

NCCS Snapshot December 18, 2006

NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES



Oak Ridge National Laboratory
U.S. Department of Energy

NCCS User Featured in Chemistry Journal



As a result of research conducted using NCCS resources, the work of ORNL scientists is highlighted on the cover of *The Journal of Physical Chemistry C*.

Research Details

- ◆ Team led by ORNL researcher Bobby Sumpter
- ◆ Resolved the molecular structure of methane layers attaching to magnesium oxide
- ◆ Results hold promise for catalytic converters, chemical sensors, and hydrogen storage
- ◆ Significant cycles used on NCCS' Phoenix (Cray X1E)
- ◆ Results to be published in the January

High-School Researchers at ORNL Land National Honor

Three Oak Ridge High School seniors recently used NCCS supercomputers to improve the process for producing biofuel. As a result, they have also won a national math and science competition and a \$100,000 scholarship.



Oak Ridge High School students Scott Molony (left), Scott Horton, and Steven Arcangeli won the Grand Prize Scholarship at the 2006–2007 Siemens Competition in Math, Science and Technology.

Project Details

- **Winners of 2006–2007 Siemens Competition in Math, Science and Technology for work in the project “Data-Intensive Computing for Complex Biological Systems (BioPilot)”**
- **Worked intensively with senior ORNL research staff**
- **Program funded by Office of Advanced Scientific Computing Research and conducted through ORNL’s Computer Science and Mathematics Division**

Biologists Look to the Future

Researchers and computational scientists from across the country gathered at ORNL recently for an NCCS-sponsored workshop to discuss biological computer simulation in the age of petascale computing.

Topics covered:

- ▶ Simulations needed to achieve scientific breakthroughs
- ▶ Scalability of codes on next generation of high-performance computers
- ▶ Effect of petascale computing on biological computer simulation



Workshop participants



*Martin Karplus,
Harvard University*

“The community agrees that increasing computer power holds great promise for providing novel insights into the workings of biomolecular machines.”
Pratul Agarwal, Principal Investigator of the Leadership Computing Facility project *Next Generation Simulations in Biology: Investigating Biomolecular Structure, Dynamics, and Function through Multi-scale Modeling*.