

National Center for Computational Sciences Snapshot The week of December 18, 2006

Oak Ridge Research Surfaces on Cover of Chemistry Journal

Four Oak Ridge researchers using high-performance computers at the National Center for Computational Sciences (NCCS) and intricate beam lines to probe molecular layering have shed new light on surface interactions. Their results hold promise for such diverse applications as catalytic converters, chemical sensors, and hydrogen storage and have landed them on the cover of a prestigious chemistry journal.

Michael Drummond, Bobby Sumpter, William Shelton, and John Larese are the authors of “An Electronic Structure Investigation of Surface-Adsorbate and Adsorbate-Adsorbate Interactions in Multilayers of CH₄ on MgO(100).” The paper will be featured in January as the cover article in the *Journal of Physical Chemistry C*, a publication of the American Chemical Society that focuses on nanomaterials and surface science.

A simple diatomic mineral commonly extracted from rocks or seawater, magnesium oxide is an ideal “bedrock” upon which shear layers of hydrocarbons may be overlaid, molecule by molecule.

Surface-adsorbate interactions are important to multi-billion dollar industries, playing a key role in activities ranging from petrochemical production to water purification. However, while many of the products we use each day are made possible by these reactions, our understanding of the process at the molecular level is far from complete. A better understanding of simplified models translates into selective process design and increased industrial competitiveness.

The Oak Ridge researchers resolved the molecular structure of successive layers of methane as they attach to magnesium oxide. In the paper the authors reveal that the arrangement of methane molecules in the first layer is determined by their interaction with both the magnesium oxide and one another. The role played by the magnesium oxide, however, becomes progressively less important, and by the third layer—and presumably subsequent layers—it plays practically no role at all. Although this conclusion is seemingly straightforward, the theoretical and experimental approaches used to arrive at this result provide a clear way to evaluate other systems in which the interactions between the surface and its attached molecules are not so well behaved or understood.

The researchers were able to resolve the interactions using NCCS computing systems, primarily the Cray X1E known as Phoenix, but also the SGI Altix known as Ram.

“We’ve cleared it up, we think,” Sumpter said. “You have to be able to do a fairly high-level calculation, and that requires a reasonably good-sized computer to do these simulations.”

According to Sumpter, the collaboration began with Larese, an experimental physicist and neutron scientist at the University of Tennessee and with Oak Ridge National Laboratory's (ORNL's) Chemical Sciences Division.

“The initial project was trying to understand what he was seeing. That's typical: Theory and computation can do two things—we can try to understand an experiment, which happens a lot, or we can actually come up with a material and tell experimentalists that they should look into it.

“It's a feedback. Without both, it's interesting but not complete, because if you don't have the experiment, it's just a piece of computational theory. With experiment, it's really there.”

Biologists Look to the Future

Researchers and computational scientists from across the country gathered at ORNL recently to discuss biological computer simulation in the age of petascale computing.

The NCCS-sponsored workshop, entitled “Future of BioMolecular Simulations: From Ab Initio to Nano-molecular Machines,” allowed members of the biological sciences community—computational biochemists, biophysicists, and developers of biomolecular simulation codes, among others—to discuss the successes and challenges of a field working to take advantage of increasingly powerful computer systems. Attendees came from Harvard, Stanford, and New York universities, the San Diego Supercomputing Center, and a variety of other institutions.

As supercomputers housed at the NCCS continue to grow in power, the codes used in biological simulation must advance as well. According to ORNL staff member Pratul Agarwal, the December 11–12 workshop enabled researchers to identify and discuss the issues they will be facing, including a variety of software and development challenges.

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

“On one side, petascale computing will provide new insights by allowing simulations to reach longer time scales; on the other side, novel methods will allow petascale science to be performed using a number of tightly coupled runs.”

The NCCS will continue to sponsor domain-focused workshops in 2007, bringing together researchers to discuss current and future computational needs in computer architecture and software design. Potential topics include materials design, climate research, and nuclear energy simulations.

High-School Researchers at ORNL Land National Honor

Three Oak Ridge High School seniors recently used National Center for Computational Sciences (NCCS) supercomputers to improve the process for producing biofuel. As a consequence, they have also won a national math and science competition and pulled in a \$100,000 scholarship.

The students—Steven Arcangeli, Scott Horton, and Scott Molony — took the Grand Prize Scholarship at the 2006–2007 Siemens Competition in Math, Science and Technology for their work with ORNL researchers in the project “Data-Intensive Computing for Complex Biological Systems (BioPilot).”

The award grows out of a collaboration between the high school and Oak Ridge National Laboratory (ORNL). The students worked intensively in the BioPilot program with senior ORNL researchers Tatiana Karpinets, Hoony Park, Chris Symons, and Nagiza Samatova. The program is funded by Office of Advanced Scientific Computing Research and conducted through ORNL’s Computer Science and Mathematics Division.

The students worked full time at the lab through the summer of 2006 and about 1 day a week since mid-August. Along the way, their ORNL partners instructed them in the fundamentals of graph theory, statistical theory, systems biology, bioinformatics, artificial intelligence, and programming in C and C++. The students also presented research papers related to the project to members of their team.

The three were naturals as individuals and as a team.

“They are really bright,” said Samatova, who served as their mentor. “What really mattered, though, is that they really worked very nicely together as a team. They are all talented, but in a complementary way.”