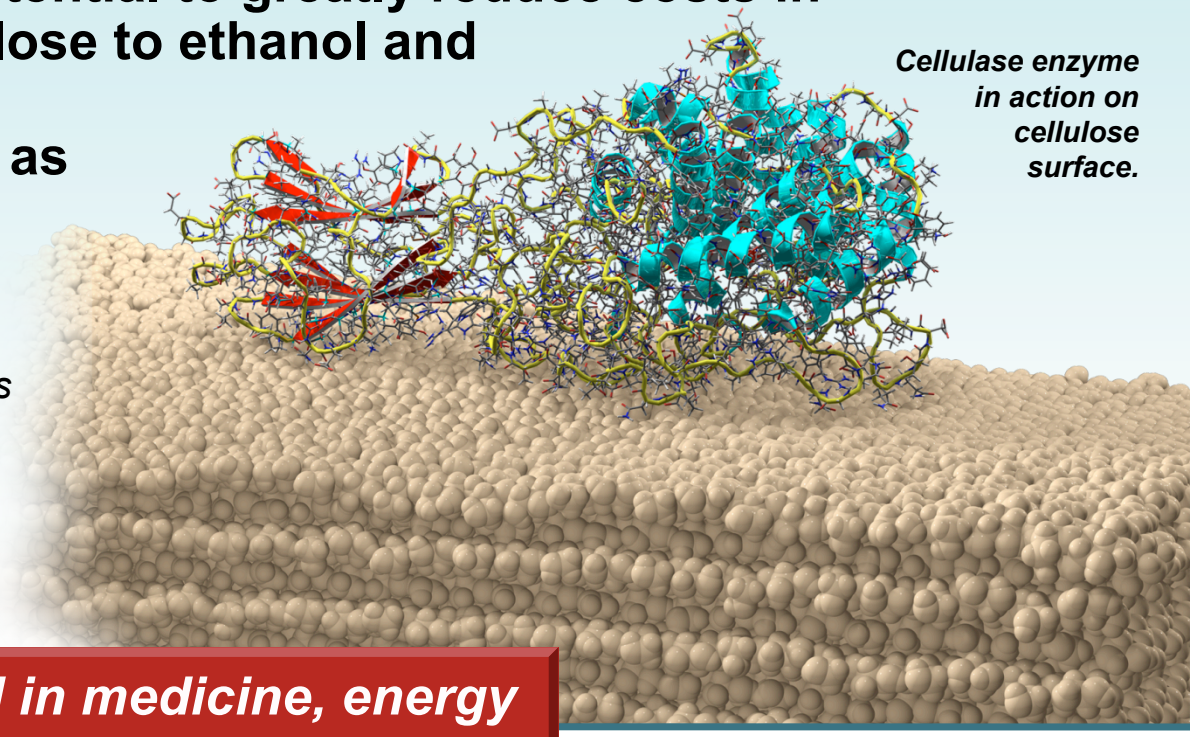
NCCS Snapshot
The Week of December 17, 2007

NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES

Oak Ridge National Laboratory
U.S. Department of Energy

Researchers at ORNL Solving Mysteries Behind Biomolecules

- **Recent biomolecular simulations on the NCCS's Jaguar supercomputer have produced major new insights into protein structure, dynamics, and functions.**
- **The research shows potential to greatly reduce costs in the conversion of cellulose to ethanol and in aiding treatment of various diseases, such as Alzheimer's and HIV**



Cellulase enzyme in action on cellulose surface.

"The implications of the fundamental understanding of biomolecular systems will be felt in many fields, including health and medicine, energy, and the environment."

Pratul Agarwal, ORNL, principal investigator for the project

Simulations show potential in medicine, energy

ORNL Hosts Computational Materials Workshop

Nardelli addresses the finer points of simulation

- **Dr. Marco Nardelli of North Carolina State University recently conducted a "Computational Materials Workshop" at ORNL**
- **The workshop, which addressed the simulation and modeling of nanostructures, was held December 10-14**
- **Besides lectures focusing on the latest research in nanoscale physics and engineering, the workshop featured hands-on exercises and simulation**

"It was a lot of work, but I am very pleased overall."

Marco Nardelli, associate professor of physics at NCSU and workshop organizer

ORNL Attends TeraGrid Workshop

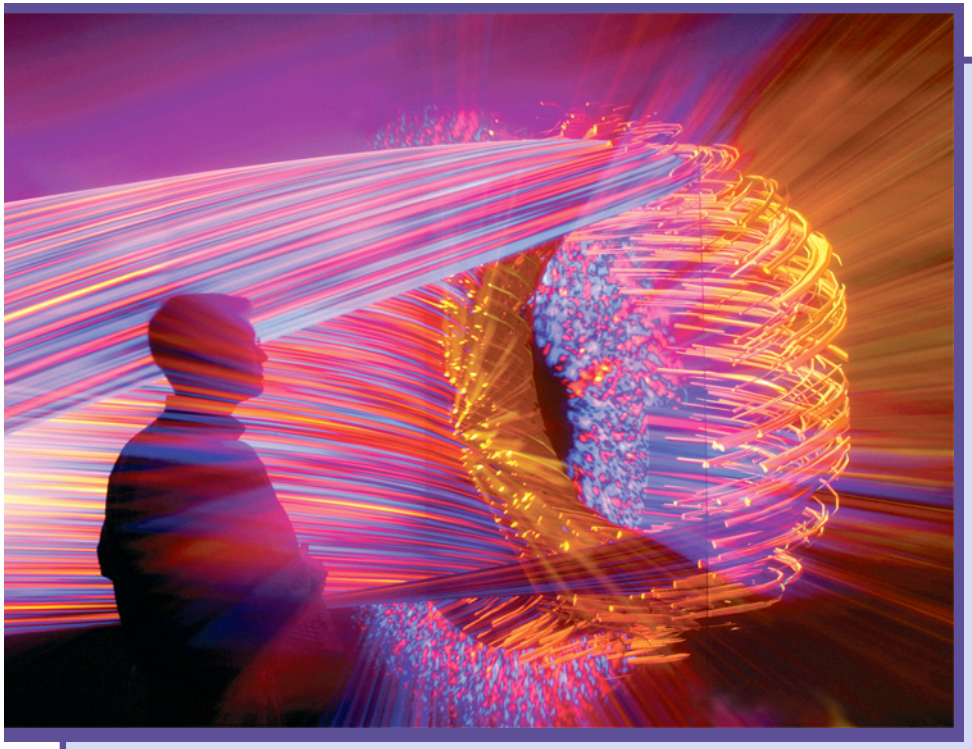
"Petascale application developers and petascale tool developers had the opportunity to get together and share expectations, plans, and needs."

Don Frederick, NCCS User Assistance and Outreach group and workshop attendee

- **A contingent from ORNL recently participated in a petascale preparation workshop at Arizona State University**
- **The workshop, titled "Building PetaScale Applications and Software Environments on TeraGrid," featured a series of presentations on algorithms, techniques, and performance tools for petascale computing**
- **Two ORNL researchers, Bronson Messer and Ricky Kendall, gave presentations**

National Science Foundation prepares for petascale at ASU

ORNL Hosts CPES Workshop



Visualization showing the structure of electrostatic potential in a three-dimensional simulation of plasma microturbulence in a fusion reactor.

- **Members of the Center for Plasma Edge Simulation (CPES) met at ORNL on December 3 and 4 for a comprehensive workshop**
- **The team is steadily uncovering the mysteries surrounding plasma edge research, a vexing field of fusion science**

The administrative support from ORNL was excellent, which includes the visitor badge arrangement, busing, food, remote participations, and projector handling."

C.S. Chang, New York University, CPES team leader

Scientists present latest breakthroughs in plasma edge research

Seminar Series Investigates New HPC Platform

Exploring LANL's Roadrunner at ORNL

- **ORNL recently hosted a seminar entitled "Early Experiences in Hybrid Computing" on a new high-performance computing platform at Los Alamos National Laboratory**
- **The seminar outlined early experiences and results of science applications on the new platform, dubbed Roadrunner**
- **The new platform will consist of general purpose processors and hardware accelerators based on the Playstation 3 video game console**

"Success will require both the development of software tools and a rethinking of current algorithmic and code development approaches and practices."

John A. Turner, LANL, computational physics group leader and seminar lecturer