The National Center for Computational Sciences at Oak Ridge National Laboratory

Douglas B. Kothe

Director of Science

Leadership Computing Facility
National Center for Computational Sciences
Oak Ridge National Laboratory

Leadership Computing Facility Mission

Our mission is to enable breakthrough science by fielding the most powerful capability computers for scientific research; building the required infrastructure to facilitate user access to these computers; working with the DOE to select a few time-sensitive problems of national importance that can take advantage of these systems; and joining forces with these teams to deliver breakthrough science.

LCF Computer Systems

Jaguar: Cray XT4 – 119 TF

- # 7 on Nov 2007
- 11,706 Dual-core Opterons
- 46 TB memory (2 GB/core)

Phoenix: Cray X1E – 18 TF

- Largest Cray vector system in the world
- 1,024 vector processors
- 2 TB shared memory

The Jaguar Cray XT4 Leadership System

Today

- 11,508 compute nodes
  - 2.6 GHz dual-core AMD Opteron processors with 4 GB memory
  - 23,016 compute cores
- 396 service & I/O nodes
- ~750 TB local storage
- 3D Torus interconnect
- 46 TB aggregate memory
- 119 TF peak performance

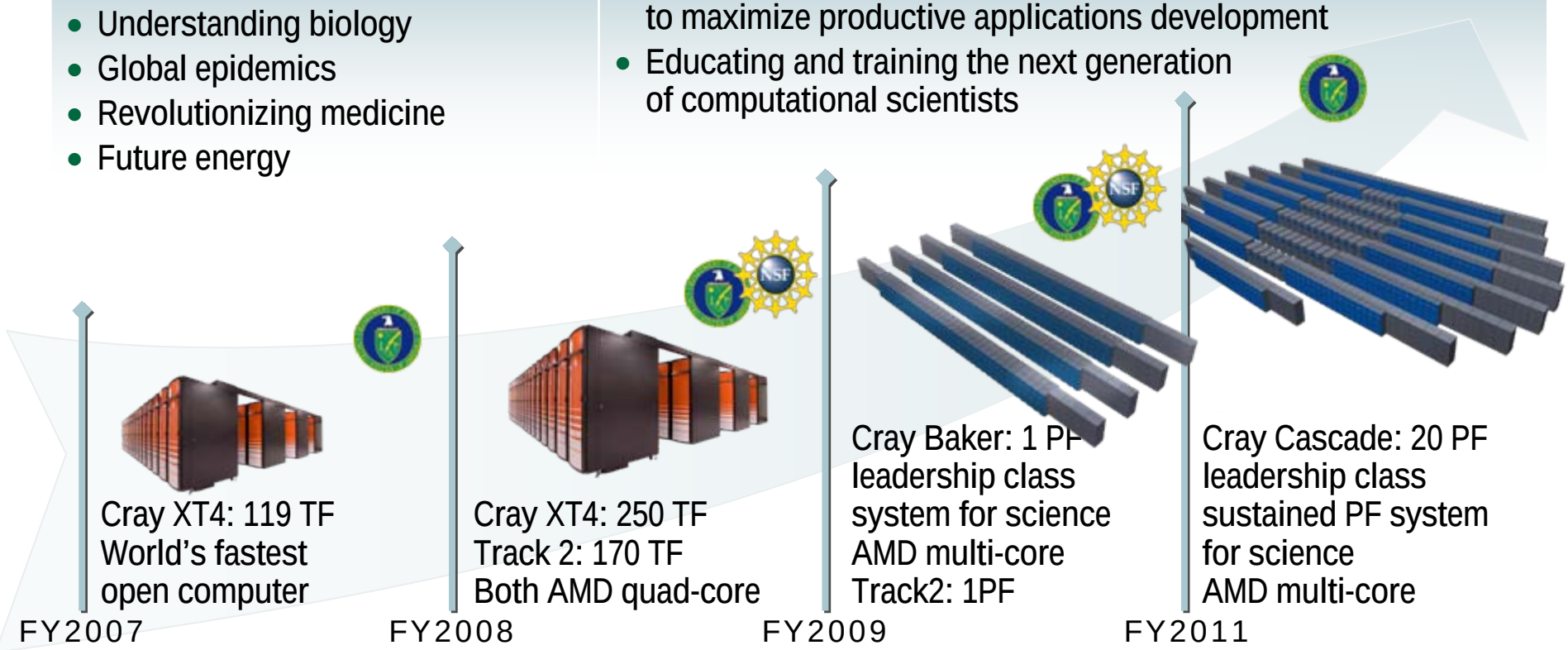
After Upgrade*

- 7,824 compute nodes
  - 2.2 GHz quad-core AMD Opteron processors with 8 GB memory
  - 31,296 compute cores
- 240 service & I/O nodes
- ~750 TB local storage
- 3D Torus interconnect
- 63 TB aggregate memory
- 275 TF peak performance

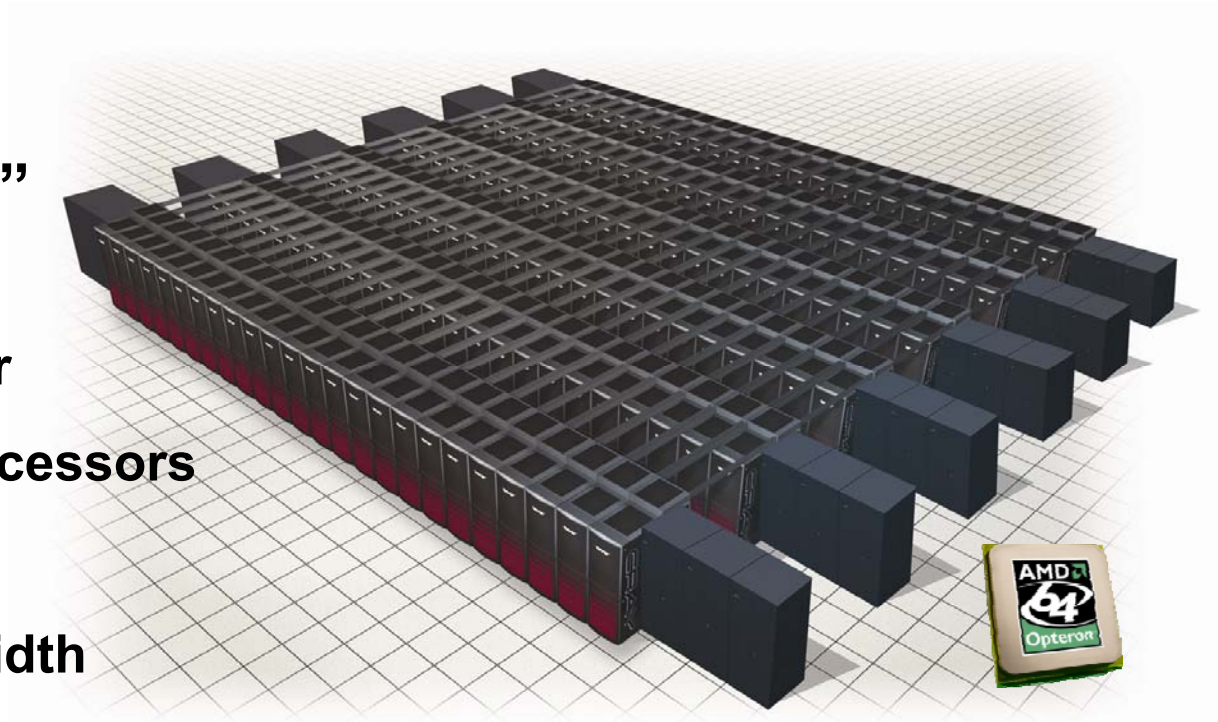
*Planned to commence in mid Dec, 2007

Near Term HPC Roadmap

Mission: Deploy and operate the computational resources needed to tackle global challenges	Vision: Maximize scientific productivity and progress on the largest scale computational problems
• Understanding the universe • Understanding earth's life-support systems • Understanding biology • Global epidemics • Revolutionizing medicine • Future energy	• Providing world class computational resources and specialized services • Providing a stable hardware/software path of increasing scale to maximize productive applications development • Educating and training the next generation of computational scientists



1 Petaflops System - Cray "Baker"



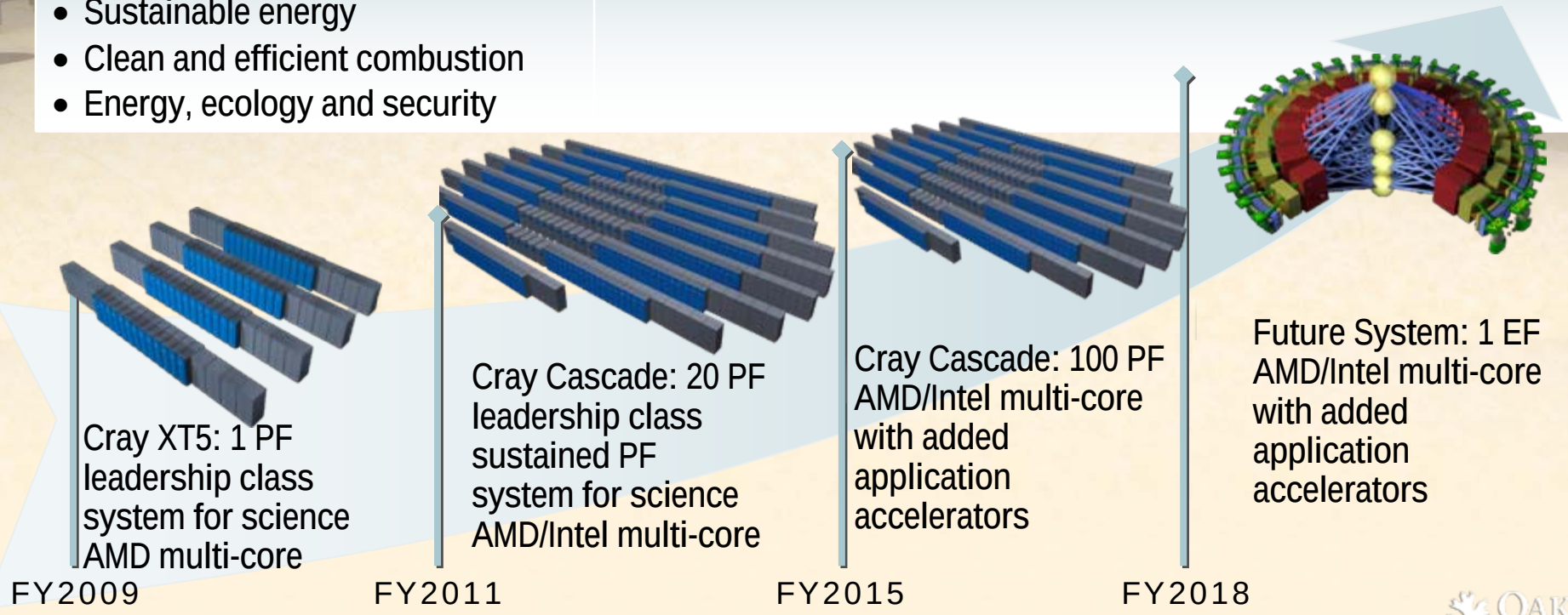
FY 2009: Cray "Baker"

- 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"
- 8 MW system power
- 144 Cabinets, 3,220 ft^2

- Phase-0 of HPCS "Cascade" program
  - Liquid cooled
  - Operating system for hybrid processors
  - Gemini interconnect

Longer Term HPC Roadmap

Mission: Deploy and operate the computational resources needed to tackle global challenges	Vision: Maximize scientific productivity and progress on the largest scale computational problems
• Understanding the universe • Materials and nanoscience • Climate change and terrestrial sequestration of carbon • Sustainable energy • Clean and efficient combustion • Energy, ecology and security	• Providing world class computational resources and specialized services for the most computationally intensive problems • Providing a stable hardware/software path of increasing scale to maximize productive applications development



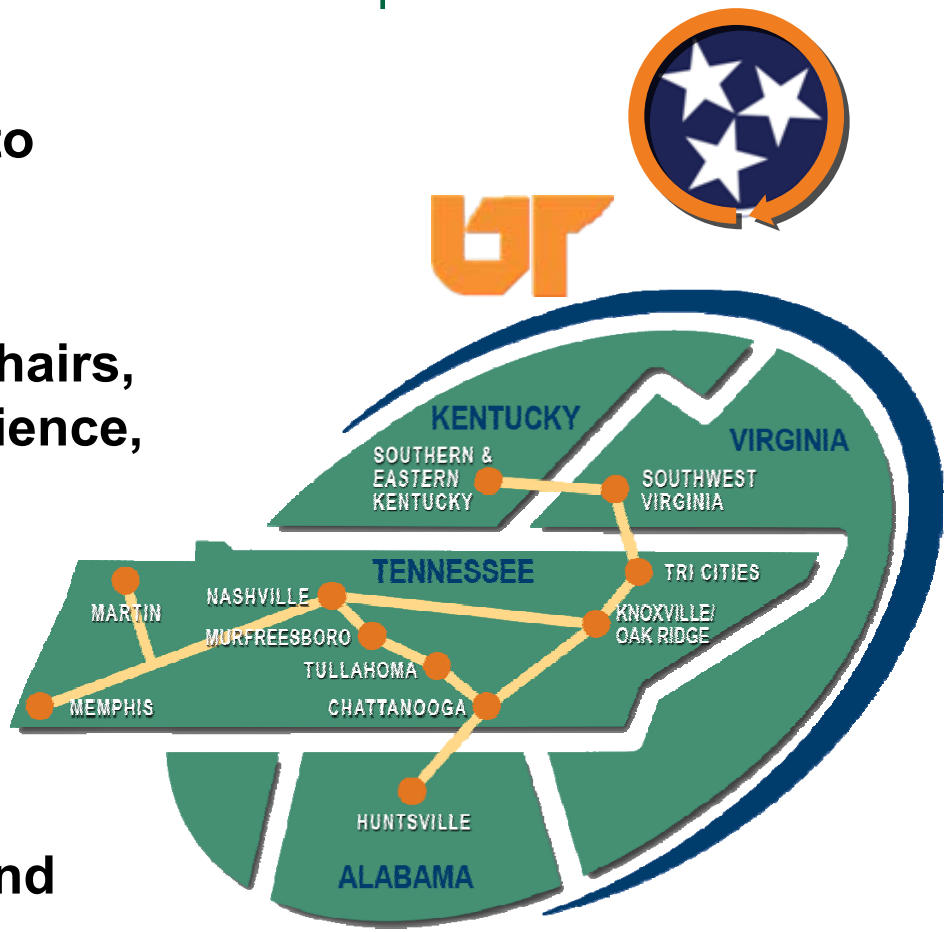
With UT we are NSF's National Institute for Computational Sciences for academia

- **1PF system to the UT-ORNL Joint Institute for Computational Sciences**
  - **Largest grant in UT history**
  - **Other partners: Texas Advanced Computing Center, National Center for Atmospheric Research, ORAU, and core universities**
- **1 of up to 4 leading-edge computing systems planned to increase the availability of computing resources to U.S. researchers**
- **A new phase in our relationship with UT**
  - **Engagement with the scientific community**
  - **Research, education, and training mission**

We are accelerating Tennessee's research enterprise: A statewide cyberinfrastructure

Create a statewide innovation environment to transform research, education, and economic development

- **Build on Joint Institute for Computational Sciences (JICS) to create bold new inter-university partnership**
- **Increase number of governors chairs, faculty, staff, and students in science, technology, engineering, and mathematics (STEM) fields**
- **Create virtual environments for collaboration, education, and experimentation**
- **Underpin advances in science and engineering**



Computer Center

Part of a three-building 365,000 ft^2 complex built in 2003

- **135,670 ft^2 building**
- **Includes a 40,000 ft^2 raised-floor computer room on two floors**
- **Staffed 24x7x365 by operators, security, electricians, and HVAC mechanics**

Systems Infrastructure—Overview
Current and projected

Networking	2007	2008	2009
LAN B/W (GB/s)	40	200	200

Archival storage	2007	2008	2009
Capacity (PB)	4	10	20
Bandwidth (GB/s)	4	10	19

Central storage	2007	2008	2009
Capacity (PB)	0.22	1.0	10.0
Bandwidth (GB/s)	10	40	200

ORNL Provides Leadership Computing to 2008 INCITE Program

- The NCCS is providing leadership computing to 30 programs in 2008 under
  the DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.
- Leading researchers from government, industry, and the academic world will use more than 75 million processor hours on the center's Cray leadership computers.
- The center's Cray XT4 (Jaguar) and Cray X1E (Phoenix) systems will provide more than 75% of the computing power allocated for the INCITE program.

Project Allocations: 145.3 million hrs

Industrial Allocations: 11.9 million hrs

INCITE 2008 Projects

Office of Science
INCITE
Advancing America's Science and Industrial Competitiveness

Astrophysics

Multi-Dimensional Simulations of Core-Collapse Supernovae **Anthony Mezzacappa (Oak Ridge National Laboratory)**
First Principles Models of Type Ia Supernovae **Stan Woosley (University of California, Santa Cruz)**
Numerical Relativity Simulations of Binary Black Holes and Gravitational Radiation **Joan Centrella (National Aeronautics and Space Administration)**

Biology

Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass **Jeremy Smith (Oak Ridge National Laboratory)**
Gating Mechanism of Membrane Proteins **Benoit Roux (Argonne National Laboratory & Univ. of Chicago)**

Chemistry

Molecular Simulation of Complex Chemical Systems **Christopher Mundy (Pacific Northwest National Laboratory)**
An Integrated Approach to the Rational Design of Chemical Catalysts **Robert Harrison (Oak Ridge National Laboratory)**

Computer Science

Performance Evaluation & Analysis Consortium End Station **Patrick Worley (Oak Ridge National Laboratory)**

Climate

The Role of Eddies in the Meridional Overturning Circulation **Paola Cessi (University of California, San Diego)**
Assessing Global Climate Response of the NCAR-CCSM3: CO_2 Sensitivity and Abrupt Climate Change **Zhengyu Liu (University of Wisconsin, Madison)**
Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean **Synte Peacock (ASC/Alliance Flash Center, University of Chicago)**
Climate-Science Computational End Station Development and Grand Challenge Team **Warren Washington (National Center for Atmospheric Research)**
Modeling Reactive Flows in Porous Media **Peter Lichtner (Los Alamos National Laboratory)**

Engineering

High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels **Jacqueline Chen (Sandia National Laboratories)**
Clean and Efficient Coal Gasifier Designs Using Large-Scale Simulations **Madhava Syamlal (National Energy Technology Laboratory)**
Landmark Direct Numerical Simulations of Separation and Transition for Aerospace-Relevant Wall-Bounded Shear Flows **Hermann Fasel (University of Arizona)**

INCITE 2008 Projects *(continued)*

Office of Science
INCITE
Advancing America's Science and Industrial Competitiveness

Fusion

Verification and Validation of Petascale Simulation of Turbulent Transport in Fusion Plasmas **Patrick Diamond (University of California, San Diego)**
Fluctuation Spectra and Anomalous Heating in Magnetized Plasma Turbulence **William Dorland (University of Maryland)**
Gyrokinetic Steady State Transport Simulations **Jeff Candy (General Atomics)**
High Power Electromagnetic Wave Heating in the ITER Burning Plasma **Fred Jaeger (Oak Ridge National Laboratory)**

Materials

Predictive and Accurate Monte Carlo Based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems **Thomas Schulthess (Oak Ridge National Laboratory)**
Electronic, Lattice, and Mechanical Properties of Novel Nanostructured Bulk Materials **Jihui Yang (GM R&D Center)**
Development and Correlations of Large-Scale Computational Tools for Flight Vehicles **Moeljo Hong (The Boeing Company)**

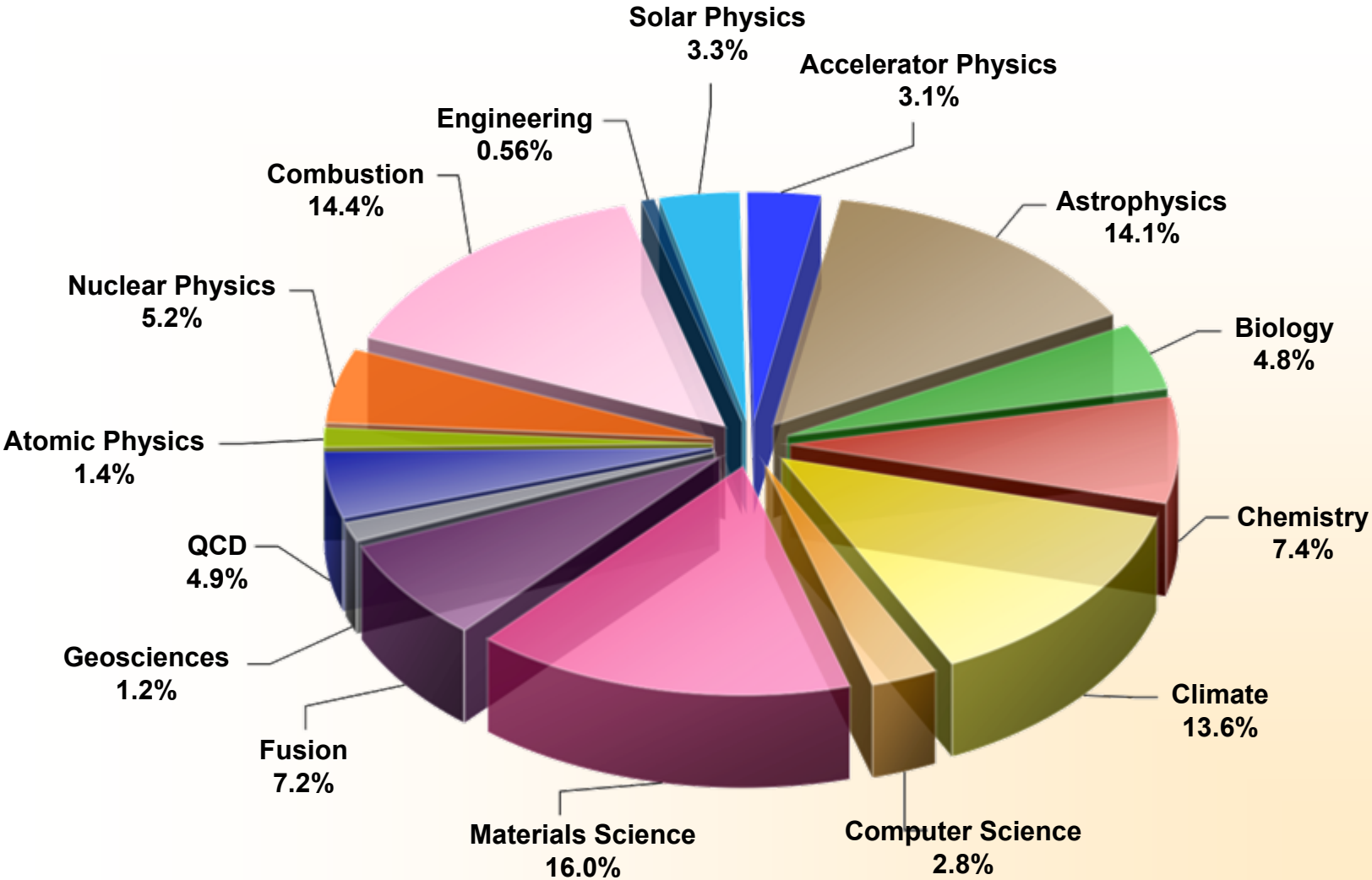
Materials **(continued)**

Bose-Einstein Condensation vs. Quantum Localization in Quantum Magnets **Tommaso Roscilde (Max-Planck Gesellschaft)**
Linear Scale Electronic Structure Calculations for Nanostructures **Lin-Wang Wang (Lawrence Berkeley National Laboratory)**

Physics

Computational Nuclear Structure **David J. Dean (Oak Ridge National Laboratory)**
Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling **Lie-Quan Lee (Stanford Linear Accelerator Center)**
Lattice QCD **Robert Sugar (University of California, Santa Barbara)**
Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences, and Fusion Energy Sciences **Michael Pindzola (Auburn University)**
Modeling Heliospheric Phenomena with an Adaptive, MHD-Boltzmann Code **Nikolai Pogorelov (University of California, Riverside)**

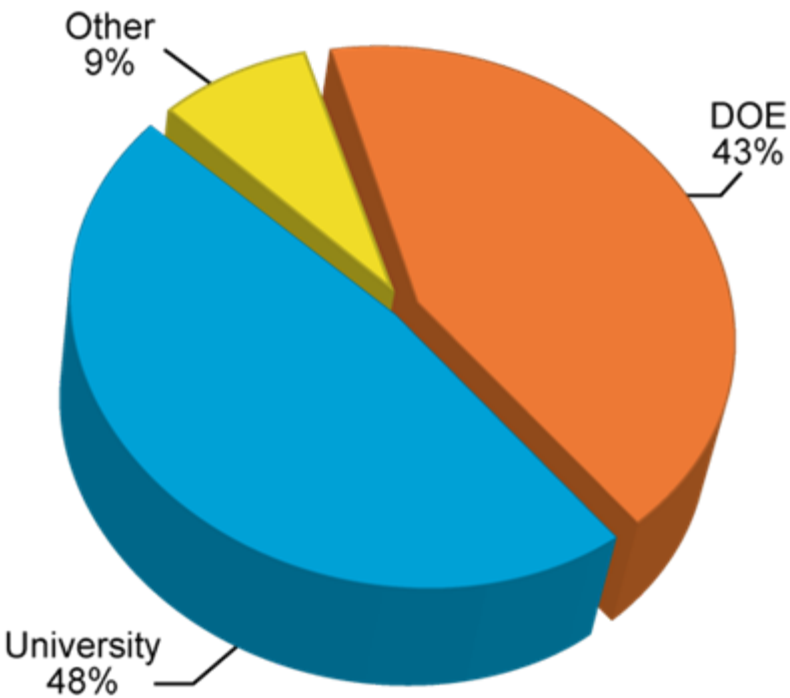
INCITE 2008 Allocations by Discipline

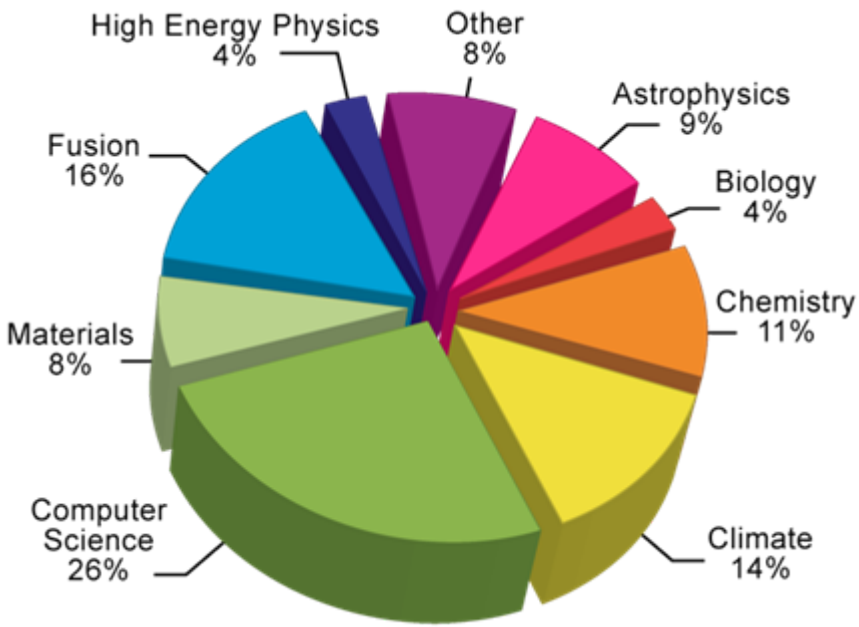


LCF General User Demographics in 2007

National and international scientific communities including industry

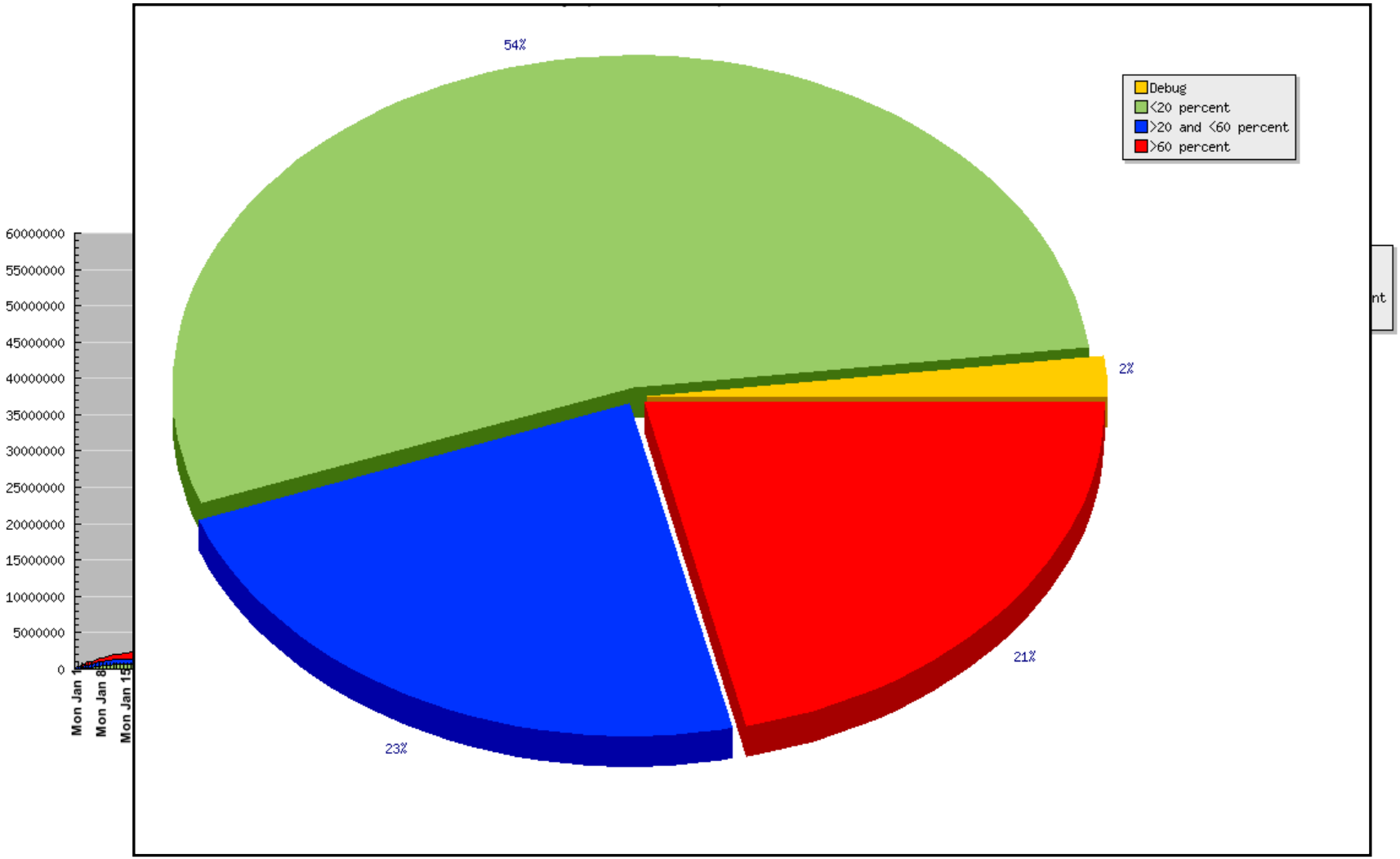
Active Users by affiliation





Percentage of Active Users by Discipline

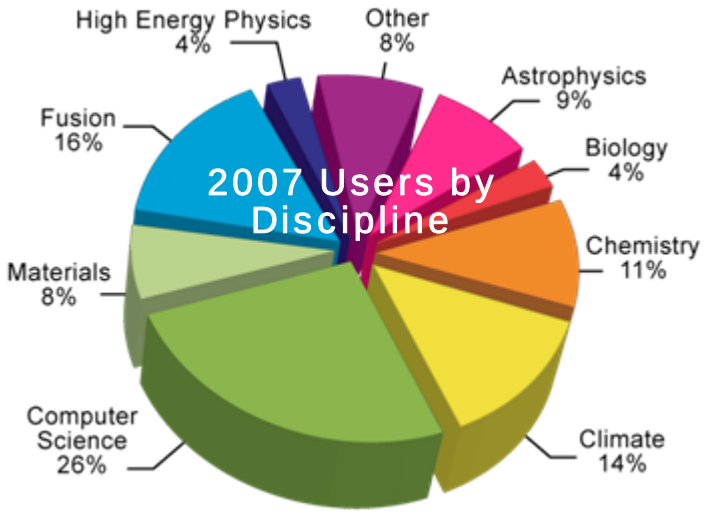
Cray System Usage at the ORNL Leadership Computing Facility in CY07



Our DOE Leadership Computing Facility
Has Become a Flagship Computational Science Enabler

- **We have delivered on an aggressive path of support and collaboration with science teams in 2005-2008**
  - INCITE Projects Committed to: 5, 22, 28, 30*
  - Users Supported: 266, 373, 685, >700*
  - Compute Hours Used (M): 13, 38, 98, 180*
  - Aggregate Compute Power (TF): 38, 79, 171, 327**
- **We have established and are adhering to tough availability, usage, and support metrics**
  - Availability: >95% for systems in place >1 year
  - Usage: >30% of usage requires >30% of resource
  - User satisfaction: >75% (on user survey)
- **We have a prudent security posture in place**
  - Moderate Security Certification & Accreditation Level granted in 2007 allows us to fully support ITAR & proprietary work vital to our industry and government users
- **We are better enabling and driving science output**
  - Require quarterly INCITE project reports
  - Track output: publications, awards, presentations
  - Publications: 85 (2005); 129 (2006); 175 (2007 est)

*2008 projections
**Includes current Jaguar upgrade



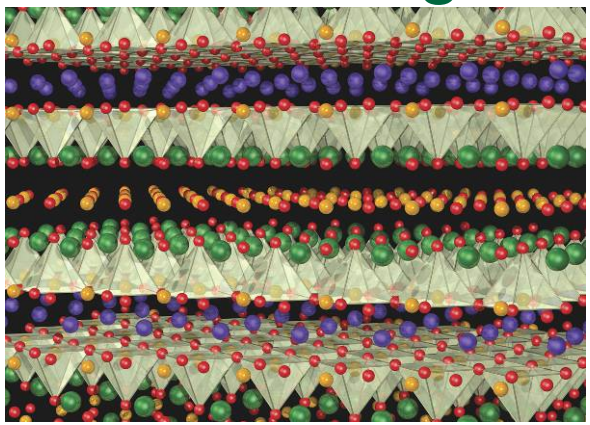
"Impressive maturing of the organization over the last year."

"Doing an outstanding job at problem resolution in a rapidly evolving environment, and in user support in a uniquely challenging area of scientific endeavor. "

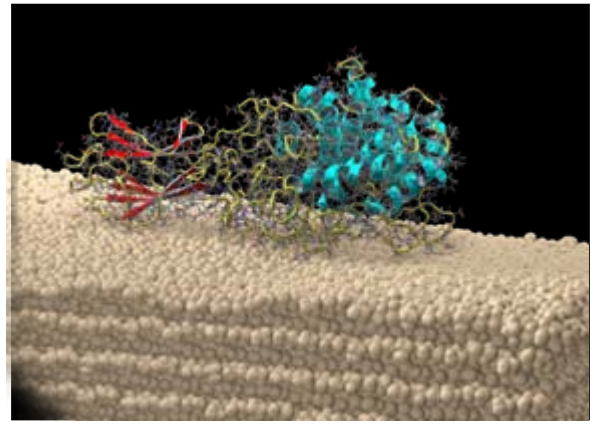
"Impressed by scientific output – the program of consultants for the scientific projects appears to be effective."

2007 DOE Operational Assessment Review

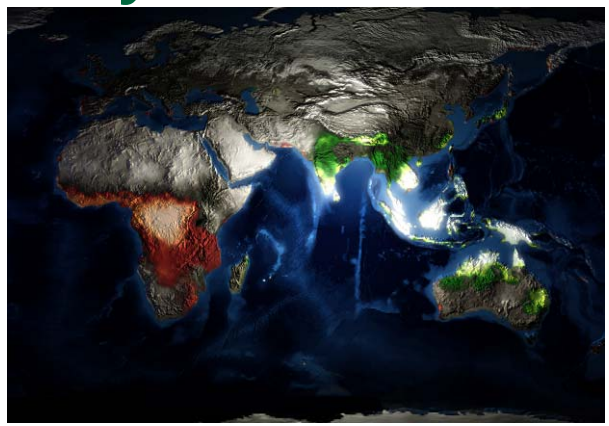
Advancing Scientific Discovery



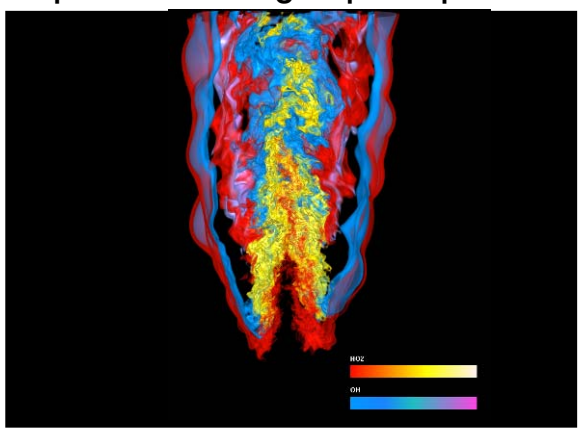
Resolved decades-long controversy about validity of 2D Hubbard model in predicting behavior of high-temperature superconducting cuprate planes



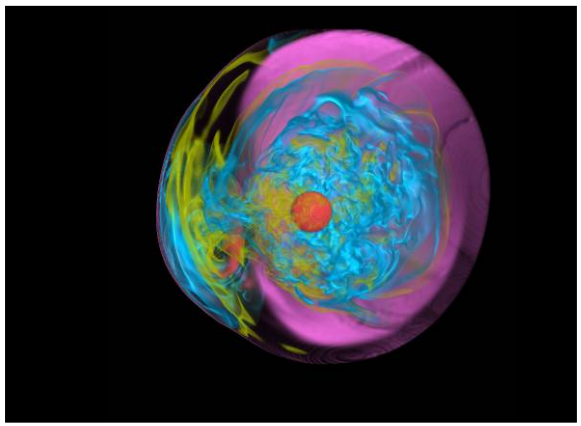
300K-atom models of cellulase enzyme on cellulose substrate reveal interior enzyme vibrations that influence reaction rates converting cellulose to ethanol



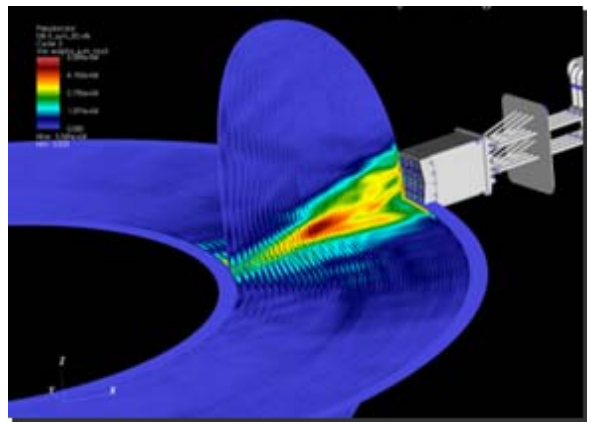
Addition and intercomparison of carbon-land models in new climate model is resolving key processes for carbon sources & sinks



Turbulence chemistry revealed in study of lifted turbulent H_2/air jet flames in ignitive coflow relevant to diesel engines and gas turbines



Instability of supernova shocks was discovered directly through simulation and core collapse pulsar mechanism was explained

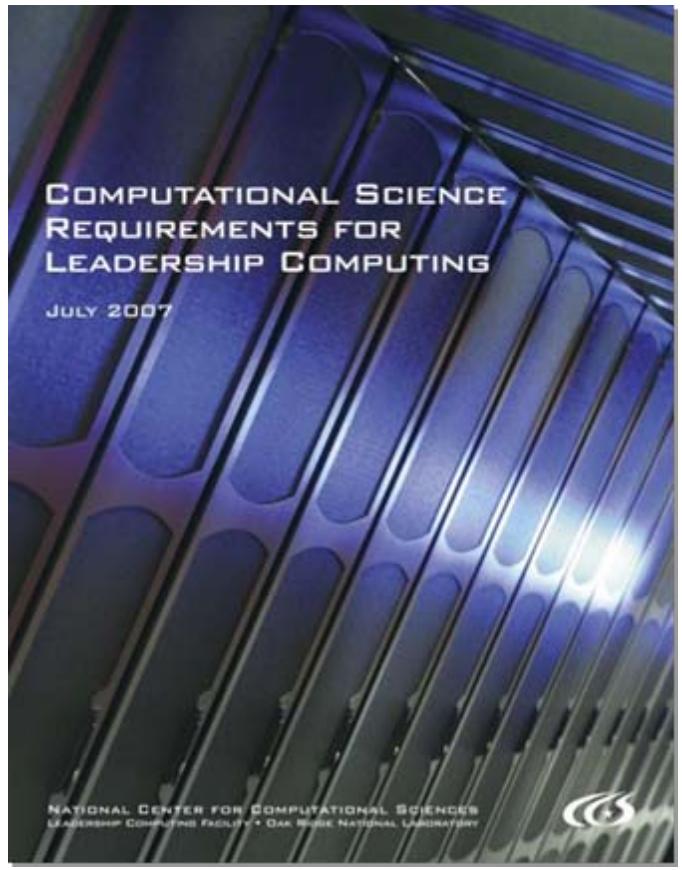


Providing increasing assurance that RF power will effectively heat ITER

Preparing for the Future

Application requirements: Process and actionable results

- **LCF Application Requirements Council (ARC)**
  - Stood up in 2006
  - Established ARC charter & reqms management process
- **LCF elicits requirements in many ways**
  - INCITE proposals
  - Questionnaires devised by LCF staff
  - One-on-one interviews
  - Existing publications/documentation
  - Analyzing source code
- **Application categories analyzed**
  - Science motivation and impact
  - Science quality and productivity
  - Application models, algorithms, software
  - Application footprint on platform
  - Data management and analysis
  - Early access science-at-scale scenarios
- **Results**
  - First annual 100+ page Application Requirements Document to be published 9/07
  - New methods for categorizing platforms and application attributes devised and utilized in analysis: guiding tactical infrastructure purchase and deployment
  - Best practice: Process being embraced and emulated by others



Planned Pioneering Application Runs in Early 2008

Cursory Look at the Simulation Specs

Code	Quad-Core Nodes	Global Memory Reqm (TB)	Wall-Clock Time Reqm (hours)	Number of Runs	Local Storage Reqms (TB)	Archival Storage Reqms (TB)	Resolution and Fidelity
CHIMERA	7824 4045	16 8	100 100	1 1	13	50	256x128x256 or 256x90x180 20 energy groups, 14 alpha nuclei
GTC-S GTC-C	3900 3900	40 60	36 36	2 2	350	550	600M grid points, 60B particles 400M grid points, 250B particles
S3D	7824	10	140	1	50	100	1B grid points, 15 μm grid spacing 4 ns time step, 23 transport vars
POP	2500	1	400	1	1	2	3600x2400x42 tripole grid (0.1°) 20-yr run; partial bottom cells; first with biogeochemistry at this scale
MADNESS	7824	48	12 2	10 12	5	50	600B coefficients
DCA++	2000 6000	16 48	12 to 24	20	1	1	Lattices of 16 to 32 sites 80 to 120 time slices $O(10^2\text{-}10^3)$ disorder realizations

Astrophysics — Fusion — Combustion — Climate — Chemistry — Materials Science

LCF 2008 Director Discretion Program

We welcome more nuclear physics collaboration and presence on our systems