

# Leadership Computing Facility Status and Plans

Presented at the  
**Scientific Impacts and  
Opportunities in Computing  
Workshop**

Buddy Bland

**January 10, 2008  
Maui, Hawaii**



# National Center for Computational Sciences Oak Ridge National Laboratory

- Leadership Computing Facility provides the most powerful open science systems in the world for government, academia, and industry
- Focuses on a small number of important applications that need the full size of these systems to solve time-sensitive problems

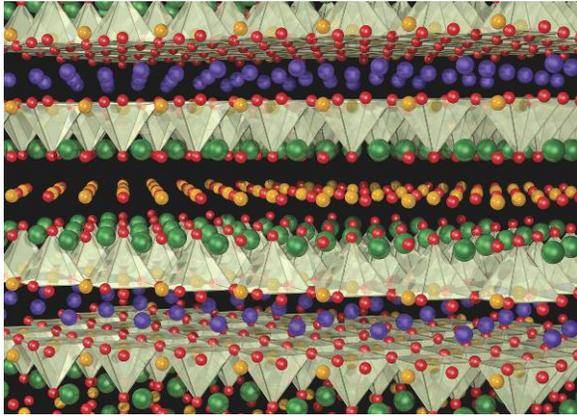


# National Center for Computational Sciences

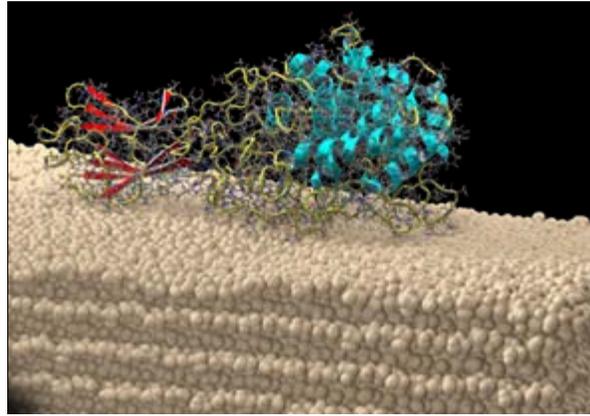
- Delivered a series of increasingly powerful and diverse set of computer systems beginning with the KSR, Intel Paragon, Compaq Alphaserver, IBM Power3 and Power4, SGI Altix, Cray X1, XT3, and XT4
- **Worked directly with application teams to port, scale, and tune codes with great success going from 100s to 10s of thousands of processors**
- **Delivered 80% of cycles for DOE INCITE Program in 2007. Will more than double the number of hours in 2008.**
- **First DOE lab with cyber security program accredited at the moderate level of controls, allowing export controlled and proprietary work**



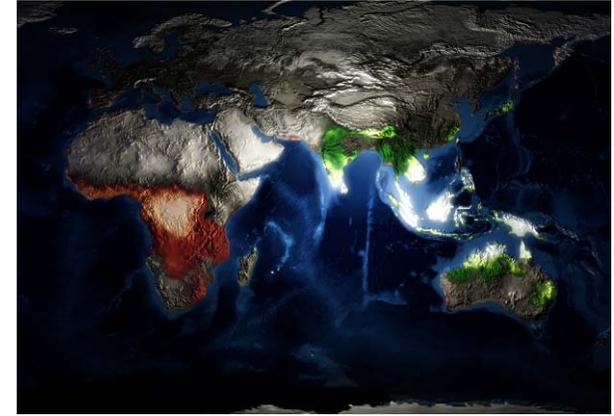
# We are advancing scientific discovery



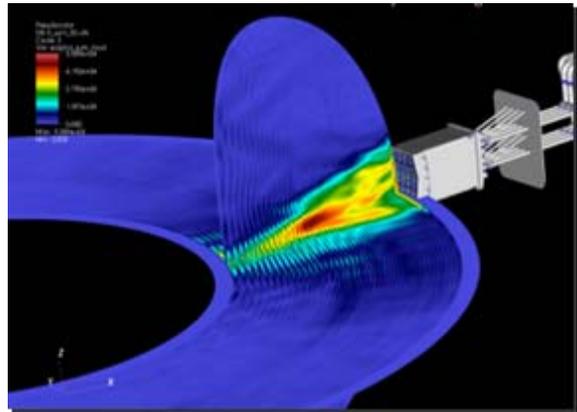
Resolved decades-long controversy about modeling physics of high temperature superconducting cuprates



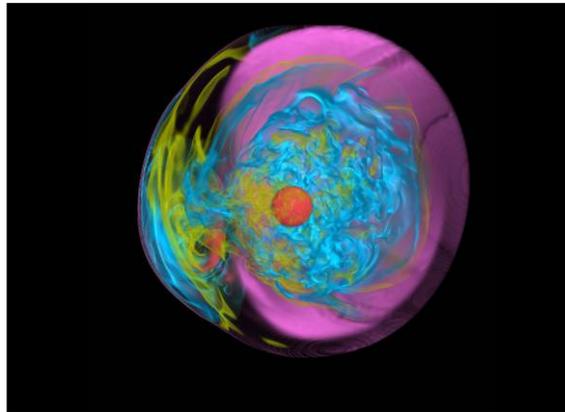
New insights into protein structure and function leading to better understanding of cellulose-to-ethanol conversion



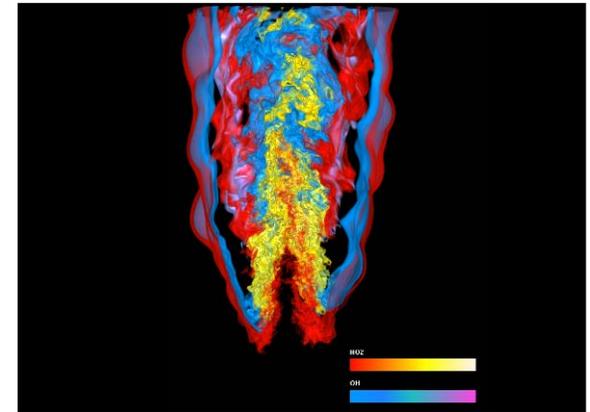
Addition of vegetation models in climate code for global, dynamic CO<sub>2</sub> exploration



First fully 3D plasma simulations shed new light on engineering superheated ionic gas in ITER



Fundamental instability of supernova shocks discovered directly through simulation



First 3-D simulation of flame that resolves chemical composition, temperature, and flow

# Jaguar: 119 TF Cray XT4 being upgraded to 250+ TF

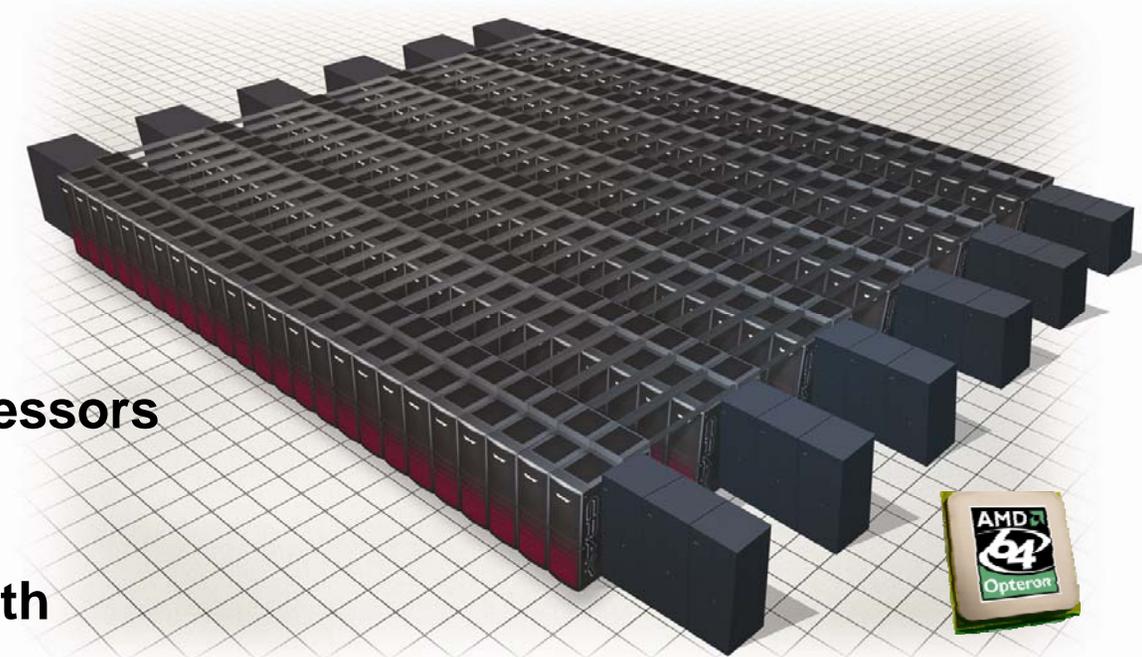
- **We are in the process of upgrading Jaguar from dual-core to quad-core Opteron processors**
- **Linux Operating System**



Compute Processors	7,832
Memory / Core	2 GB
System Memory	62 TB
Disk Bandwidth	41 GB/s
Disk Space	900 TB
Node Size	4-core, 35 GF

# 1 Petaflops System - Cray "Baker"

## FY 2009: Cray "Baker"

- 1 Petaflops system
  - 38 GigaFlops processor
  - 27,000+ Quad-core processors
  - 2 GB per core
  - 200+ GB/s Disk bandwidth
  - Dual-socket 8-core SMP "nodes" with 16 GB
  - 6.5 MW system power
  - 144 Cabinets, 3,220 ft<sup>2</sup>
- 
- Phase-0 of HPCS "Cascade" program
    - Liquid cooled
    - Linux Operating system with support for heterogeneous processors
    - Gemini interconnect

# Storage for an avalanche of data

## *Center wide shared file systems*

- “Spider” will be available later this year to provide a shared, parallel file system for all LCF systems
  - Based on Lustre file system
- Planned bandwidth of over 200 GB/s with multi-petabytes (8-12 PB) of capacity
- HPSS provides archival storage for all system
- HPSS has been upgraded with two additional tape libraries to add additional capacity and bandwidth



# Visualization and Data Analytics

## Visualization

Once users have completed their runs, the Visualization task group helps them make sense of the sometimes overwhelming amount of information they generate.

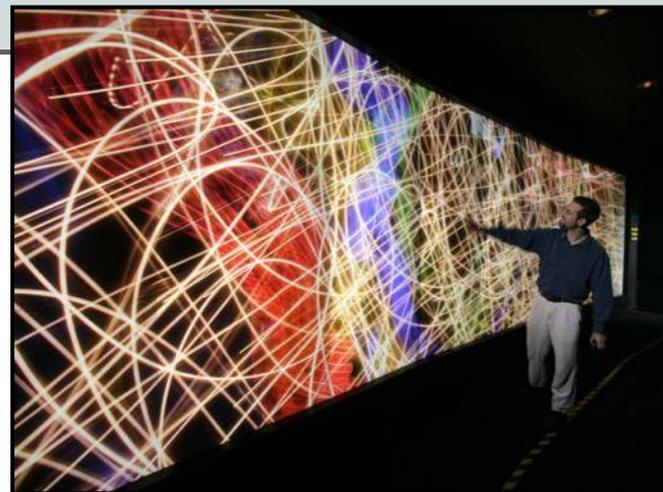
- Viewing at a 30'x8' PowerWall
- Upgraded cluster with GPUs for remote visualization



## End-to-End Solutions

Researchers must analyze, organize, and transfer an enormous quantity of data. The End-to-End task group streamlines the work flow for system users so that their time is not eaten up by slow and repetitive chores.

- Automate routine activities, ex. job monitoring at multiple sites
- Data Analysis



Visit us at: <http://nccs.gov>

Contact us at: [help@nccs.gov](mailto:help@nccs.gov)

Questions?

Buddy Bland

[BlandAS@ornl.gov](mailto:BlandAS@ornl.gov)

865-576-6727