

# **NCCS Snapshot**

## **The Week of March 24, 2008**

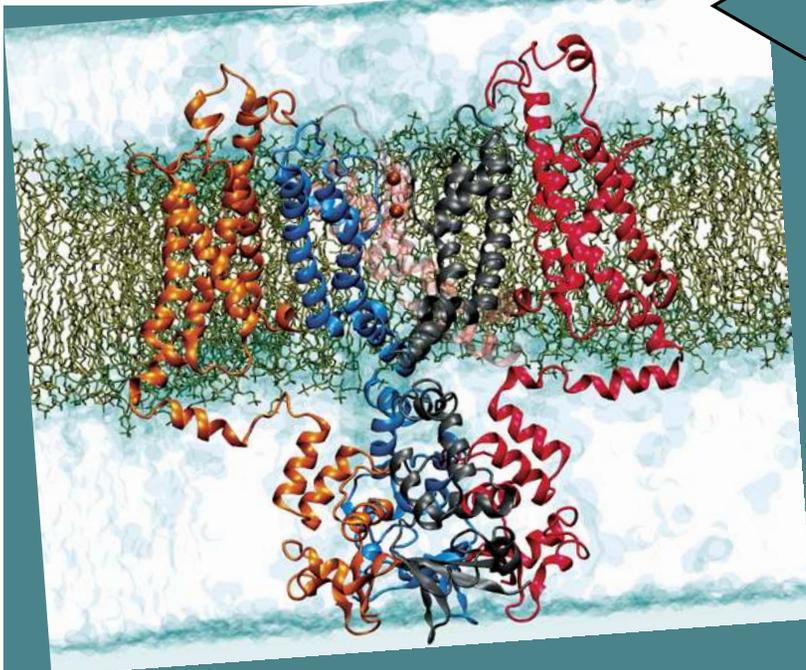
**NATIONAL CENTER**  
FOR COMPUTATIONAL SCIENCES



Oak Ridge National Laboratory  
U.S. Department of Energy

# Scientists Use NCCS to Model Potassium Channel

*Supercomputers to reveal in atomistic detail all steps from open to closed ion channel*



Researchers use NCCS supercomputers to illuminate the workings of the voltage-gated potassium channel, simulated here in its open state in a membrane environment.

- Scientists are using NCCS resources to simulate in unprecedented detail the voltage-gated potassium channel
- The channel is a membrane protein that responds to spikes of electricity by changing shape to allow potassium ions to enter a cell
- If the switch operates normally, the potassium channel opens when activated and closes when resting—but if gating malfunctions, cardiovascular or neurological disease can result

*“The study will serve as a future road map for simulating, visualizing, and elucidating the workings of molecular nanomachines.”*

Professor Benoît Roux, Argonne National Laboratory and the University of Chicago

# ORNL Offers HPC to Universities



*Laboratory to open supercomputing facilities to students, faculty*

- ORNL will grant access to its supercomputing systems to university students and faculty through a collaborative program with Oak Ridge Associated Universities (ORAU)
- Two grants will be awarded each year, with each recipient team receiving \$75,000 for three years
- The laboratory will make available its leading computer systems, relevant staff, and possibly other necessary resources to those teams that receive grants

*"We all become stronger if we can bring the best of what the lab has to offer coupled with the best of what the university community has to offer."*

**Thomas Zacharia, Associate Laboratory Director, ORNL Computing and Computational Sciences Directorate**



# NCCS Alters HPSS Storage System

## *New system dubbed Site-Style*

- The NCCS has modified the accounting system to its High Performance Storage System (HPSS), allowing users to separate data by specific projects
- As usage of HPSS space increases over time, Site-Style will enable the NCCS to better determine which projects need additional space
- The team that oversaw the transition was made up of NCCS staff members Vicky White, Mitchell Griffith, Chris Fuson, Jason Hill, and Bill Renaud

*“The principal investigators can actually monitor what users are storing, such as the number of files and the amount of data.”*

Mitchell Griffith, NCCS staff member

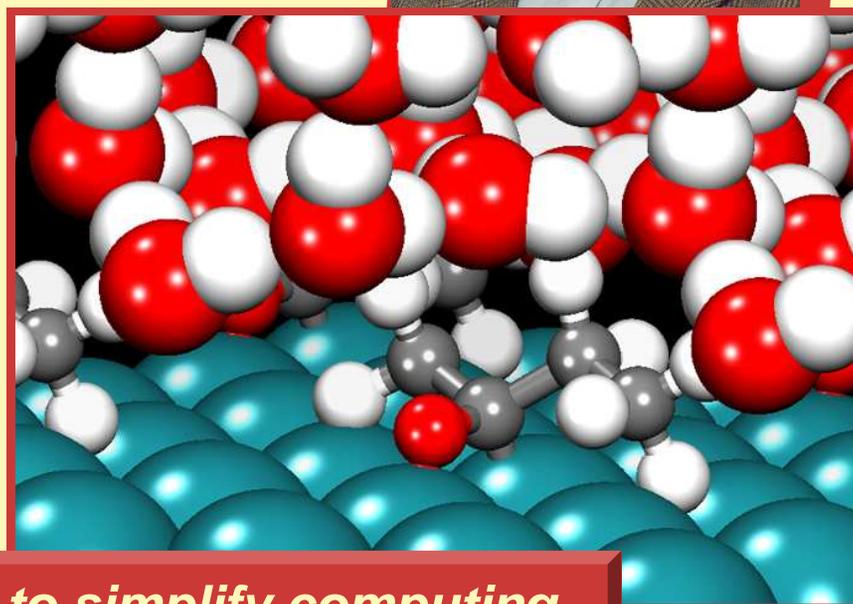
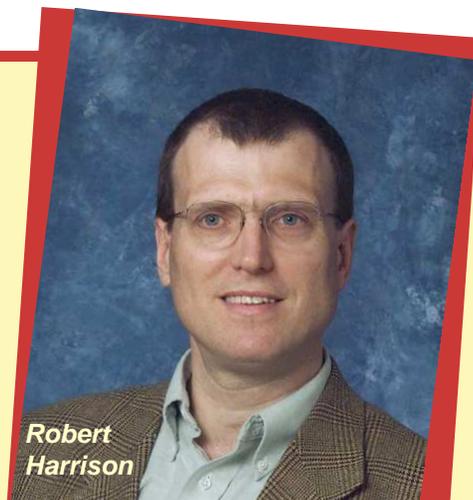


# MADNESS opens the door to parallel worlds

*“MADNESS [Multiresolution ADaptive Numerical Environment for Scientific Simulation] takes over much of the responsibility of scheduling and even placement of computation.”*

Robert Harrison, ORNL Computational Chemist

- **MADNESS provides fast numerical computation in many dimensions with guaranteed precision. It provides a very high-level programming interface while striving to express essentially all available parallelism**
- **The NCCS Seminar Series featured ORNL chemist Harrison discussing MADNESS and emerging applications in chemistry, molecular physics, and nuclear physics that are built within the framework**



*Programming environment to simplify computing*