National Center for Computational Sciences Snapshot
September 25, 2006

Science Highlights

Scientists at Oak Ridge National Laboratory's (ORNL's) National Center for Computational Sciences (NCCS) are using groundbreaking computer simulations on the Cray XT3 (Jaguar) to uncover the incredible role molecular motors play in the process of life.

Harvard University Professor Martin Karplus is the principal investigator on the INCITE project "Molecular Dynamics Simulation of Molecular Motors." According to Karplus, Harvard's Theodore William Richards Professor of Chemistry, the goal is to understand how motors in living things function. His team is currently looking at two motors, both of which play major roles in everyday biological processes. The first motor, dubbed F_1ATP-synthase, is responsible for the manufacture of ATP, or adenosine triphosphate, the molecule that, says Karplus, "supplies energy for our every action." The rotary motor, believed to be the smallest in nature or otherwise, turns food into usable energy, allowing the numerous processes necessary for life to take place. F_1ATP-synthase, which Karplus labels "highly efficient," in many ways resembles an automobile engine, with the exception of performance, where it excels; the shaft rotates a thousand times a second, producing three molecules of ATP each time, for a total of 3,000 molecules per second.

The function of the second motor, DNA polymerase, is not as clear, says Karplus. It also serves a vital biological function: copying nucleic acid to make new cells and bacteria or reproducing DNA. Essentially, the motor uses one strand of DNA as a template and makes a copy. He calls DNA polymerase "high-fidelity" because it is especially good at duplicating without mistakes (with an overall error rate of 1 in 100,000). Too many errors and the organism will die, says Karplus. The polymerase motor essentially sits on the nucleic acid it intends to copy and jumps from step to step, adding one base (the letters of the genetic code: C,G,A, and T) at a time. The movement from base to base is known as translocation, which is at the heart of Karplus's research. His team is trying to better understand the relationship between energy and translocation.

Karplus, who has worked with such science greats as Linus Pauling and Charles Coulson, is no stranger to the marriage of computers and science. Approximately 30 years ago, he was a member of the first team to simulate the molecular dynamics of biomolecules. The code, dubbed CHARMM for "Chemistry at Harvard Macromolecular Mechanics" is used by thousands of researchers today and has been sold to pharmaceutical companies for drug design.

He points to a variety of possible applications for his research at NCCS. A deeper understanding of the high-fidelity mechanism might be used to repair the polymerase and eliminate mistakes in duplication. By inhibiting the F_1ATP-synthase motor, it might be possible to prevent cancers from spreading. The motors themselves are being explored in the realm of nanotechnology, and their sheer efficiency makes them of interest to all branches of science.

"Very exciting things have come out of [the simulations]," says Karplus, adding that his team is applying for a new grant. They are also currently in the process of writing two new papers detailing the research. If his past success is any indication, the results could very well prove to be invaluable.

NCCS Scientific Computing

A staff member of the NCCS recently went "out of his way" to meet the needs of one of the system users. Mark Fahey traveled to California to spend three days working with researcher Jeff Candy. Candy is the principal investigator for the LCF Project "Exploring Advanced Tokamak Operating Regimes Using Comprehensive GYRO Gyrokinetic Simulations."

Candy was originally scheduled to come to ORNL to work with Fahey, but due to scheduling issues, it worked out better for Fahey to travel to meet with him instead. Over the three days of work, the researchers were able to interact and collaborate on code development and testing without the barrier of over 2,000 miles between them. Ultimately they were able to accomplish much more in a shorter period of time. The result of their work is a new version of Candy's code, GYRO, now updated to version 6.0.0. According to Fahey, "the release would have happened much later without the trip."

Candy is quick to point out the benefits of working with the NCCS and its staff members. In an August 26, 2006, article in HPCWire (http://www.hpcwire.com/hpc/830483.html), he points out the value of Fahey's assistance, saying, "I just want to repeat that Mark Fahey of ORNL has been a crucial person in this effort, especially for code optimization. He sees things we sometimes don't. I have nothing but great things to say about him."

NCCS Facilities

The progress on the second floor of the Computational Sciences Building at ORNL is on schedule. The construction is taking place to ready the facility to house the Cray XT3, which will be upgraded to 100 TF in early 2007 and ultimately to 250 TF in late 2007. The mechanical contractor has completed the process of installing 12-inch pipe for chilled water and the electrical contractor is nearly finished supplying power to the second floor. Twenty-six 30-ton air conditioners will be delivered by the end of the week and will be added to the six air conditioners already on the second floor. When finished, the air conditioners will cool about 4 megawatts of power. The completion of the current construction work is an important step on the path to deliver the petascale machine by late 2008.

ORNL'S Jaguar the Fastest Computer in the World for GTC

Stephane Ethier of the Princeton Plasma Physics Laboratory was able to use 10,368 of Jaguar's 10,424 processors in a run last week of the gyrokinetic toroidal code (GTC), making Jaguar the fastest system in the world for running the code.

The GTC code is used to simulate microturbulence in a fusion reactor. Last week's run was able to advance 5.4 billion particles per step per second, a 13 percent improvement over the previous record of 4.8 billion particles per step per second set on Japan's Earth Simulator.

More information about this milestone will be included in the next Snapshot.