National Center for Computational Sciences Snapshot
July 25, 2006

Science Highlights

Life's smallest components might one day be a huge asset to mankind. Researchers at Oak Ridge National Laboratory (ORNL) are slowly unlocking the secrets behind biomolecules—microscopic wonders of nature with enormous potential. According to Dr. Pratul Agarwal, an associate staff scientist at ORNL, biomolecules are "very efficient machines that work at the molecular level, performing all functions of living cells," such as proteins and DNA. Dr. Agarwal is using the immense resources of the National Center for Computational Sciences (NCCS) to computationally model biomolecules.

The main purpose of his research is to discover how these biomolecules function, deciphering their structure and dynamics so that one day they can be used to solve some of mankind's most pressing problems. For example, the research could lead to the building of better proteins and enzymes for drug design. A more immediate possibility, however, is the conversion of cellulose into ethanol, a fuel that could potentially replace gasoline at the pump for supply and environmental reasons.

Dr. Agarwal and his partners in the research, the National Renewable Energy Laboratory and scientists from Cornell University, hope that studying the dynamics of cellulose will lead to a solution and a more readily available, environmentally friendly fuel. Although Dr. Agarwal began his research only 6 months ago, other scientists around the world have been working on the problem for 5 years. "Molecules are extremely difficult to study," says Agarwal, adding that the traditional techniques of x-ray crystallography, nuclear magnetic resonance (a sort of MRI for molecules), neutron-scattering, and biochemical studies are extremely expensive and time-consuming. Besides the cost and time involved, says Agarwal, experiments can also be limiting.

"Computational techniques using the NCCS's resources allow us to complement and extend the information from experimental studies," he says, adding that the NCCS also allows the researchers "to explore those aspects of biomolecules that are beyond the reach of experimental techniques."

NCCS Systems

Right on schedule, the NCCS passed the hardware acceptance milestone of the dual-core upgrade of Jaguar from 25 to 50 TeraFLOPS. The upgrade started on July 11th and was completed on July 19th, when all of the diagnostic tests for the system had run without failure after checking out the CPUs, memory, and interconnection network of the upgraded system.

The upgrade involved physically removing all 1,303 compute-node boards from the Cray XT3 (Jaguar). For each node board, the heat sinks were removed from each of the four processors, and the thermal transfer compound was cleaned off of the heat sink. Then the four single-core Opteron™ processors were removed and replaced by the new dual-core ones. New thermal transfer compound was applied to each of the processors, and the heat sinks were reinstalled. Finally, the memory on each node was doubled by installing four, 2-GB dual in-line memory modules (DIMMs). The covers were replaced, and the node was returned to its slot in the cabinet to be checked.

While the node upgrades were under way, another team was doubling the bisection bandwidth of the system by completing the torus in the “Y” dimension of the system. This task required removing all the overhead cables, using new 7-meter cables to rewire the system, and replacing all of the overhead cable trays to accommodate the larger cables. Finally, two new power supplies were added to each cabinet, and the diagnostic control computer in each cabinet was upgraded to support the new dual-core chips and their higher power consumption. The failure rates of the components in this initial upgrade were as follows:

- Of the 5,212 Opteron™ chips replaced, a total of eight failed, five were replaced, and three were fixed by reseating the processor.

- Of the 5,212 new 2-GB DIMMs installed, 13 failed and required replacement.

- Of the 168 new 7-meter cables, two had to be replaced.

It is important to note that this was the first upgrade of an XT3 system to dual-core processors and the first upgrade to the 7-meter cables. Cray had a team of 13 people at ORNL to complete the upgrade.

The machine has now been turned over to Cray’s software team, which will verify the dual-core software on the system. This process is expected to take 2 weeks because Cray has never had a dual-core system of this size for internal testing. Upon completion of the software checkout, the NCCS will start the acceptance-test activities, with the goal of completing acceptance by August 11th.

LCF and INCITE Projects

On July 14th, project updates were sent to the Principal Investigators (PIs) for all Leadership Computing Facility (LCF) and Innovative and Novel Computational Impact on Theory and Experiment (INCITE) projects. Each update contained detailed charts outlining each project’s usage of its allocated processor hours on each system, as well as a list of the project milestones to be updated by the PI. The goal of the updates was to collect information from the researchers regarding their progress as of the third quarter of fiscal year 2006 and to identify ways the NCCS staff can assist the researchers as they seek to achieve breakthrough science using the resources of the NCCS.