National Center for Computational Sciences Snapshot
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Science Highlights

Imagine a world with a virtually unlimited source of clean, safe energy, with almost no by-products or waste and zero risk of a nuclear meltdown. While it might sound like a pipe dream, fusion reactors could one day be a reality. Their potential is being explored by computational physicists like Jeff Candy of General Atomics, who is using the enormous resources of Oak Ridge National Laboratory's (ORNL's) National Center for Computational Sciences (NCCS) to model transport-related phenomena in tokamak plasmas.

A tokamak is a doughnut-shaped device that houses the plasma in a fusion reactor. According to Candy, the plasma, or fuel, is turbulent, and such turbulence is extremely difficult to simulate. Because of this plasma turbulence, a tokamak lacks "perfect containment," and heat leaks out of the plasma. The key, says Candy, is knowing the rate at which the heat in the plasma is leaking, because while some loss is necessary, too much can be detrimental. "Turbulence is necessary for a tokamak reactor," says Candy, adding that his GYRO code computes "optimal turbulence," finding the perfect balance of heat and alpha-particle production and loss. Managing turbulence affects potential tokamak reactors in a number of ways, including the cost, which will no doubt be a key factor in bringing fusion reactors to reality.

Candy's primary allocation at the NCCS is divided into five research subtopics, with different scientists studying particular aspects of the simulations. These individual projects take advantage of the GYRO code and Candy's allocation but are not interrelated. Because tokamaks are extremely complicated (Candy compares studying them to studying climate, with multiple factors at multiple scales), research on these individual subtopics is necessary for a thorough understanding of all the factors involved. So far the team has run several successful simulations on the Cray X1E (Phoenix).

Candy also has an allocation at the NCCS to study turbulence at multiple scales. While the turbulences of ions and electrons have been studied separately in the past, Candy hopes to use his GYRO code to gain a "real, theoretical, broad understanding of ion-electron turbulence." This allocation has led to enormous simulations on the NCCS's Cray X1E supercomputer, with "very nice results," says Candy. These results will be presented at the International Atomic Energy Agency's 21st Fusion Energy Conference in Chengdu, China, in mid-October.

Candy's work at the NCCS could eventually lead to a better understanding of tokamak plasmas and some day help deliver clean, safe energy to a world in need. With projects such as ITER (an international effort aimed at determining the feasibility of fusion power for human consumption) already under way in France, the environmental side effects of conventional power production could one day be a thing of the past.

NCCS Systems

The latest upgrade to the Cray XT3 (Jaguar) has been completed, and the system was returned to general production use on Monday, August 21. Jaguar is now operating at 54 teraflops, making it one of the world's most powerful open scientific supercomputing systems. NCCS and Cray staff members worked together last week installing the upgrade and making sure the system passed a rigorous acceptance test. According to project director Buddy Bland, "The upgrade went very smoothly and on schedule."

The latest upgrade doubled the performance of the XT3. The machine now has the ability to perform 54 trillion mathematical calculations per second, aiding researchers by providing the tools essential to running the larger simulations that will lead to significant scientific discoveries. However, the work is just beginning, as Jaguar's operating capacity will soon double again. The Department of Energy's (DOE's) Leadership Computing Facility is on schedule to upgrade the supercomputer to 100 teraflops by the end of the year. The center aims to reach a petaflop, or 1 quadrillion mathematical calculations per second, by 2009.

Last week's upgrade involved replacing all 5,212 processors with Cray's latest dual-core processors, doubling the memory, and adding additional interconnect cables to double the bisection bandwidth. Jaguar now features more than 10,400 processing cores and 21 terabytes of memory. Other improvements included an upgrade to the Lustre file system, increasing the capacity of the system from 50 to 100 terabytes. As a result, users will be able to run larger simulations much faster and with increased efficiency. In addition, InfiniBand®, a high-speed network connection, was successfully integrated on a test node, indicating that it is possible to connect the Lustre file system to Jaguar at a much greater bandwidth than had previously been obtained.

The NCCS is committed to making these transitions smooth for the user community. In the days leading up to the return of the XT3 to production use, the users were informed of the significant upgrades that had been performed and other system changes as well. As a result of the improvements, there also had to be adjustments to how jobs are entered into the queuing system. As an aid to the users, NCCS staff provided instructions and tips to assist the researchers as they began working on the system again. In addition, workshops are being planned for the near future that will help users of the system revise their advanced codes to take full advantage of the resources available at the NCCS.

NCCS Outreach

DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program and the NCCS were featured in a recent article on *HPCwire*. The article highlighted the INCITE program and the decision to expand it to include industry, government, and university research. Doug Kothe, Director of Science for the NCCS, and Jeff Candy, a principal scientist in the Energy Group of General Atomics and current INCITE participant, were extensively interviewed about the expanded program. Candy stated that INCITE and the NCCS have allowed him and his research team to make tremendous progress on their project. Candy says, "The availability of the substantially more powerful Cray machines made ORNL even more attractive for our work. ORNL has an extremely receptive, helpful staff that jumps immediately on problems."

The complete article can be found at http://www.hpcwire.com/hpc/830483.html.