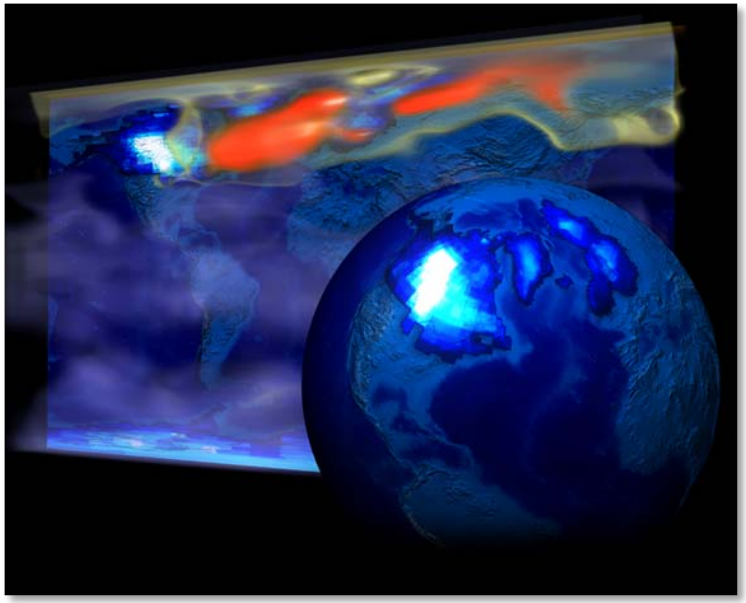
For the Week of July 20th,2009

Oak Ridge Supercomputers Provide First Simulation of Abrupt Climate Change

Researchers use 'Phoenix' and 'Jaguar' to study climate's past and future

- ORNL's Jaguar, the world's fastest supercomputer for open science, is simulating abrupt climate change and shedding light on a period of natural global warming in Earth's relatively recent history.
- The work, led by scientists at the University of Wisconsin and the National Center for Atmospheric Research is featured in the July 17 issue of the journal *Science*.
- The data from these simulations may soon find their way into IPCC's data repository and reports as we struggle to understand our effect on the Earth's climate.



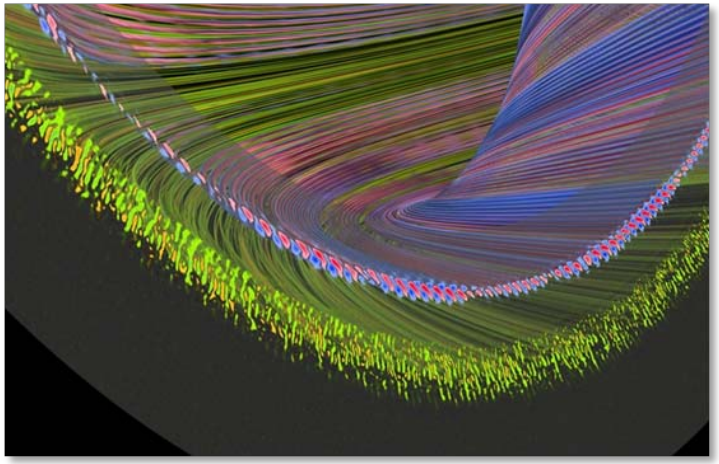
Simulations show deglaciation during the Bølling-Allerød, Earth's most recent period of natural global warming.
Image credit: Jamison Daniel, National Center for Computational Sciences

"Our simulation is an important step in assessing the likelihood of predicted abrupt climate changes in the future because it provides a rigorous test of our model against the major abrupt changes observed in the recent past." – Co-principal Investigator Zhengyu Liu

Fusion Gets Faster

New optimizations, enhanced I/O increase speed of GTC by more than 100 percent

- Thanks to the OLCF's Scott Klasky and a diverse team of collaborators, the fusion code GTC recently became twice as fast on the center's Jaguar supercomputer.
- These advances are the result of software enhancements by Cray Inc. and a combined team effort of physicists, vendors, and computational scientists from numerous organizations.
- The various technical improvements include a new Cray compiler, optimizations to the code itself, and further I/O enhancements to ADIOS—an I/O middleware package created by Klasky and collaborators at Georgia Tech and Rutgers.



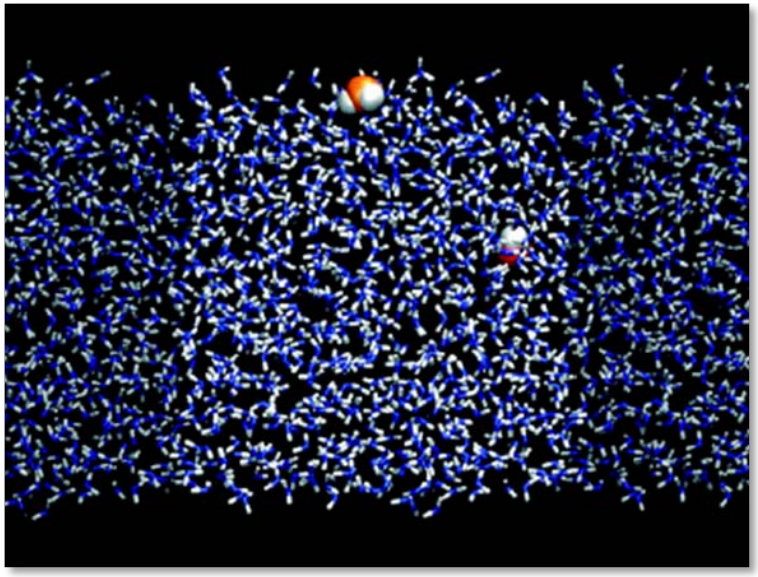
Researchers are using Jaguar to perform the largest fusion simulations in history. The image above is from a plasma microturbulence simulation experiment using resources of the OLCF. Image credit: Chris Ho, Chad Jones, and Kwan-Liu Ma of UC Davis and the SciDAC Institute for Ultrascale Visualization.

"In order to advance the science, collaboration is essential. High-performance computing is more than benchmark numbers; it is about advancing scientific breakthroughs and that is accomplished by achieving high performance from both the code and the computing system [Jaguar]."
– Zhihong Lin of UC–Irvine

Supercomputing Charts Unfamiliar Waters

Simulations explore the air–water interface

- Christopher Mundy, a physical chemist at PNNL and Doug Tobias, a chemistry professor at the UC–Irvine, are exploring the mysteries of aqueous interfaces on OLCF's Jaguar supercomputer.
- The interface is the world of unknowns that lies between water and air and is commonly known to have a dramatically different electronic structure than bulk water.
- With their remaining computer time, the team members hope to create a consistent picture of the chemistry and thermodynamics present in aqueous interfacial systems.



INCITE researchers are using their allocation on the Cray XT Jaguar to study the interface of water and air.
Image courtesy: Christopher Mundy, Pacific Northwest National Laboratory

"We want to characterize the system both structurally and thermodynamically and compare it to experimental measurements. We can then begin to explain, with greater confidence, specific reaction mechanisms that are important for many chemical processes used in industry."
– Principal Investigator Christopher Mundy