National Center for Computational Sciences Snapshot The Week of June 9, 2008

Pass the Proton

Simulation explores mechanism for proton transfer in water

Magic happens at the nanoscale. From antibacterial coatings to fuel-cell-powered cars, tomorrow's inspiring new technologies depend on today's researchers learning how to control the novel behavior of small-scale systems in a predictable way.

A team of materials scientists led by Jorge Sofo of Penn State University and Thomas Schulthess of Oak Ridge National Laboratory (ORNL) has used ORNL's Jaguar supercomputer to successfully simulate such a system. Working from fundamental principles of quantum mechanics, the team accurately simulated the behavior of water in the presence of the common catalyst titanium dioxide. The work not only improves our understanding of a process that is already important in areas such as fuel cells and the geosciences; it also prepares the way for simulations of ever more complex systems.

"This whole simulation sets the stage for a lot more work on more complicated systems," explained Paul Kent, a member of the team who worked extensively on the computer application used in the research. "This is much more than a proof of concept because we've got a lot of science out of this, but the idea is obviously to move on to more complicated materials."

Specifically, the team simulated the process by which water passes protons from one molecule to another. While a molecule of water—H_2O—contains two hydrogen atoms and one oxygen atom, one of the hydrogens will occasionally break off. The nucleus of this hydrogen—a proton—can then be exchanged with other hydrogens in other water molecules, transporting the proton through the water. The simulation shows that first-principles molecular dynamics—in this case performed using the Vienna Ab-Initio Simulation Package—can be used to explore this process.

The process itself is very fast and localized. To capture the behavior of water molecules, the simulation tackled a system of 700 atoms in steps of a half femtosecond each. Equivalent to a half-quadrillionth of a second, a half femtosecond is to a second as a second is to 63 million years. To get enough useful information, the simulation proceeded through more than 20,000 time steps to get to 10 picoseconds, or 10 trillionths of a second of data, making it one of the largest such simulations undertaken to date.

The simulation put the water in contact with titanium dioxide for two primary reasons. First, the catalyst spurred the process enough for a 10-picosecond simulation to yield sufficient results. Second, technologies such as fuel cells typically use catalysts, and the group aims to improve our understanding of the processes involved and thereby improve the technologies.

The computer specialists were able to compare their results with results from a team of experimentalists led by Dave Wesolowski of ORNL, which evaluated the same system of water and titanium dioxide molecules using neutron-scattering techniques. The collaboration illustrates the benefits of experiment and computer simulation working together.

"One of the cool things about this work is that the neutron scattering gives us a fingerprint for the dynamics of the water," Kent explained. "And we can, in our simulations, go off and compute that fingerprint as well. So we've got this cross reference, and as closely as we're looking, it seems to be accurate. The cross reference is by no means everything, but it gives a hint that the dynamics in the simulation are pretty good and that we're justified in looking in more detail."

He stressed that these simulations are unlikely to lead to great technological innovation in the short term, but they are a necessary step along the way.

"For example, proton transport is critical for fuel cells," he noted. "This is clearly a major motivation for learning what we can about proton transport in water—on a surface that is well characterized and clean and where the neutron-scattering people can do measurements. Looking at a fuel cell membrane is much more complicated, so this is a prerequisite."

ORNL/Oak Ridge High School Team Up to Find Global Temperature

Students tackle pesky climate problem

In June, it may be 30°F in Anchorage, Alaska, 90°F in Oak Ridge, Tennessee, and 115°F in Baghdad. So what is the earth's global temperature, the "real" temperature, which, say, an observer on Mars might "read," and how can you determine it here on earth?

That is the question Oak Ridge High School (ORHS) graduating seniors Casey Jaeger and Helen Ren chose for their 2007–08 Math Thesis project, for ORHS mathematics teacher Benita Albert.

Jaeger's research ultimately led him to the Cray XT4 teraflops computer, named Jaguar, at the NCCS. The students worked with mentor John Drake, group leader of the Computational Earth Sciences Group, in the Computer Sciences and Mathematics Division at ORNL.

"This is an example of a simple question with a complicated answer," Drake said. "The whole global warming debate assumes we have a clear answer. This kind of research puts kids in the position to question assumptions and to examine first hand the scientific premises underlying an important issue."

The students approached the problem of finding a finite global temperature for the entire planet, from different vantage points. Ren took the point of view of the stationary observer. "The temperature measured at one place will differ from the temperature measured at another," Drake said. "So we have to ask, how can we express that, and we have mathematical language we can use."

"This is what Helen [Ren] and I set out to do: find novel approaches to the multiscale dilemma that is our climate," said Jaeger. "If we can supply our climate modeling algorithms with data that suit the multiscale nature of our planet, we believe results will begin to improve."

Jaeger started with a spherical model of the earth in a MATLAB algorithm. "The idea of my crude model was simple: calculate a global average temperature by sampling a small pool of data from the earth's climate. If the sample accurately represents a multiscale function, such as earth's temperature, the calculated average would be quite close to the exact average (from historical data)."

When averaging an NCEP (National Center for Environmental Prediction) temperature function, Jaeger's model initially produced skewed results. He introduced a set of latitudinal zones that corrected his sampling error. This small tweak allowed his model to accurately average each of the 712 temperature functions it sampled, providing a global average temperature closely correlated to existing decades of actual data.

In her research, Ren's method considered global warming and the relationship among CO_2, temperature, and dust. "I looked into a way to calculate the global average temperature from a stationary observer model, which requires that a global integral over the earth be developed, based on unevenly spaced data points," she explained.

Real temperature data obtained from the NCEP produced an average of 285.5 K (54.23°F), with a standard deviation of 1.3. "We found that sampling fewer data points for the analytic test function gives us a solution closer to the true value (the value obtained by averaging the results from NCEP data for past decades, a global average that is most generally accepted by the scientists), than sampling fewer points from real temperature data. That actually gives a less accurate solution," she said.

Jaeger began doing his calculations on his laptop, but it ultimately led him to the high-tech world of supercomputing, where the grown-up scientists play: the NCCS's Jaguar. "When we started sampling multiscale functions, the laptop's processing took more than 25 hours to derive a simple average," Jaeger said. "So we had to create a version of my algorithm that would run on a parallel computing system."

The pair started their project at ORNL in the summer of 2007 before entering grade 12. They worked on it through the school year. Encouraged by Ms. Albert, Jaeger and Ren entered the national Siemens Competition in Math, Science and Technology and represented ORHS at the regional finals at Georgia Tech.

<u>NCCS Director Gives Congressional Testimony</u>

Hack talks climate in D.C.

NCCS director James (Jim) Hack recently testified before the U.S. Senate on the intricacies of climate modeling. Hack spoke at the hearing on *Improving the Capacity of U.S. Climate Modeling for Decision-Makers and other End-Users* on May 8, 2008, before the committee on Commerce, Science, and Transportation.

The hearing was aimed at assessing the ability of computers to accurately predict present and future climate scenarios, at both the regional and local scales, with a focus on application development and network operation. The future of climate modeling was also a major topic of discussion.

Computational climate models play an increasingly important role in providing policymakers with information which they in turn use to draft and examine legislation related to climate change. One of the world's foremost experts on climate modeling, Hack stressed future investments in computational algorithms to improve the accuracy of future-predicting climate models and a "close and continuing collaboration between the climate, facilities, applied mathematics, and computer science communities."

Hack is in charge of a new program at Oak Ridge National Laboratory to coordinate the various climate-related research activities taking place at the lab in different organizations. "There is no single pacing item to the advancement of climate change science, but a collection of interrelated science and technology challenges," he said. "Many of the issues discussed in this testimony speak to the need for a balanced investment portfolio in computational infrastructure, climate science, computer science, and applied mathematics. In the short and long term, computational capability remains a significant bottleneck and should remain a high-priority investment . . . . State-of-the-art climate models embody our best understanding of the many complex processes that are central to the climate system," said Hack, adding "They are the best available tools for exploring how the climate system works and how it is likely to evolve."

Representatives from the National Oceanic and Atmospheric Administration, Microsoft, and the University of Alaska–Fairbanks, among others, also gave testimony during the hearing.

<u>NCCS Big Presence at CUG '08</u>

Researchers descend on Helsinki

The (NCCS) enjoyed a major presence at the annual Cray Users Group (CUG), held May 5–8 in Helsinki, Finland.

The conference theme this year was "Crossing the Boundaries." The event featured numerous educational seminars, including general sessions, tutorials, and birds-of-a-feather sessions. The ORNL presence this year was so significant, in fact, that the organization had its own parallel session during the conference, which included four talks, all conducted by ORNL staff.

The NCCS’s James Rogers unveiled ORNL’s coming new petascale system in a talk titled **“**Reaching a Computational Summit: The 1 PFLOP Cray XT at the Oak Ridge National Laboratory.” The new system is destined to be one of the most powerful open-science supercomputers in the world, enabling groundbreaking discoveries in the fields of climate, alternative energy, astrophysics, and many more.

The NCCS also looked to the future in a talk by Trey White of ORNL titled “Exascale Computing: Science Prospects and Application Requirements,” in which White discussed a recent NCCS document on the requirements necessary to push supercomputing to the exascale.

“The conference was very informative,” said the NCCS’s Mark Fahey, who is also treasurer of CUG. “There was a lot of information about the quad-core architecture, and the interactive sessions provided a very useful, engaging setting.”

ORNL will be hosting next year’s CUG meeting in Atlanta.