

# **NCCS Snapshot**

## **The Week of March 10, 2008**

**NATIONAL CENTER**  
FOR COMPUTATIONAL SCIENCES



Oak Ridge National Laboratory  
U.S. Department of Energy

# Big Machines Model Small Wonders

## NCCS Supercomputers shed light on nanotechnology



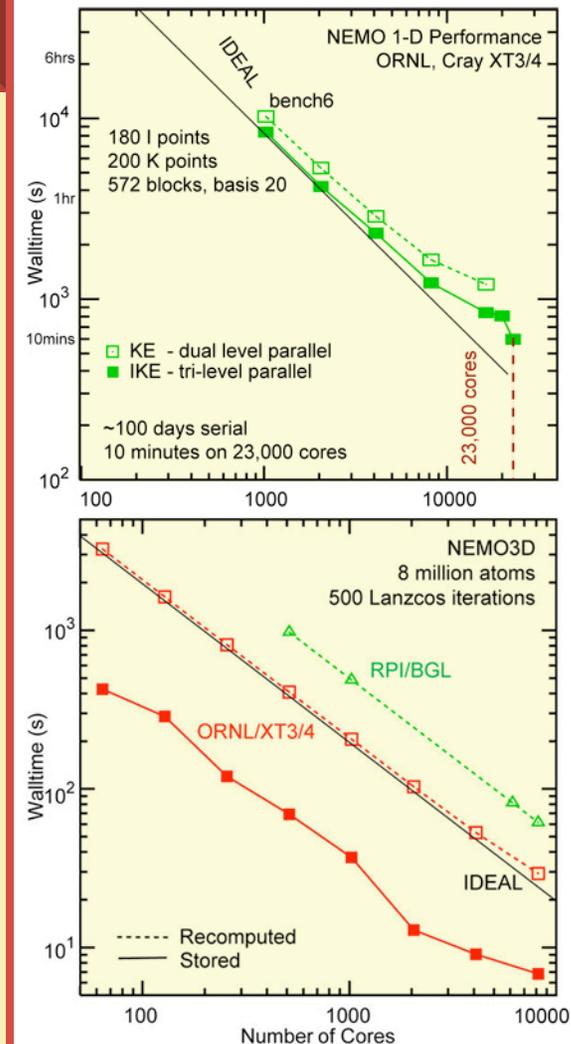
Gerhard Klimeck

- Dr. Gerhard Klimeck is using NCCS supercomputers to perform cutting edge nanoelectronic simulations, making devices smaller and faster.
- Klimeck's NEMO (nanoelectronic modeling) 3D code has scaled extremely well on the NCCS's Jaguar – so well in fact, that Klimeck used it to bolster his case for a PetaApps award.

- His NEMO 1D code, when scaled to 23,000 cores, did in ten minutes what would have taken a serial machine 100 days

*“For real device engineering, you need turnaround that happens in a few minutes, to try different ideas, concepts, and trend analysis rapidly.”*

Gerhard Klimeck, NCCS investigator



# HPCWire Interviews Doug Kothe



## NCCS Director of Science waxes petascale



- ◆ **HPCwire** contributing editor Steve Conway recently interviewed NCCS Director of Science Doug Kothe about petascale computing.
- ◆ Kothe discussed an NCCS survey used to gauge the needs and capabilities of researchers wishing to use petascale computing systems.
- ◆ “Petascale systems will greatly enhance research but bring with them numerous technical challenges,” Kothe says.

*“HPC centers will collaborate to optimally map the applications to the platform and continue to work with the researchers and vendors to ensure that the science demands of today and the future are met with leadership computing resources.”*

Doug Kothe, NCCS Director of Science



# What a Long, Strange Trip It's Been

- On February 22, Bobby Whitten of the National Center for Computational Sciences (NCCS) was the speaker at the University of Tennessee (UT) Science Forum.
- The presentation was divided into two parts: the history of the lab and the NCCS and the possible future impact of supercomputing.



*"The UT Science Forum was an outstanding venue to share ORNL's rich scientific research history. It was my pleasure to be a part of the forum as a representative of the NCCS."*

**Bobby Whitten, NCCS researcher**

***NCCS researcher tells history of ORNL***