

NCCS Snapshot

The Week of September 24, 2007

NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES



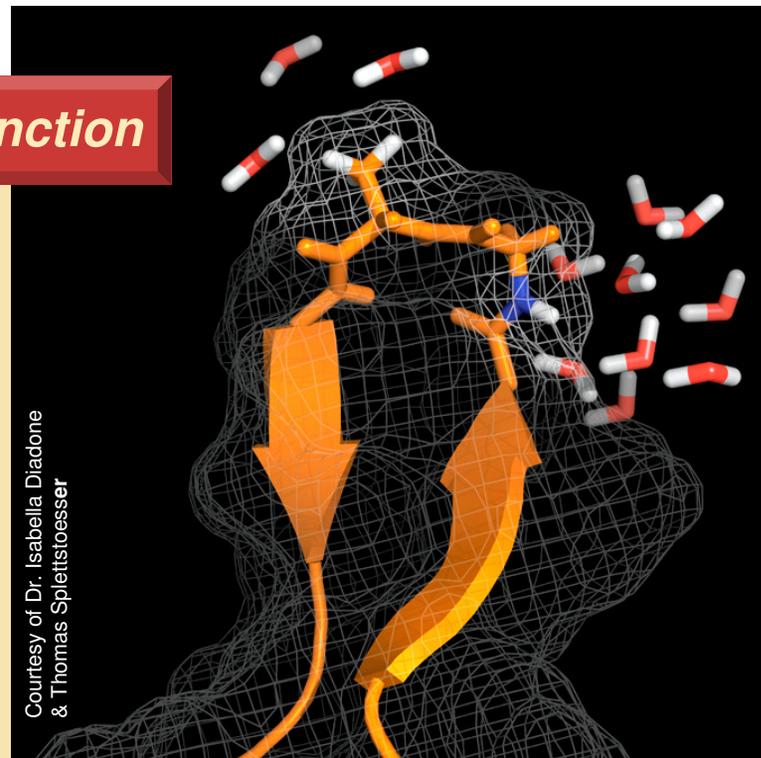
Oak Ridge National Laboratory
U.S. Department of Energy

Simulation Helps Unlock the Secrets of Protein Folding

Water determines shape, shape determines function

- Proteins are the workhorses of the body; they fight infections, turn food into energy, copy DNA, and catalyze chemical reactions
- The function of a protein is determined by its shape, which researchers now think may be a reaction to contact with water
- Once more fully understood, the research applications range from rational drug design to useful functions in nanotechnology and bioenergy

“Understanding the mechanism by which proteins fold up into unique three-dimensional architectures is a holy grail in molecular biology.” – Jeremy Smith, Oak Ridge National Laboratory



Courtesy of Dr. Isabella Diadone
& Thomas Splettoesser

Simulation model of a peptide surrounded by V-shaped, red-and-white water molecules. How the water hydrates the peptide is found to decide the shape the peptide adopts.

Legislators Learn How HPC Contributes to Competitiveness

- ▶ Senator Lamar Alexander and Congressmen Zach Wamp and Bart Gordan visited the NCCS on August 30 to see how the organization is advancing the legislation “America COMPETES” (Creating Opportunities to Meaningfully Promote Excellence in Technology, Education, and Science)



- ▶ Sean Ahern, visualization lead for the NCCS Scientific Computing Group, discussed several projects at the NCCS, including alternative energy and medical research, which advance the “America COMPETES” mission

Sean Ahern, left, demonstrates the EVEREST PowerWall for (L to R) Oak Ridge Operations Manager Gerald Boyd, ORNL Director Thom Mason, Congressman Zach Wamp, and Senator Lamar Alexander.

NCCS research exemplifies “America COMPETES”

NCCS Boosting Power to Building for Petascale System

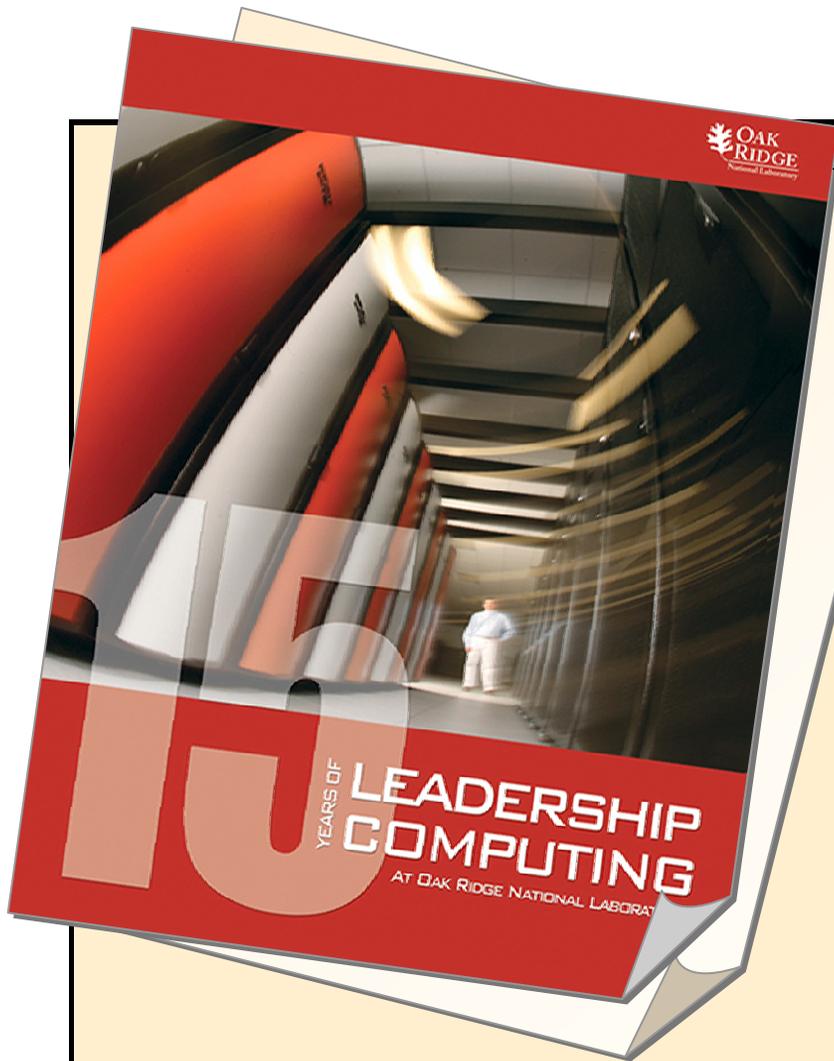
Power doubled to accommodate new supercomputer

- NCCS is doubling the power available to its computer room in anticipation of the world's first petascale supercomputer
- The added power from the Tennessee Valley Authority, which will be available in December 2007, is necessary because the Cray "Baker" supercomputer, which will have a peak performance of more than 1,000 trillion calculations a second (1 petaflop), will itself require more than 6 megawatts of power

Workers unload a generator that will help to increase power at the NCCS from 7.3 to 14 megawatts



NCCS Publication Wins Design Award



Award is one of many for ORNL, designers

- ◆ A promotional publication from the NCCS recently won an American Graphic Design Award
- ◆ The promotional magazine, entitled “15 Years of Leadership Computing,” chronicled the history of supercomputing at ORNL from 1992 to the NCCS’s current status as one of the top high-performance computing centers in the world