

# **NCCS Snapshot**

## **The Week of September 10, 2007**

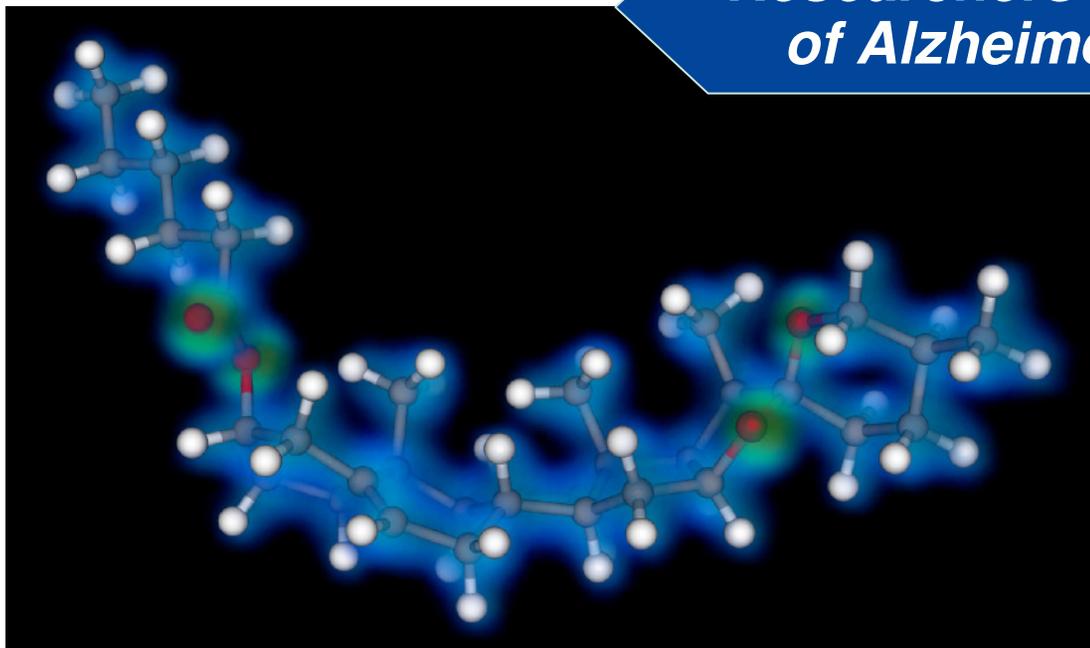
**NATIONAL CENTER**  
FOR COMPUTATIONAL SCIENCES



Oak Ridge National Laboratory  
U.S. Department of Energy

# Next-Generation Pharmaceuticals Fight Brain Theft

*Researchers explore the effectiveness of Alzheimer's drugs mechanisms*



*The model shows a quantum mechanical orbital calculation for a drug used in the simulation.*

*"Hopefully this method will become more widespread in industry and lead to better drug design."*

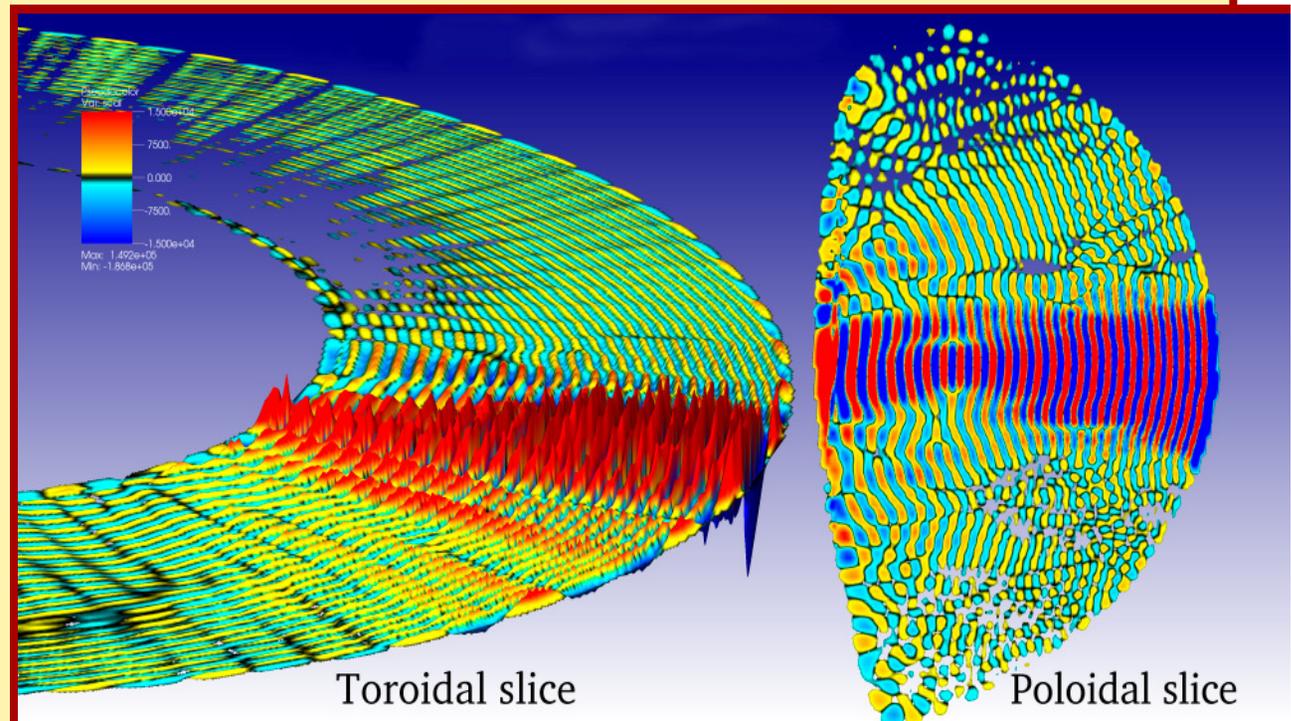
**Phil LoCascio, Oak Ridge National Laboratory**

- **ORNL's Ed Uberbacher and colleagues use the Cray XT4 Jaguar supercomputer and other systems to discover the mechanisms by which a new type of Alzheimer's drug may stop the progression of plaque formation and disassemble the fibrils that make up the plaques**

# Radio Waves Are Hot Enough for ITER

- Radio waves will heat ITER plasma ten times hotter than the sun
- Experiments on smaller reactors suggested radio wave heating might not work
- Jaguar simulations allay fears, verify that radio-wave heating should work on ITER

AORSA ITER Simulation  
of RF Heating



*Fusion researcher shows that when it comes to heating plasma, bigger is better*

# NCCS Experts Address How HPC Enables Scientific Discovery

*Kothe and Whitten reach out to public and policymakers in 2007*



*Doug Kothe*

- Science Director Doug Kothe speaks at DOE's Energy Efficiency and Renewable Energy program office in Washington, D.C.
- Senior User Support Specialist Bobby Whitten delivers his fifth talk of the year, to Knoxville's Sertoma service club

*"It's important for the public to know that we do what we do so we can keep America competitive and that there are advantages locally, regionally, nationally, and globally."*

**Robert M. Whitten, National Center for Computational Sciences**



*Bobby Whitten*