

# NCCS Snapshot

## The Week of November 17, 2008

NATIONAL CENTER  
FOR COMPUTATIONAL SCIENCES



Oak Ridge National Laboratory  
U.S. Department of Energy

# Oak Ridge Supercomputer is World's Fastest for Science

*Jaguar breaks petascale barrier*

- A Cray XT high-performance computing system at ORNL is the world's fastest supercomputer for science
- The Cray XT, called Jaguar, has a peak performance of 1.64 petaflops per second, incorporating 1.382 petaflops XT5 and 266 teraflops XT4 systems
- In a matter of a few days, Jaguar has already run scientific applications ranging from materials to combustion on the entire system

*"This accomplishment is the culmination of our vision to regain leadership in high-performance computing and harness its potential for scientific investigation."*

Raymond L. Orbach,  
Undersecretary for Science  
for the Department of Energy

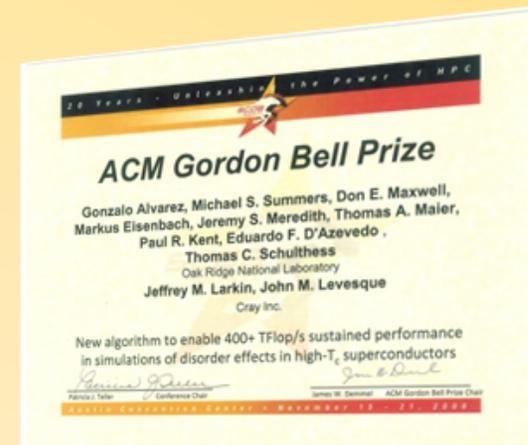


# ORNL supercomputer simulation wins prize for fastest-running science application

*Materials simulation breaks 1.3 petaflops*



- A team led by ORNL's Thomas Schulthess received the prestigious 2008 Association for Computing Machinery (ACM) Gordon Bell Prize at SC08.
- The award was given to the team for attaining the fastest performance ever in a scientific supercomputing application.
- The team achieved 1.352 petaflops on ORNL's Cray XT Jaguar supercomputer with a simulation of superconductors.
- By modifying the algorithms and software design of the DCA++ code, the team was able to boost its performance tenfold with the help of Cray Inc.



# Library of Flames Illuminates Design of Advanced Combustion Devices

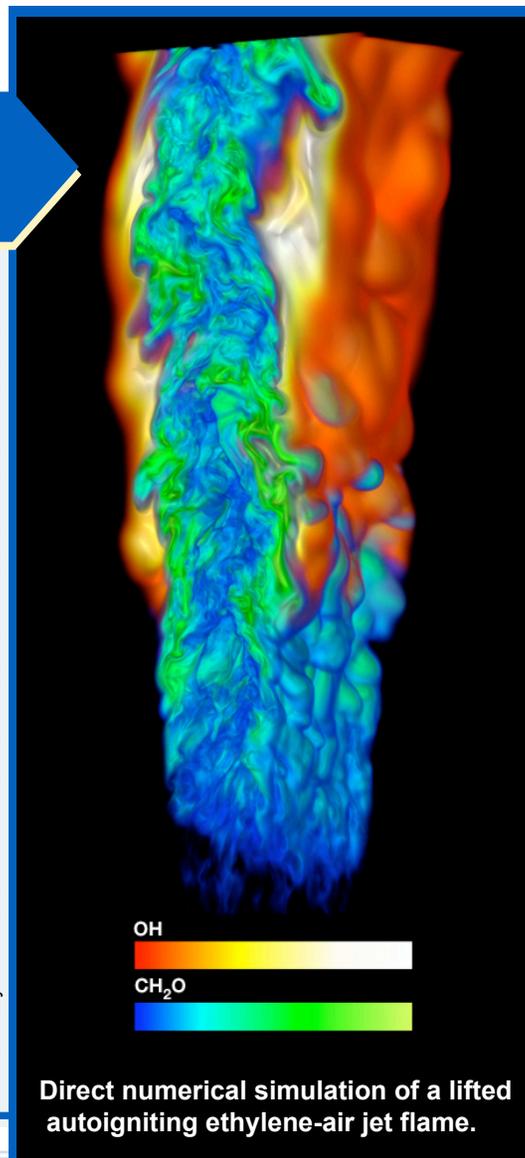
*Next-generation engines and industrial burners may use less fuel, emit fewer pollutants*

- Supercomputers at the NCCS are hastening the arrival of advanced combustion devices that will consume less energy and emit fewer pollutants
- The result is a library of science data that captures complex aero-thermo-chemical interactions and provides insight into how flames stabilize, extinguish, and reignite
- These libraries will assist in the design of next-generation combustion devices burning alternative fuels

*“If low-temperature compression ignition concepts employing dilute fuel mixtures at high pressure are widely adopted in next-generation autos, fuel efficiency could increase by as much as 25 to 50 percent.”*

**Jackie Chen, Project Principal Investigator**

Courtesy H. Yu of SNL and K. L. Ma of SciDAC Institute for Ultrascale Visualization.

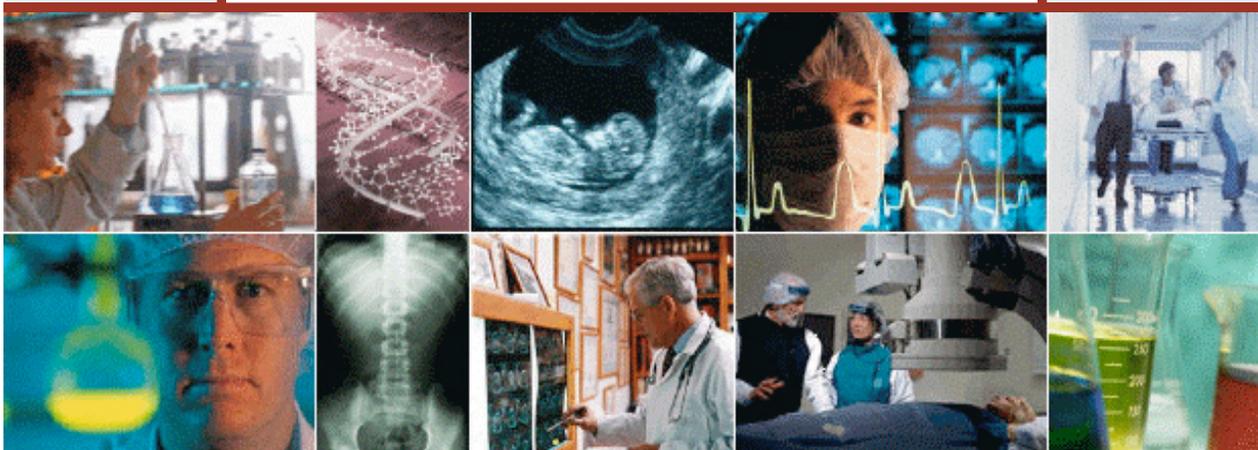


# ORNL, GUMC Ink Formal Collaboration

- A recently established partnership between ORNL and Georgetown University Medical Center (GUMC) will help researchers battle diseases such as cancer
- ORNL hosts the world's most powerful computing complex, while GUMC is a leading biomedical research facility and is one of America's

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Georgetown UNIVERSITY MEDICAL CENTER



- comprehensive cancer centers
- The partnership will give GUMC researchers access to ORNL's leading supercomputing systems and ORNL expertise in protein and drug modeling

*New relationship lends supercomputing resources to biological research*

# Cray Workshop Promotes Supercomputing Skills

- More than 24 computational scientists gathered recently at ORNL to hone their Cray XT4 and XT5 supercomputer skills and share tips and experiences
- The 2008 Cray XT Quad-core Workshop was held at ORNL October 15-17, and was co-sponsored by NICS and the NCCS.
- The workshop featured hands-on sessions to help users make the most of ORNL's two Cray XT supercomputers and talks on a range of issues important to users



*Researchers gather to work with experts from ORNL and vendors*