visualization with VisIt

June 4, 2010

For many HPC projects, visualization is a crucial aspect of analyzing research results. This workshop introduces users to VisIt, a scientific visualization software developed within DOE for analyzing and

visualizing extreme-scale simulation datasets. The class alternates between lecture discussions and hands-on exercises and is designed to introduce class participants to VisIt in an interactive setting. Active sessions included working with ORNL’s visualization cluster, LENS.

Crash Course in Supercomputing

June 17 and 18, 2010

This course taught students the basics of parallel programming necessary to compute on leadership-class systems like Jaguar. Day one taught students to program, compile, and run code in a UNIX environment. It also taught the basics of makefiles, common UNIX commands and VI editor commands. Day two covered more advanced topics such as parallelization, as well as MPI and OpenMP, the two leading parallel programming libraries. By the close of the two-day course, students put each of these newly learned concepts together by programming, compiling, and running a program.

SciApps

August 3–6, 2010

With exascale computing on the horizon, adapting existing codes to run efficiently on hybrid architectures is a key goal for the HPC community. The goal of this workshop was to offer a cross-disciplinary venue to facilitate interactions among current and potential leadership-class computing users, explore opportunities to strengthen application development, and obtain insight into near-term and medium-term application requirements and scientific mission goals. Approximately 70 interdisciplinary researchers gathered at ORNL for the Scientific Applications (SciApps) Conference and Workshop to share experience, best practices, and knowledge about how to sustain large-scale applications on leading HPC systems while looking toward building a foundation for exascale research. Funded by the American Recovery and Reinvestment Act, SciApps 2010 was co-hosted by OLCF Scientific Computing Group Leader Ricky Kendall and Director of Science Doug Kothe.





Day one of the workshop included an overview of the OLCF, and OLCF Project Director Buddy Bland provided a summary of the architecture of exascale computing. Computational scientist Rebecca Hartman-Baker led a discussion about the Joule metric program for testing the speed and accuracy with which supercomputing applications solve problems. Day two's talks described sustaining the present computing resource capabilities and looking toward the potential for future resources. On the final day, topics included software engineering practices as well as sustaining climate science's petascale research. The conference concluded with a roundtable discussion led by Kendall.

Proposal Writing Webinars

January 24, 2011

The OLCF teamed up with the Argonne Leadership Computing Facility (ALCF) for an "INCITE Proposal Writing Lecture/Webinar" to provide both prospective and returning users the opportunity to get specific answers to questions about the proposal and review process for INCITE. Representatives from INCITE, OLCF, and ALCF were present at the event.

OLCF Users Meeting

May 12, 2010

The OLCF Users Meeting focused on the research teams who have been granted allocations on Jaguar through the INCITE program. New OLCF users were introduced not only to the upgraded Jaguar system, but also to the various support groups available to them at OLCF. The OLCF Users' Council also met on this day to elect a new chair. This elected council member will act as the voice of the users, presenting user views, opinions, and ideas to OLCF management.

XT5 Hex-Core Workshop

May 10–12, 2010

The Cray XT5 Hex-core workshop focuses on familiarizing new, returning, and potential users with the Cray XT5 systems located at ORNL: the OLCF's Jaguar and the National Institute for Computational Sciences' (NICS's) Kraken. The workshop featured lectures from NCCS, NICS, and Cray staff covering key topics like XT5 architecture, using debuggers on the XT5, and developing applications capable of scaling to 100,000 or more cores. Hands-on sessions throughout the workshop allowed participants to access Jaguar and/or Kraken using their own codes and work one-on-one with NCCS, NICS, and Cray staff members to resolve any issue.—*by Caitlin Rockett*



High School Students Build Their Own Supercomputer—Almost—at ORNL



ARC students at ORNL working on a cluster of Mac minis.

Learning how to link multiple processors and build a computer network is probably not the way most high school students envision summer vacation.

However, for the third straight year, students and teachers from around Appalachia gathered at ORNL this summer for interactive training from some of the world's leading computing experts. The summer camp, a partnership between ORNL and the ARC Institute for Science and Mathematics, took place July 12–23. The OLCF hosted 10 students from various backgrounds and parts of the region.

“They get to learn HPC basics, and it’s a chance for them to live on their own for a couple of weeks,” said Bobby Whitten, an HPC specialist at ORNL and facilitator of the OLCF program.

The course was titled “Build a Supercomputer—Well Almost.” And that they did. With the help of ORNL staff, collaborators, and interns from universities, the high-school students went to work building a computer cluster, or group of computers communicating with one another to operate as a single machine, out of Mac mini CPUs. The students’ cluster did not compute nearly as fast as the beefed-up cluster right down the hall—Jaguar, which is ranked number three in the world—but it successfully ran the high-performance software installed. Through the program students received a foundation in many of the things that make a supercomputer work.

After a crash course in computer hardware, students learned how to connect the CPUs to one another via Ethernet cables and ran tests to determine whether the processors were indeed connected. After creating personal accounts to log on to their cluster, they were taught how to install a communication protocol, which formats messages into a

common language computers can send and receive. Finally, the students installed and ran high-performance software capable of solving large-scale computations, which is the forte of supercomputers.

Course instructor Jerry Sherrod, a professor at Pellissippi State Community College and ORNL collaborator, had the students list 10 things that they had learned during the 2 weeks. Answers scribbled on notebook paper ranged from “what a Beowolf cluster is” and “binary code—what a computer understands, made of 1s and 0s” to light-hearted comments such as “Jerry is a saint.”

Students filled out anonymous comment sheets to describe their experiences and suggest improvements. “I learned so much in my short time here. I only wish we had more time,” one entry said. Another suggestion went straight to the point: “This program needs to be longer, by an extra 2 weeks!”

Stephanie Poole, an ORNL intern and student at Pellissippi State who worked with the ARC students, felt they would benefit from having a solid foundation of computing principles and a small knowledge base of the field. “We started from the very beginning and then went into networking,” Poole said. Participating student Kenziah Terefenko playfully noted, “A lot of the material went straight over my head, but I can now crimp on a mean Ethernet cable!”

Whitten explained that in addition to the technical knowledge the students receive, the program tries to improve skills in other areas as well. “[Students] work on team building, collaboration, and communication,” he said, noting that students had to give an oral presentation at the end of the course. Instructors used team-building exercises not only to instill the idea of working as a group, but also to illustrate topics related to HPC the students may not have gotten otherwise.

For example, to show how multiple processors communicate with one another to quickly solve problems, students were given a lengthy math problem. One student was chosen to operate as a single “node” and try to solve the problem individually, while the other students worked on specific aspects of the problem and collaborated toward a faster correct answer.

Whitten happily notes that one of his students from that program’s first year, 2008, is heading off to Cornell University in the fall to study biomechanical engineering.—*by Eric Gedenk*

High-Impact Publications

Astrophysics

Endeve, E., C.Y. Cardall, R.D. Budiardja, and A. Mezzacappa. "Generation of Magnetic Fields by the Stationary Accretion Shock Instability." *Astrophysical Journal* 713, no. 2 (2010): 1219–1243.

Kasen, D., F.K. Ropke, and S.E. Woosley. "The Diversity of Type Ia Supernovae from Broken Symmetries." *Nature* 460, no. 7257 (2009): 869–872.

Schekochihin, A.A., S.C. Cowley, W. Dorland, G.W. Hammett, G.G. Howes, E. Quataert, and T. Tatsuno. "Astrophysical Gyrokinetics: Kinetic and Fluid Turbulent Cascades in Magnetized Weakly Collisional Plasmas." *Astrophysical Journal Supplement Series* 182, no. 1 (2009): 310–377.

Biology

Maffeo, C., R. Schopflin, H. Brutzer, R. Stehr, A. Aksimentiev, G. Wedemann, and R. Seidel. "DNA-DNA Interactions in Tight Supercoils Are Described by a Small Effective Charge Density." *Physical Review Letters* 105, no. 15 (2010): 158101.

Schulz, R., B. Lindner, L. Petridis, and J.C. Smith. "Scaling of Multimillion-Atom Biological Molecular Dynamics Simulation on a Petascale Supercomputer." *Journal of Chemical Theory and Computation* 5, no. 10 (2009): 2798–2808.

Tainer, J.A., J.A. McCammon, and I. Ivanov. "Recognition of the Ring-Opened State of Proliferating Cell Nuclear Antigen by Replication Factor C Promotes Eukaryotic Clamp-Loading." *Journal of the American Chemical Society* 132, no. 21 (2010): 7372–7378.

Chemistry

Baer, M., C.J. Mundy, T.M. Chang, F.M. Tao, and L.X. Dang. "Interpreting Vibrational Sum-Frequency Spectra of Sulfur Dioxide at the Air/Water Interface: A Comprehensive Molecular Dynamics Study." *Journal of Physical Chemistry B* 114, no. 21 (2010): 7245–7249.

Kimmel, G.A., J. Matthiesen, M. Baer, C.J. Mundy, N.G. Petrik, R.S. Smith, Z. Dohnalek, and B.D. Kay. "No Confinement Needed: Observation of a Metastable Hydrophobic Wetting Two-Layer Ice on Graphene." *Journal of the American Chemical Society* 131, no. 35 (2009): 12838–12844.

Climate

Evans, K.J., M.A. Taylor, and J.B. Drake. "Accuracy Analysis of a Spectral Element Atmospheric Model Using a Fully Implicit Solution Framework." *Monthly Weather Review* 138, no. 8 (2010): 3333–3341.

Washington, W.M., R. Knutt, G.A. Meehl, H.Y. Teng, C. Tebaldi, D. Lawrence, L. Buja, and W.G. Strand. "How Much Climate Change Can Be Avoided by Mitigation?" *Geophysical Research Letters* 36 (2009): L08703.

Engineering

Boykin, T.B., M. Luisier, M. Salmani-Jelodar, and G. Klimeck. "Strain-Induced, Off-Diagonal, Same-Atom Parameters in Empirical Tight-Binding Theory Suitable for [110] Uniaxial Strain Applied to a Silicon Parametrization." *Physical Review B* 81, no. 1 (2010): 125202.

Li, T.W., A. Gel, M. Syamlal, C. Guenther, and S. Pannala. "High-Resolution Simulations of Coal Injection in a Gasifier." *Industrial & Engineering Chemistry Research* 49, no. 21 (2010): 10767–10779.

Phillips, P., and M. Jarrell. "Comment on 'X-ray Absorption Spectra Reveal the Inapplicability of the Single-Band Hubbard Model to Overdoped Cuprate Superconductors.'" *Physical Review Letters* 105, no. 19 (2010): 199701.

Fusion

Malkov, M.A., P.H. Diamond, L.O. Drury, and R.Z. Sagdeev. "Probing Nearby Cosmic-Ray Accelerators and Interstellar Medium Turbulence with MILAGRO Hot Spots." *Astrophysical Journal* 721, no. 1 (2010): 750–761.

Xiao, Y., and Z.H. Lin. "Turbulent Transport of Trapped-Electron Modes in Collisionless Plasmas." *Physical Review Letters* 103, no. 8 (2009): 085004.

Yan, Z., M. Xu, P.H. Diamond, C. Holland, S.H. Muller, G.R. Tynan, and J.H. Yu. "Intrinsic Rotation from a Residual Stress at the Boundary of a Cylindrical Laboratory Plasma." *Physical Review Letters* 104, no. 6 (2010): 065002.

Geosciences

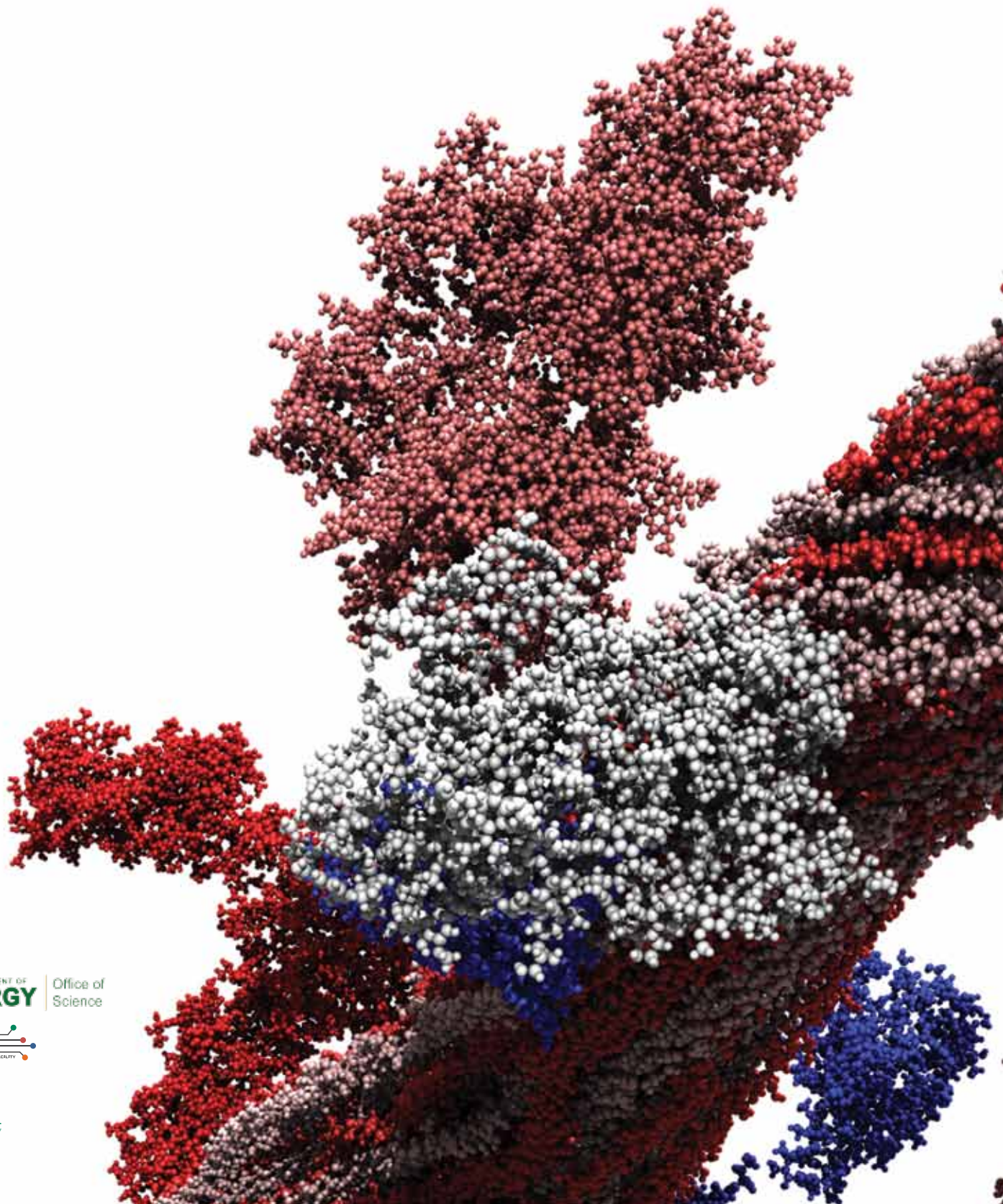
Roy, M., T.H. Jordan, and J. Pederson. "Colorado Plateau Magmatism and Uplift by Warming of Heterogeneous Lithosphere." *Nature* 459, no. 7249 (2009): 978–U102.

Materials

Maier, T.A., G. Alvarez, M. Summers, and T.C. Schulthess. "Dynamic Cluster Quantum Monte Carlo Simulations of a Two-Dimensional Hubbard Model with Stripelike Charge-Density-Wave Modulations: Interplay between Inhomogeneities and the Superconducting State." *Physical Review Letters* 104, no. 24 (2010): 247001.

Wang, Y.G., X.F. Xu, and J.H. Yang. "Resonant Oscillation of Misch-Metal Atoms in Filled Skutterudites." *Physical Review Letters* 102, no. 17 (2009): 175508.

Zhang, Y., X.Z. Ke, C.F. Chen, J. Yang, and P.R.C. Kent. "Thermodynamic Properties of PbTe, PbSe, and PbS: First-Principles Study." *Physical Review B* 80, no. 2 (2009): 024304.



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