

NCCS Snapshot

The Week of June 9, 2008

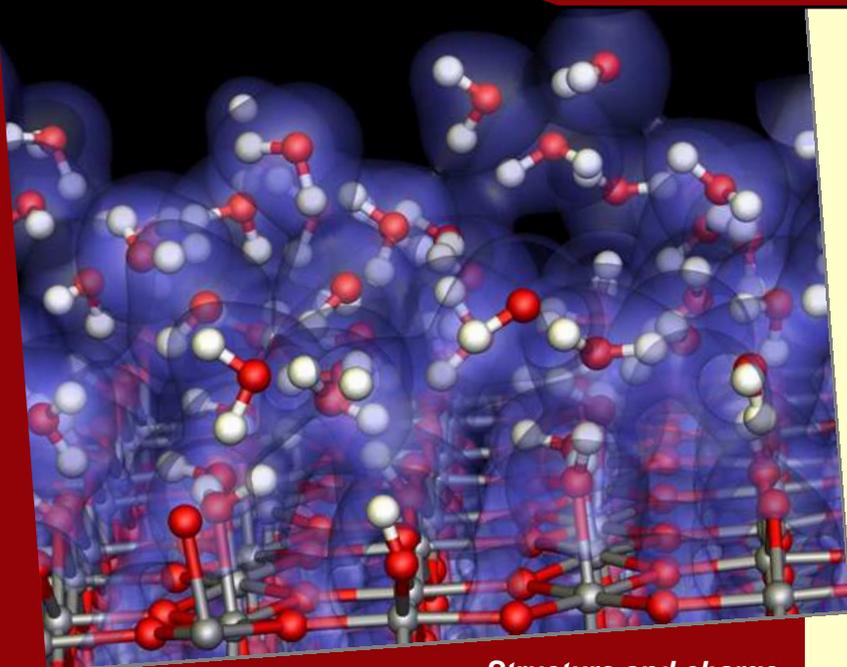
NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES



Oak Ridge National Laboratory
U.S. Department of Energy

Pass the Proton

Simulation explores mechanism for proton transfer in water



Structure and charge density of water on a titanium dioxide surface from large scale ab initio molecular dynamics calculations. (Courtesy Paul Kent, ORNL and Jorge Sofo, Penn State Univ.)

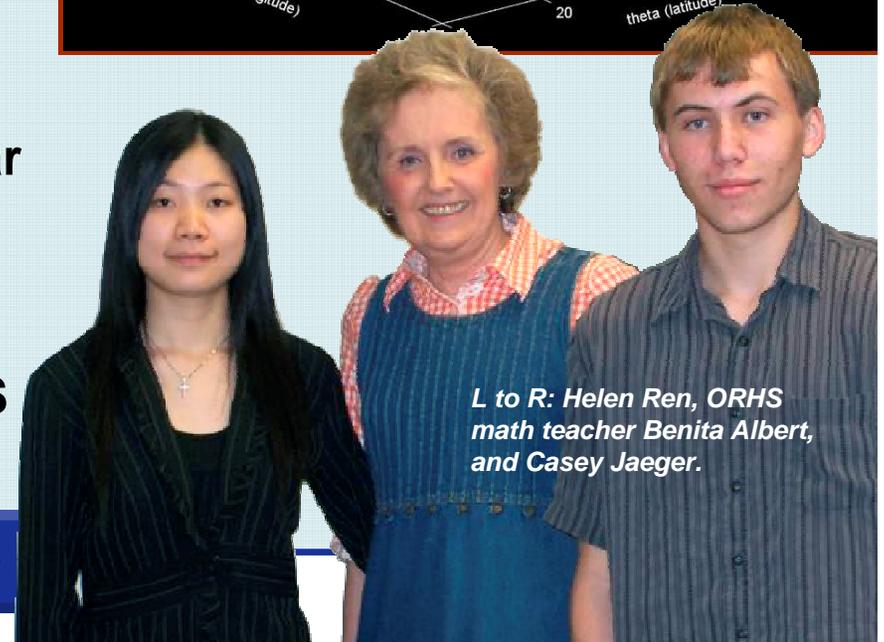
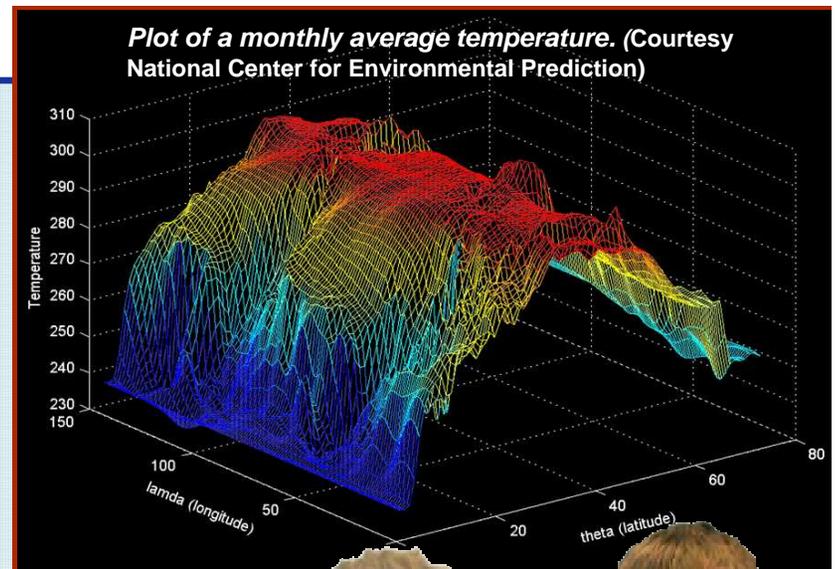
- A team of materials scientists has used ORNL's Jaguar supercomputer to successfully simulate the behavior of water in the presence of the common catalyst titanium dioxide
- The work improves our understanding of an important process in fuel cells and the geosciences and prepares the way for simulations of more complex systems
- The simulation also shows that first-principles molecular dynamics can be used to explore this process

"This whole simulation sets the stage for a lot more work on more complicated systems."

Paul Kent, ORNL researcher and team member

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

- Two Oak Ridge High School students recently attempted to figure out a “global” temperature for the earth, using computation as their main tool
- The two ORHS seniors, Casey Jaeger and Helen Ren, working with ORNL’s John Drake, took different computational approaches, each yielding remarkably accurate results
- Casey used the NCCS’s Cray XT4 Jaguar to help resolve his model
- Casey and Helen entered the national Siemens Competition in Math, Science and Technology, and represented ORHS at the regional finals at Georgia Tech



L to R: Helen Ren, ORHS math teacher Benita Albert, and Casey Jaeger.

Student uses Jaguar to tackle climate

NCCS Director Gives Congressional Testimony

Jim Hack



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 *Improving the Capacity of U.S. Climate Modeling for Decision-Makers and other End-Users* hearing on May 8, 2008
- Hack stressed future investments in computational algorithms and a continuing collaboration between the various disciplines involved in climate modeling

“State-of-the-art climate models embody our best understanding of the many complex processes that are central to the climate system.”

Jim Hack, NCCS Director

NCCS Big Presence at CUG '08



CUG 2008 HELSINKI • MAY 5–8, 2008
CROSSING THE BOUNDARIES

- ORNL once again enjoyed a major presence at the annual Cray Users Group (CUG), held from May 5-8 in Helsinki, Finland
- The ORNL presence was so significant that the organization had its own parallel session during the conference, which included four talks, all conducted by ORNL staff
- ORNL will host next year's Cray Users Group meeting in Atlanta, Georgia

"The conference was very informative. There was a lot of information about the quad-core architecture and the interactive sessions provided a very useful, engaging setting."

Mark Fahey, NCCS staff member and CUG Treasurer

Researchers descend on Helsinki