National Center for Computational Sciences Snapshot
The Week of May 12, 2008

Jaguar Upgrade Brings ORNL Closer to Petascale Computing
NCCS supercomputer doubles peak performance

Upgrades to Oak Ridge National Laboratory's Jaguar supercomputer have more than doubled its performance, increasing the system's ability to deliver far-reaching advances in climate studies, energy research, and a wide range of sciences.

The system recently completed acceptance testing, running applications in climate science, quantum chemistry, combustion science, materials science, nanoscience, fusion science, and astrophysics, as well as benchmarking applications that test supercomputing performance.

The Jaguar system, a Cray XT4 located at ORNL's National Center for Computational Sciences, now uses more than 31,000 processing cores to deliver up to 263 trillion calculations a second (or 263 teraflops).

"The Department of Energy's Leadership Computing Facility is putting unprecedented computing power in the hands of leading scientists to enable the next breakthroughs in science and technology," said ORNL Director Thom Mason. "This upgrade is an essential step along that path, bringing us ever closer to the era of petascale computing [systems capable of thousands of trillions of calculations per second]."

Jaguar was among the most powerful computing systems within DOE's Office of Science even before the recent upgrade and has delivered extraordinary results across a broad range of computational sciences.

"The leadership capability at Oak Ridge has been delivering real scientific results," said Michael Strayer, associate director for advanced scientific computing research in the DOE Office of Science. "Benoît Roux of the University of Chicago used Jaguar to simulate in unprecedented detail the voltage-gated potassium channel, a membrane protein that responds to spikes of electricity by changing shape to allow potassium ions to enter a cell. This work has the potential to help us understand and control certain forms of cardiovascular and neurological disease."

Climate scientists are calculating the potential consequences of greenhouse gas emissions and the potential benefits of limiting these emissions. Combustion scientists are modeling the most efficient designs for engines that use fossil fuels and biofuels. Fusion researchers are using the system to lead the way toward a clean and plentiful source of electricity. Physicists are exploring the secrets of the universe, illuminating its most elusive mysteries. And materials scientists are searching for the next revolution in technology.

"This is an important advancement," said Thomas Zacharia, ORNL associate laboratory director for computing and computational sciences. "Leading researchers need many orders of magnitude more computing power and infrastructure than we can yet provide, and they have shown us how they will use these new resources, whether it be to predict the consequences of climate change at the regional level, design new materials with predetermined properties, discover new chemical catalysts, explore more efficient ways to manufacture biofuels, or simulate all important aspects of new reactor designs."

"The U.S. Department of Energy and its Oak Ridge National Laboratory have been making huge strides in providing more and more simulation capabilities to advance some of the world's most important scientific and engineering research—and invaluable partners with Cray to push the leading edge of supercomputing," said Peter Ungaro, president and CEO of Cray. "This upgrade is another big milestone in leadership computing and we, along with many others around the world, are looking forward to learning about the scientific breakthroughs that are borne as a result of this powerful new computing capability."

With its new power, Jaguar will be able to double its contribution to DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, which is revolutionizing key areas of science by facilitating the world's most challenging computer simulations. The NCCS will host 30 INCITE projects in 2008 from universities, private industry, and government research laboratories, contributing more than 140 million processor hours on Jaguar.

Radio Waves Will Make Reactor Hotter Than the Sun

Simulation provides insight into fusion power possibilities

In 2007 a fusion research team led by Fred Jaeger and Lee Berry of Oak Ridge National Laboratory (ORNL) achieved a performance of more than 87 trillion calculations per second, or teraflops, on a key computation that consumes more than half of the simulation time on the Cray XT4 Jaguar supercomputer at the National Center for Computational Sciences (NCCS). At the time of Jaeger and Berry's simulation, only eight nonclassified computers in the world could beat Jaguar's speed. The simulation provided insight into how best to heat an experimental reactor that is scheduled to begin operating in 2016. Formerly known as the International Tokamak Experimental Reactor, ITER is a multinational project that will be an important step toward developing commercial fusion power plants.

ITER will use antennas to launch radio waves carrying 20 megawatts of power into the reactor. That's the power equivalent of a million compact fluorescent light bulbs. These waves will heat the deuterium and tritium fuel to fusion temperatures—about ten times hotter than the surface of the sun. The deuterium and tritium form plasma, a state of matter created when gases become so hot that electrons get energized and fly off their atoms. In addition, the radio waves can drive currents that help confine the plasma. Jaeger's simulations will contribute to understanding how to make the most of the wave power in both heating and controlling the plasma.

“This run is the first two-dimensional simulation of mode conversion in ITER,” Jaeger said of the 2007 simulation, which explored the conversion of fast electromagnetic waves to slow electrostatic waves. Before this run, mode conversion in ITER was simulated in only one dimension, although scientists could simulate mode conversion in two dimensions for smaller tokamaks. “We need to know which types of waves are present because different waves can interact differently with the plasma.”

Jaeger’s team uses AORSA, a software code that solves Maxwell’s equations for the electromagnetic wave fields in the plasma. For the 2007 simulation, the code employed 22,500 processor cores—98 percent of the machine’s capacity—to calculate the interplay between radio waves and particles in the plasma as well as the current produced by the interaction. A mesh of 500 by 500 cells, or 250,000 individual cells—more than triple the resolution of earlier simulations—gave the team the ability to examine interactions in fine-grained detail.

Upon analyzing the energy distributions of the very-high-energy ions created when radio waves heat the plasma, the scientists found that in some cases these ions increased the fusion reaction rate. They learned the optimal frequency for driving current in the ITER plasma and identified the heat-loss channels that limit this current. In addition, comparing ITER with current tokamaks, they found stronger central focusing of radio waves in ITER, which bodes well for its ability to keep plasma hot enough for fusion.

In 2008, Jaguar was upgraded from dual-core to quad-core processors. An early evaluation of application performance on the upgraded machine resulted in two significant changes. First, the speed of the key computation increased from 87 to 152 teraflops, with further improvements expected. Second, another important computation was reconfigured to take advantage of new machine capabilities. This reconfiguration resulted in a 50 percent reduction in the computation’s runtime.

The AORSA team is part of a Scientific Discovery through Advanced Computing (SciDAC) project known as the SciDAC Center for Simulation of Wave-Plasma Interactions. The team includes plasma scientists, computer scientists, and applied mathematicians from ORNL; the Massachusetts Institute of Technology; Princeton Plasma Physics Laboratory; General Atomics; CompX, Inc.; Tech-X Corporation; and Lodestar Research Corporation.

Recent Publications

“Evolution of Nonthermal Particle Distributions in Radio Frequency Heating of Fusion Plasmas,” P. T. Bonoli et al., *Journal of Physics: Conference Series* **78**, 012006 (2007).

“Experimental and Numerical Characterization of Ion-Cyclotron Heated Protons on the Alcator C- Mod Tokamak,” V. Tang et al., *Plasma Physics and Controlled Fusion* **49**, 873 (2007).

The Wizard Behind the Curtain

Cray Center of Excellence makes breakthrough science possible

The groundbreaking research that takes place at ORNL requires much more than the world's fastest supercomputers. Behind the success of these miraculous machines lies a suite of dedicated, talented people whose job it is to ensure that the potential of these computational powerhouses is realized.

Take ORNL's Cray XT4, named Jaguar, for example. One of the world's fastest computers for open science research, Jaguar currently peaks at 119 teraflops and tackles some of the world's most pressing scientific questions: What is the mechanism behind the implosion of core-collapse supernovas? How can we make automobiles more environmentally friendly and efficient? What are the main obstacles preventing the feasibility of fusion energy? The computational simulations addressing these dilemmas don't run themselves. They rely on a relationship between researchers in specific fields and "liaisons" at ORNL to ensure that the codes being implemented make the most of their allotted computing time.

To help researchers better tailor their codes to the Cray architecture, ORNL and Cray founded the Cray Center of Excellence (COE) on the ORNL campus in the spring of 2005. Headed by John Levesque, the COE features two other Cray employees who are likewise experts in using Cray systems. As new systems are delivered to ORNL, the COE staff assists principal investigators (PIs) in porting and optimizing the most important scientific applications to the new machines. Currently, says Levesque, the COE is working on six to eight applications, tweaking the various codes so that they achieve maximum performance on the latest Cray systems.

Originally created to challenge the Earth Simulator in Japan, the COE has grown into an essential component of the supercomputing successes at ORNL. As the relationship between Cray and ORNL grew stronger, so did the need for further collaboration. Levesque volunteered to head the organization, and his philosophy behind its success is simple. "Let's allow the Office of Science researchers to concentrate on breakthrough science, and we will deal with the problems of the machine," he said.

For example, Jackie Chen of Sandia National Laboratories is currently using Jaguar to run S3D, a combustion modeling code that Chen hopes will help engineers design diesel engines and industrial boilers with greater efficiency and fewer emissions. Chen's research has shown promising results, but as Jaguar prepares to implement quad-core processors, S3D will need to be modified to take advantage of the system's new power, precisely the work of the COE. When S3D is finally optimized for the quad-core architecture, Chen's research will be that much stronger and diesel engines that much closer to becoming cleaner and more effective.

Other promising optimizations are in the works as well. For instance, the COE's Nathan Wichmann is currently working on altering the fusion code known as GTC for the quad-core architecture. Fusion energy could one day provide the world with a cleaner, more abundant energy source. With minimal nuclear byproduct and virtually no emissions, this experimental phenomenon has the potential to revolutionize the way the world harvests its energy. The research being done at ORNL is primarily concerned with ITER, a prototype fusion reactor under construction in France to test the feasibility of fusion power production for mass consumption.

But the COE does more than optimize codes—much more. The organization has a strong educational component, both for ORNL staff and remote users conducting science on NCCS systems such as Jaguar. The COE offers workshops for education and troubleshooting, including an upcoming 3-day workshop for Office of Science and National Science Foundation users who will soon be conducting their research on the updated machines at the center.

ORNL's Scientific Computing Group, headed by Ricky Kendall, features liaisons that work side by side with PIs to address any problems with codes and ensure maximum performance. All members of the Scientific Computing Group participate in and complete COE educational initiatives, further providing PIs with a strong assistance component when tackling today's state-of-the-art science.

"This close interaction between Cray and Oak Ridge has been very successful," said Levesque.

Recently, the COE has begun working on libraries for a variety of applications as well. COE staff have begun to optimize certain routines, but as Levesque says, "there are so many libraries and so many routines in the libraries that we can't do everything, but we try to identify the most important and have those ready for the applications."

As ORNL's high-performance computing (HPC) component continues to grow, pushing the limits of computational simulations with ever bigger systems tackling ever bigger problems, the COE will no doubt continue to play a major role in the laboratory's success. While today's supercomputers may seem almost supernatural, they are only the visible proof of the hard work of numerous people engaged in the most challenging science imaginable. The COE is just one of many wizards behind the curtain.

NCCS Hosts Workshop Series

Cray, Lustre, NCCS systems on agenda

The NCCS recently continued its outreach success with a series of workshops aimed at educating the wider HPC community.

A total of three workshops, held at ORNL, were hosted in mid-April, beginning with the NCCS Cray XT workshop on April 14, 15, and 16. Staff from the NCCS, ORNL's Joint Institute for Computational Sciences, Cray, and chipmaker AMD discussed XT issues, researchers participated in hands-on sessions with the Cray XT system, and computational scientists gathered with vendors and ORNL's staff experts to discuss strategies for making the most of their time on Cray XT supercomputers.

The Lustre workshop, held April 16, focused on helping application scientists get the most from the Lustre File System. The workshop was presented by Oleg Drokin and Wang Di, two file system engineers with Sun Microsystems and both seasoned Lustre developers.

Closing out the workshop series was the NCCS Users Meeting on April 17 and 18. PIs and members of their research teams gathered with NCCS staff and vendors to discuss challenges and solutions in areas such as porting and scaling of applications on the XT system. Each project new to the Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program was invited to give a 10-minute presentation. NCCS staff also gave presentations highlighting the complete range of resources, capabilities, and services available to the center's users.

"These workshops are so helpful for the researchers," said John Levesque, director of Cray's Supercomputing Center of Excellence. "By helping them profile their applications, we can immediately identify the bottlenecks and often actually fix the problems before the end of the workshop."

R.I.P. Cheetah

ORNL supercomputer has left the building

A former supercomputing heavyweight has been retired from the NCCS. Before its removal, the IBM Power4 system dubbed Cheetah performed dutifully throughout its 6 years of service.

Ranked as the eighth fastest computer in the world in 2002, Cheetah was involved in numerous computational science breakthroughs. However, it is perhaps best known for providing 40% of the cycles for the U.S. contribution to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC), which in 2008 shared the Nobel Peace Prize with former Vice President Al Gore.

"Cheetah came in as an extremely stable, well-tested system," said ORNL Computational Scientist Dr. John Drake. "Almost from day one, we were doing productive science. Due to its stability, it was well suited to the IPCC task."

Cheetah comprised 27 cabinets, each containing one node. Each node's 32 Power4 processors ran at 1.3 GHz, giving Cheetah a peak performance of almost 4.5 teraflops. The system had 1.1 terabytes of memory and 40 terabytes of disk space.

ORNL will continue to provide leadership computing through Jaguar, a Cray XT4 currently being upgraded with quad-core processors to a peak performance of 250 teraflops; Phoenix, a Cray X1E; and Eugene, an IBM BlueGene/P.