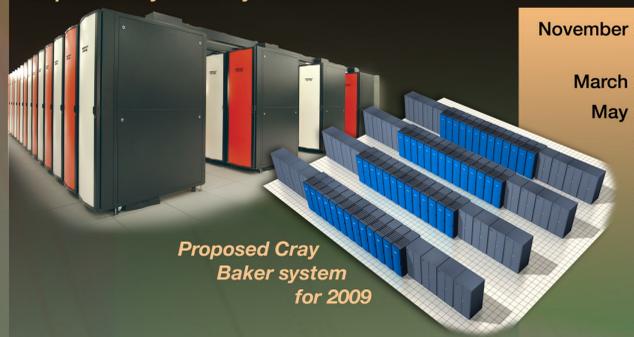## Panel 1 — HARDWARE

NICS

Computing Resources for the Future at the National Institute for Computational Sciences (NICS)


Proposed Cray 170 TF system

Proposed Cray Baker system for 2009

Schedule

November 2007	NSF access to DOE system
March 2008	Delivery of XT4
May 2008	In production
2009	Delivery of "Baker" system
2010	Upgrade "Baker" CPUs

Networks

- 20-year IRU on dark fiber to Atlanta and Chicago
- Capability of up to:
  - 10 Gb/s connections
  - 40 Gb/s or 100 Gb/s connections
- Connected to every major research network
  - TeraGrid: OC-192
  - Internet2: OC-192
  - CHEETAH: OC-192
  - ESnet: OC-192 with OC-48 backup link
  - UltraScience Net: 2xOC-192
  - Gloriad: OC-192
  - NLR: 2xOC-192
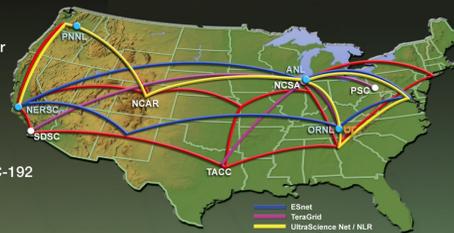
Facilities

Computer Center

Part of a three-building 365,000 ft² complex built in 2003

- 135,670 ft² building
- Includes 40,000 ft² raised-floor computer room on two floors
- Staffed 24/7/365 by operators, security, electricians, and HVAC mechanics

Joint Institute for Computational Sciences Building

- 50,000 ft² building
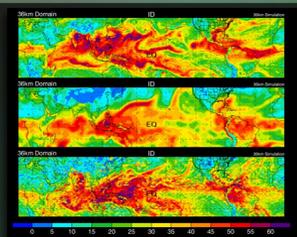- Offices, classrooms, and laboratories
- Distance-learning infrastructure

HARDWARE

ENABLING TRANSFORMATIONAL SCIENCE

Panel 2 — APPLICATIONS

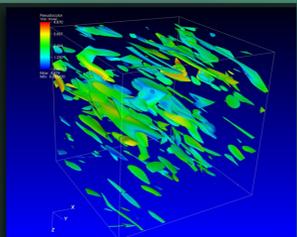# NICS

NSF and ORNL 2011 Model Problems

WRF
Climate

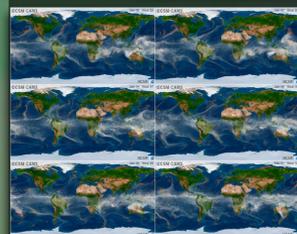Global cloud-resolving model for 0.1–1 km nature and real-data simulations

DNS/CFD
Combustion

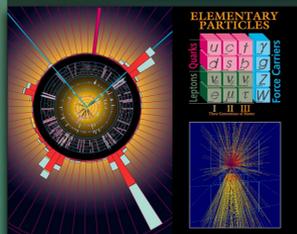12,288³-mesh resolution simulation of fully developed homogeneous turbulence

POP, CICE, HOMME
Climate

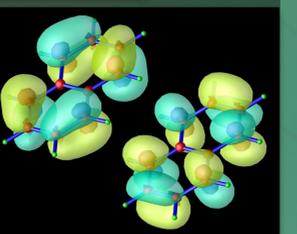Ensemble of ten 200-year simulations with ultra-high resolution

MILC
High Energy Physics
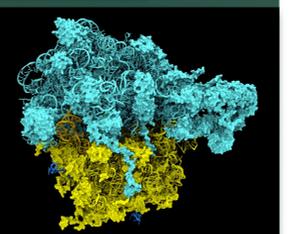
84³ x 144 lattice in lattice-gauge QCD

PARSEC
Materials

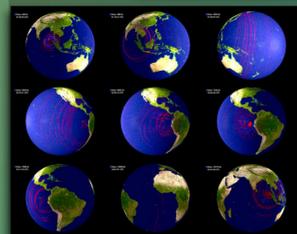Modeling of 30,500 transition-metal atoms

NAMD
Biology

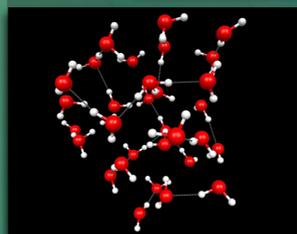100 million atoms solvated in 30 million water molecules

SPECFEM3D
Climate

Seismic probe simulations of Earth's interior to a resolution period of 1 second

GAMESS
Chemistry

Molecular dynamics of liquid water using high-accuracy first-principles calculations

APPLICATIONS

ENABLING TRANSFORMATIONAL SCIENCE

Panel 3 — EDUCATION

NICS

Education, Outreach, and Training Mission

Keeping the United States at the leading edge of simulation science by instructing and broadening the participation of a community of researchers poised to use leadership computing resources

Internships

Existing programmatic mechanisms bring nearly 1000 undergraduates, graduate students, postgraduates, faculty members, postdoctoral research associates, and others to the co-located ORNL.

Annual internships allow undergraduate and post-graduate students to be co-located on the NICS site and work under the guidance of NICS staff and researchers in areas critical to all functions of a petascale facility:

- Computer science in user support and operations
- Future technologies
- Research activities with on-site users

Workshops and Web Resources

NICS will introduce specific HPC and technology to students and researchers to give them the skills and knowledge to run on petascale systems:

- SC08: "Introduction to Petascale Computing"
- "Petascale Laboratory for Simulation Science" in 2008
- January 2008 Hands-on Workshop at NICS
- Other topical workshops will be held on location at NICS or at partner institutions

In general, seminars and workshops will be accessible via video on the web. Extensive documentation will also be web-based.

Classes

NICS will leverage partner education activities, such as the University of Tennessee's Interdisciplinary Graduate Minor in Computational Science.

NICS is promoting leadership computing education to students and researchers in curricula offered by academic institutions:

- Classes and seminars on high performance scientific computing
- Hands-on tutorials on porting and optimizing code for the NICS system
- High-impact educational and visual materials suitable for K–12

Increasing Participation

To broaden the participation of under-represented demographic groups in leadership computing, planned partnership activities include:

- "Introduction to Petascale Computing" workshops for Grace Hopper and Richard Tapia Conferences

ORNL's Research Alliance in Math and Science Program has paired hundreds of students with mentors for summer internships.

Partner Activities

Our partners have very strong and multifaceted outreach activities at all levels, involve a substantial fraction of their science and engineering undergraduates in research, and have substantial efforts at K–12 levels.

NICS will have a major impact on many of these activities by providing both educational materials and opportunities for direct involvement in the research of participating faculty.

EDUCATION

ENABLING TRANSFORMATIONAL SCIENCE

Panel 4 — REGION

NICS

Outstanding Academic and Natural Resources in East Tennessee

REGION

ENABLING TRANSFORMATIONAL SCIENCE