NCCS Snapshot The Week of January 26, 2009

Oak Ridge Leadership Computing Facility





ORNL's Petaflop Jaguar Completes Acceptance Testing Most powerful scientific computer

- The petascale upgrade to ORNL's *already tackling critical challenges* Jaguar supercomputer has completed acceptance testing
- A rigorous acceptance test of functionality, performance, and stability shows that Jaguar is the world's most powerful tool for computational science
- At a peak performance of 1.6 petaflops and with two applications over 1 petaflop, Jaguar is the world's most powerful computer



NCCS Announces Early Petascale Applications



Plan view of structure & charge density of water on a titanium dioxide surface from large scale ab initio molecular dynamics calculations. (Courtesy Paul Kent, ORNL, and Jorge Sofo, Penn State Univ.) **Pioneering science will put Jaguar to the test**

- At a peak performance of 1.6 petaflops and with two applications over 1 petaflop, Jaguar is the world's most powerful computer
- To test the mettle of the new system, ORNL has granted early access to a number of projects that can utilize a majority of the machine
- Pioneering research applications, scheduled to run until mid-2009, will push computational science to new limits, prepping Jaguar for the nearly 40 upcoming INCITE projects

"We expect these projects to deliver important results . . . early simulations on Jaguar will also help us harden the system for a broader collection of projects later in the year." Doug Kothe, NCCS Director of Science



Tracking CFC's in a Global Eddying Ocean Model

- Oceans play a critical role in the earth's balance of heat, water, and chemicals such as CO₂ and chlorofluorocarbons (CFCs)
- Using Jaguar, researchers have for the first time carried out a global eddy resolving model that has run a 100-year simulation
- The model carried not only CFCs, but also a host of other tracers that yielded valuable information about ocean ventilation pathways and timescales



First-ever 100-year simulation of the ocean at a fine enough scale to include the relatively small, circular currents known as eddies.

"This will help researchers better understand the role of the ocean in uptake and redistribution of gases such as anthropogenic (man-made) CO₂." Synte Peacock, principal investigator

Ocean ventilation provides clues to climate change

4 Managed by UT-Battelle for the U.S. Department of Energy



ORNL Hosts Online HPC Classes

Top: ORNL Director Thom Mason addresses class attendees. Bottom: DOE Oak Ridge Operations Assistant Manager for Science Johnny Moore with faculty and students.



Lab begins relationship with four new institutions

- ORNL is offering a high-performance scientific computing class to four historically black colleges and universities
- Attending the classes are students and faculty from Morehouse College, Knoxville College, Claflin University, and Jackson State University
- The survey course, featuring about 25 students and



faculty, will meet twice a week via atellite at ORNL. There they will learn the basics of using the system, arallel programming, model design, and visualization

"It's our expectation that this will give us the sort of scientific workforce we need to meet the challenges of the 21st century." **ORNL Director Thom Mason**



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