National Center for Computational Sciences Snapshot
The Week of May 21, 2007

Fusion Team Reaches 73 TF on Jaguar

AORSA code simulates use of radio 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 73 trillion calculations per second (73 teraflops) on the National Center for Computational Sciences (NCCS) Cray XT4 Jaguar supercomputer.

The team was able to use 22,500 processors for its AORSA code, which calculates the interaction between radio waves and particles in 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 made 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 450 by 450, providing more than 200,000 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.

"This allows us to look at the waves in ITER," Jaeger explained. "We need much more resolution with ITER because it's so big and the wavelength is so small."

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 both in 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 Corp.; and Lodestar Research Corp.

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>NCCS Staffers Featured at Cray User Meeting</u>
Seattle meeting focuses on HPC advances in technology and engineering

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

The theme for the meeting, sponsored by the Boeing Company, was "New Frontiers" in recognition of the technological and engineering advances enabled by high-performance computing (HPC).

NCCS staffers Josh Lothian and Don Maxwell of the High-Performance Computing Operations group and Makia Minich of the Technology Integration group were among those discussing the combined Cray XT3 and XT4 Jaguar system at the NCCS. Their presentation, entitled **"**XT7? Integrating and Operating a Conjoined XT3+XT4 System," discussed the processes and tools used to move production work from the XT3 to the combined system as well as ongoing operation of the combined system.

Minich also discussed use of the infiniband interconnect on the XT3, and Maxwell and Lothian were among the presenters for "Real Time Health Monitoring of the Cray XT Series Using the Simple Event Correlator (SEC)."

Other NCCS presenters at the meeting included the following:

- Bobby Whitten, who discussed the work of the User Assistance and Outreach group;
- Richard Barrett of the Scientific Computing group, who discussed strategies for solving linear systems of equations using the new Chapel programming language and the efficiency of XT3XT4 parallel I/O software stacks;
- Weikuan Yu of the Technology Integration group, who discussed the performance of biological applications that use field-programmable gate arrays and joined Barrett in discussing the efficiency of XT3XT4 parallel I/O software stacks;
- Mark Fahey of the Scientific Computing group, who discussed the optimization of a direct numerical simulation solver for turbulent combustion on the XT3 and techniques for parallel I/O on Cray XT systems;
- Bronson Messer of the Scientific Computing group, who discussed supernova simulation with the CHIMERA code and application requirement analysis for ORNL's Leadership Computing Facility;
- Arnold Tharrington of the Scientific Computing group, who discussed the NCCS acceptance test harness and regression test framework; and
- Trey White of the Scientific Computing group, who discussed multiresolution timers for scalable performance debugging.

NCCS Staffers Discuss HPC for Nuclear Applications

Kothe and Kendall participate in CESC2007 conference

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 to scientists and engineers focused on nuclear energy and reactor simulation. Kothe chaired the session entitled "HPC Systems and Nuclear Energy," which featured Kendall as well as 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 involves assembling a team that includes experts such as domain scientists, computational scientists, computer scientists, mathematicians, and statisticians.

Kendall also reviewed the facilities available at the NCCS and the projects included under the Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.