National Center for Computational Sciences Snapshot
The Week of June 4, 2007

<u>Radio Waves Will Make Reactor Hotter Than the Sun</u>

Fusion code simulates waves to heat and control ITER reactors

A fusion research team led by Fred Jaeger and Lee Berry of Oak Ridge National Laboratory (ORNL) has achieved a performance of more than 75 trillion calculations per second (75 teraflops) on the National Center for Computational Sciences (NCCS) Cray XT4 Jaguar supercomputer.

The team employed 22,500 processor cores for its AORSA code, which calculates the interaction between radio waves and particles in a fusion plasma as well as the current produced by the interaction.

The team's research is focused on simulations of the multinational ITER fusion reactor, an especially daunting challenge. According to Jaeger, the simulation of wave-particle interactions in ITER is difficult for two primary reasons: First, ITER will be much larger than existing fusion devices, and second, densities reached in the fusion plasma will cause the wavelength to be very small compared to the size of ITER. As a result, calculations performed in the simulation must be an order of magnitude higher in resolution than previous calculations.

Jaeger's team is now able to simulate a mesh of 500 by 500 cells, providing 250,000 individual cells. This is more than triple the resolution of earlier simulations, which provided meshes of about 256 by 256, or something over 65,000 cells.

The ITER reactor will use antennas to shoot radio waves carrying 20 megawatts of power into the plasma. These waves will both heat the plasma—which must reach a temperature about ten times hotter than the center of the sun—and create a current that controls the plasma. Jaeger's simulations will help the reactor's designers configure the antennas to make the most of that power in both heating the plasma and controlling it.

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 the Massachusetts Institute of Technology; Princeton Plasma Physics Laboratory; General Atomics; CompX, Inc.; Tech-X Corporation.; and Lodestar Research Corporation.

AORSA solves Maxwell's equations—four equations that encompass electromagnetic theory—in very hot plasma, working out both the propagation of the waves and the absorption of energy by the plasma. According to Jaeger, it is the first code that solves the integral wave equation in more than one dimension without making any approximation about the size of the wavelength.

<u>Jaguar Calculations Help Turn Vehicle Exhaust into Power</u>
Researchers simulate materials that turn heat into electricity

Materials researchers are using ORNL's Cray XT4 Jaguar system to help recover the energy that flows out your car's tailpipe.

A team led by Jihui Yang of General Motors is performing first-principles calculations of thermoelectric materials capable of turning waste heat into electricity. The team's efforts will take us a step toward capturing and using the 60 percent of the energy generated by an automobile's engine that is lost through waste heat.

Yang has been working with Changfeng Chen of the University of Nevada–Las Vegas to examine an especially promising lead-tellurium-based material for use as a thermoelectric converter. The team has been able to simulate various properties of the material in a more than 1,000-atom supercell, several times larger than previous simulations of its type.

Yang noted that the calculations would have been impossible had the team not had access to leadership computing facilities.

"Quantum mechanical ab initio calculations are usually done with 200 to 300 atoms," Yang explained. "We're doing calculations with a unit cell of more than 1,000 atoms. People would not be able to dream of doing these calculations without a large computing facility."

Yang's simulations are part of a $13 million, 5-year Department of Energy (DOE)-sponsored program entitled "Developing Thermoelectric Technology for Automotive Waste Heat Recovery." While he would not predict when the materials he simulates might appear in vehicles, he did note that DOE's goal is to have a demonstration of the technology—which promises to improve fuel economy and reduce fuel consumption—in the next 3 to 5 years.

Yang said he is very pleased with the help he has received from the NCCS, especially in using massively parallel computers. He said User Assistance and Outreach Group leader Julia White has been especially supportive.

He also noted that the simulations being performed on Jaguar are important beyond the properties of a single material, no matter how promising. He said the methodology being developed by the team will pave the way for researchers to simulate materials that have not yet been created, dramatically reducing the time to and cost of innovative materials advancements.

"The general approach can be designated as material by design," he explained.

Workshop Focuses On Tools for Petascale and Beyond

Explosion in number of processors challenges developers

Software developers from the United States and Europe gathered at ORNL May 23 and 24 in an effort to simplify the process of writing scientific applications for high-performance computers.

Their project, known as the Parallel Tools Platform Project, focuses on the Eclipse integrated development environment. It will bring a range of tools to the application developer's desktop, both streamlining the code-writing process and making the resulting application more efficient. It will also allow researchers to focus less on computer codes and more on the scientific breakthroughs they bring.

"These are people that are not that interested in writing the programs," said workshop organizer Greg Watson of IBM. "They want to get science to happen. I think if we can come up with tools that really help them do that, that will certainly be a big benefit."

Eclipse is a widely used open-source environment for developing commercial software. It makes a programmer's life more manageable by bringing together tools such as editors, debuggers, and revision-control systems. The ORNL workshop focused on tailoring Eclipse for applications that run on massively parallel supercomputers such as the NCCS's Cray leadership system. About 30 developers gathered at the workshop—organized by Watson, Rich Graham of the NCCS Technology Integration Group, and Craig Rasmussen of Los Alamos National Laboratory —to discuss additional tools such as debugging, analysis, and optimization for heavily parallel supercomputers.

The project is an acknowledgement of the unique challenges of writing an application that will run on thousands of processors.

"Often what happens is you write a code and you test it on a small number of processors and it works fine," Watson said, "and then you try it on 10,000 or 100,000 processors, and it breaks for some reason."

Staffers Share Expertise with Cray Community

Cray user meeting features presentations from all four NCCS groups

NCCS staff and researchers were out in force at the 2007 meeting of the Cray User Group, held May 7–10 in Seattle.

NCCS staff were presenters in more than a quarter of the meeting's technical sessions. All four NCCS groups—Scientific Computing, Technology Integration, High-Performance Computing Operations, and User Assistance and Outreach—were represented among the presenters.

The meeting was sponsored by the Boeing Company, which is itself an NCCS user. The theme was “New Frontiers” in recognition of the technological and engineering advances enabled by high-performance computing (HPC).

Mark Fahey of the Scientific Computing Group was elected treasurer of the user group and named to its board of directors. Trey White, also of the Scientific Computing Group, was named local arrangements chair for the group’s 2009 meeting, which will be hosted by ORNL.

Kothe and Kendall Discuss HPC for Nuclear Community
NCCS is committed to bringing state-of-the-art computing to nuclear field

NCCS Director of Science Doug Kothe and Ricky Kendall, leader of the Scientific Computing Group, contributed their expertise to the 2007 Computational Engineering and Science Conference held recently in Washington, D.C.

The conference focused on bringing HPC resources, algorithms, and software to scientists and engineers who are building advanced modeling and simulation application tools for nuclear energy. Kothe was invited to chair the session entitled “HPC Systems and Nuclear Energy”; Kendall was invited to speak in the session, which also included speakers from Los Alamos and Argonne national laboratories.

Kendall’s talk— “How Will I Get My Code to Scale on the Cray XT System (or Any Big Machine)?”—explained how scientists can prepare to perform research on leadership supercomputers such as the NCCS’s premier Cray XT4 Jaguar system.

He touched on common attributes of all scalable codes, and outlined the process and support needed to make any code ready for leadership computing systems. This process includes assembling a team that includes experts such as domain scientists, computational scientists, computer scientists, mathematicians, and statisticians.

“The nuclear energy field is committed to taking advantage of high-performance computing in the near future and realizes it needs to catch up relative to other fields,” Kothe said. “The Leadership Computing Facility at ORNL is committed to playing an important role in this renaissance by providing computing resources and modeling and simulation expertise.”

Scientists Look to the Horizon for Computing Challenges
Gathering anticipates systems capable of a million trillion calculations a second

ORNL hosted a “town hall meeting” on Simulation and Modeling at the Exascale for Energy, Ecological Sustainability, and Global Security (E3SGS) May 17 and 18. The Oak Ridge meeting was the second in a series of three workshops (Lawrence Berkeley National Laboratory hosted the first meeting on April 17 and 18, and Argonne National Laboratory hosted the final meeting held May 31 and June 1) initiated by DOE to advance its 10-year vision for focusing computational science capabilities on solving the most urgent national and global problems. The Oak Ridge town hall attracted more than 270 participants from universities, national laboratories, government agencies, and other research strongholds across the country.

Thomas Zacharia, associate laboratory director for computing and computational sciences, hosted the event at Oak Ridge and remarked that "Modeling and simulation at the terascale enabled by resources at the Leadership Computing Facility at Oak Ridge National Laboratory and the DOE INCITE program have demonstrated significant scientific advances in chemistry, materials sciences, climate, combustion, astrophysics, and fusion. Meeting petascale requirements for these computational domains is on the horizon, and computational resources at the exascale are required to make significant mission-driven advances in energy, climate, biology and astrophysics. These workshops are making significant strides toward identifying those requirements and laying the groundwork for the enabling technologies necessary to deliver exaflops to the scientific community."

The town hall meetings were aimed at engaging leading U.S. scientists and engineers, computer scientists, and mathematicians in identifying research topics that need extreme scales of computational capability and developing the computer architectures; scalable algorithms and computing tools; and data management, analysis, visualization, and storage systems required to advance from petascale to exascale scientific computing.

Michael Strayer, director of DOE's Office of Advanced Scientific Computing Research, was the opening speaker for all three workshops. Attendees participated in plenary and breakout sessions focused on ten applications and infrastructure research areas of global importance. The recommendations formulated in the breakout sessions by leading experts in their applications areas from all three town halls will be combined into a report for DOE's use in developing the strategy for the E3SGS initiative.