



# **Computing and Computational Sciences**

Presented at

**Fall '03 Workshop**

**Research Alliance for Minorities**

by

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Oak Ridge, Tennessee**

**OAK RIDGE NATIONAL LABORATORY  
U. S. DEPARTMENT OF ENERGY**

<http://www.csm.ornl.gov/Internships/>

“The Research Alliance for Minorities (RAM) Program is based on the belief that national laboratories and universities, working hand in hand, offer the best opportunity to make a real impact on the quality of a diverse workforce.”

Program sponsored by the Mathematical, Information and Computational Sciences (MICS) Division of the Office of Advanced Scientific Computing Research, U.S. Department of Energy

# Goals

## Short Term

- Increase number of underrepresented minorities (African American, Hispanic American, Native American and women) who pursue degrees in science, mathematics, engineering, and technology

## Long Term

- Increase number of underrepresented individuals with advanced degrees in science, mathematics, and engineering in the workforce

<http://www.csm.ornl.gov/Internships/RAM>

# Oak Ridge National Laboratory was established during World War II

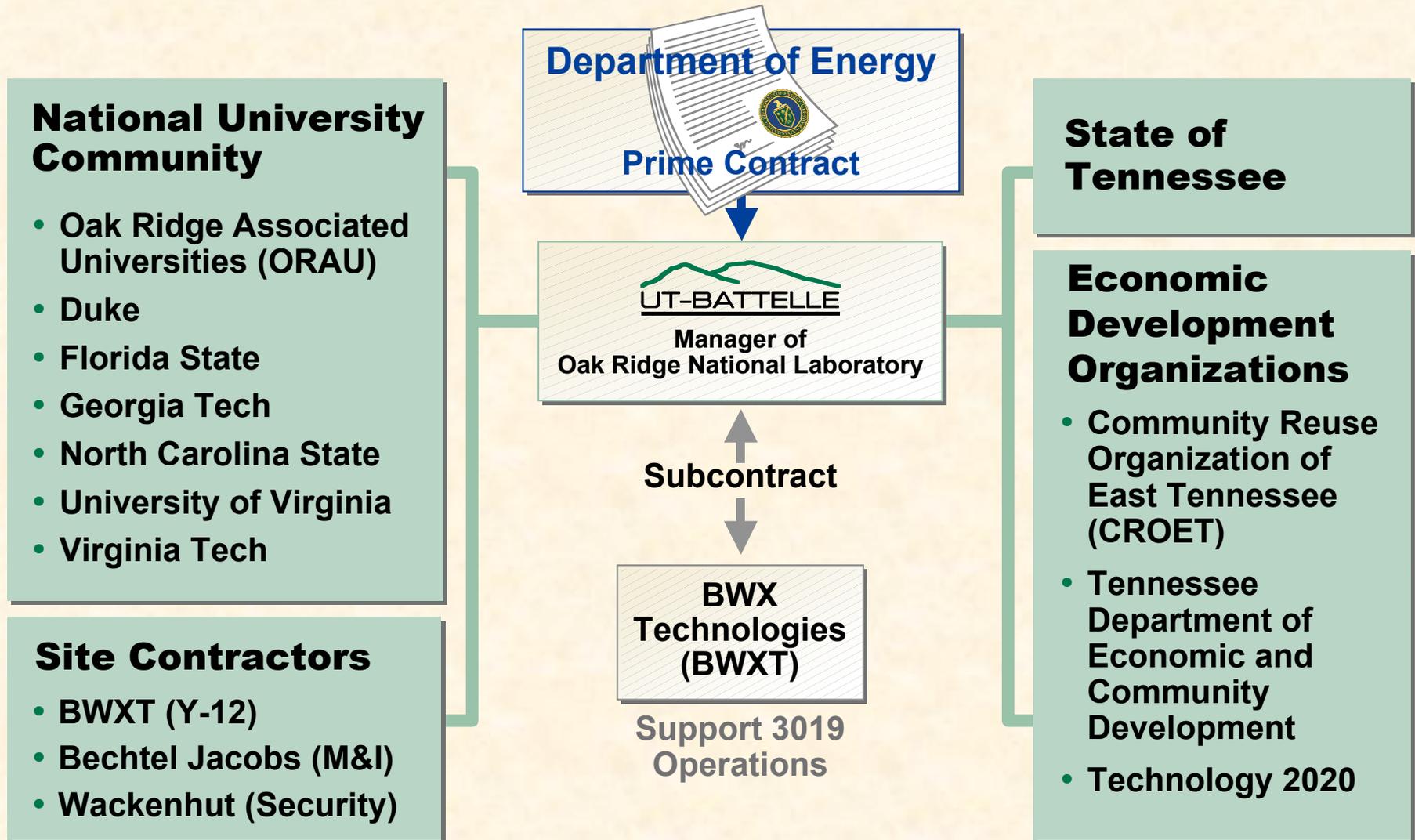


**Senator  
Kenneth D. McKellar**

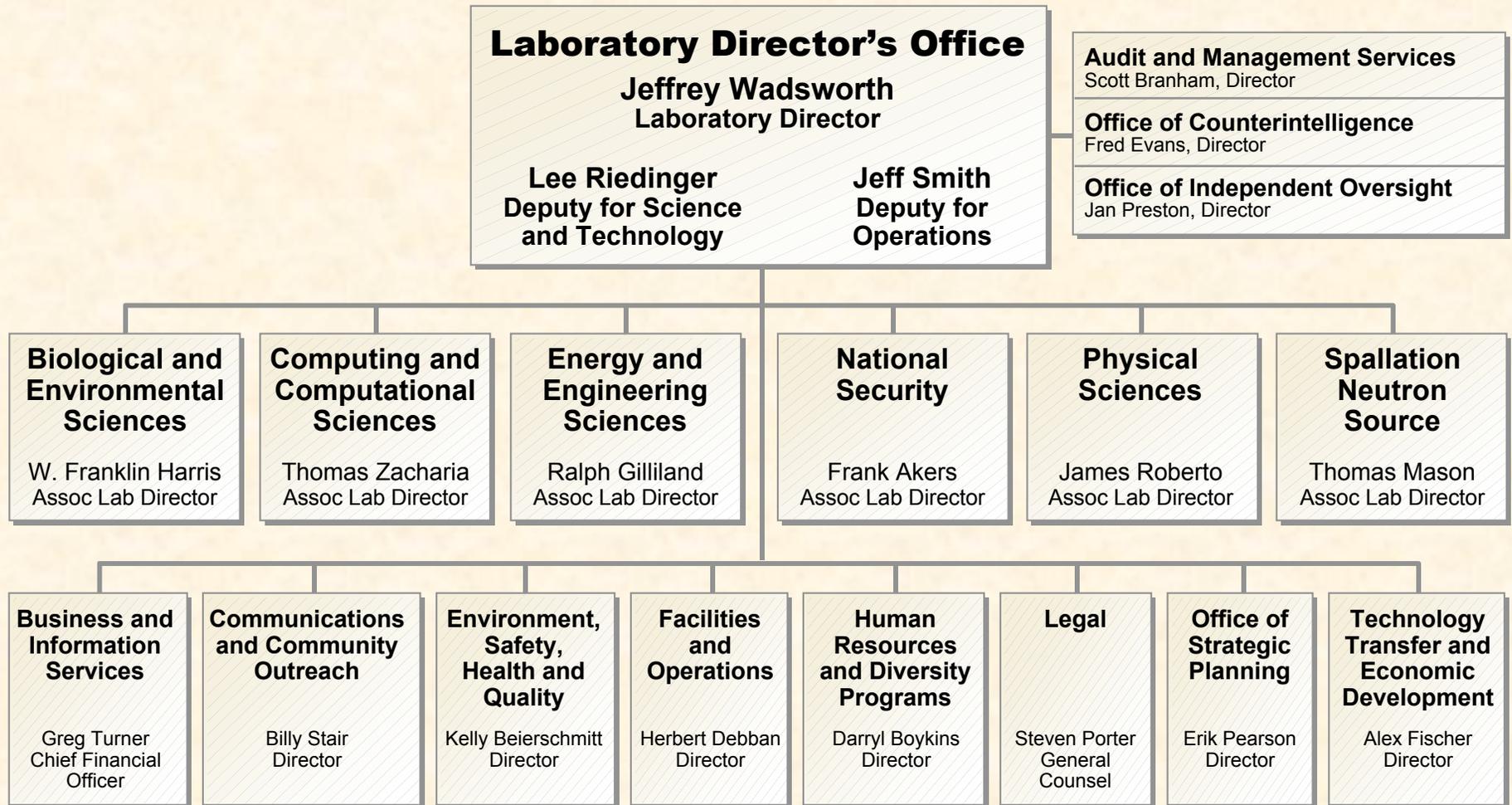


**The Graphite Reactor was the world's first  
continuously operated nuclear reactor**

# We operate with many partners



# Oak Ridge National Laboratory



# Oak Ridge National Laboratory today

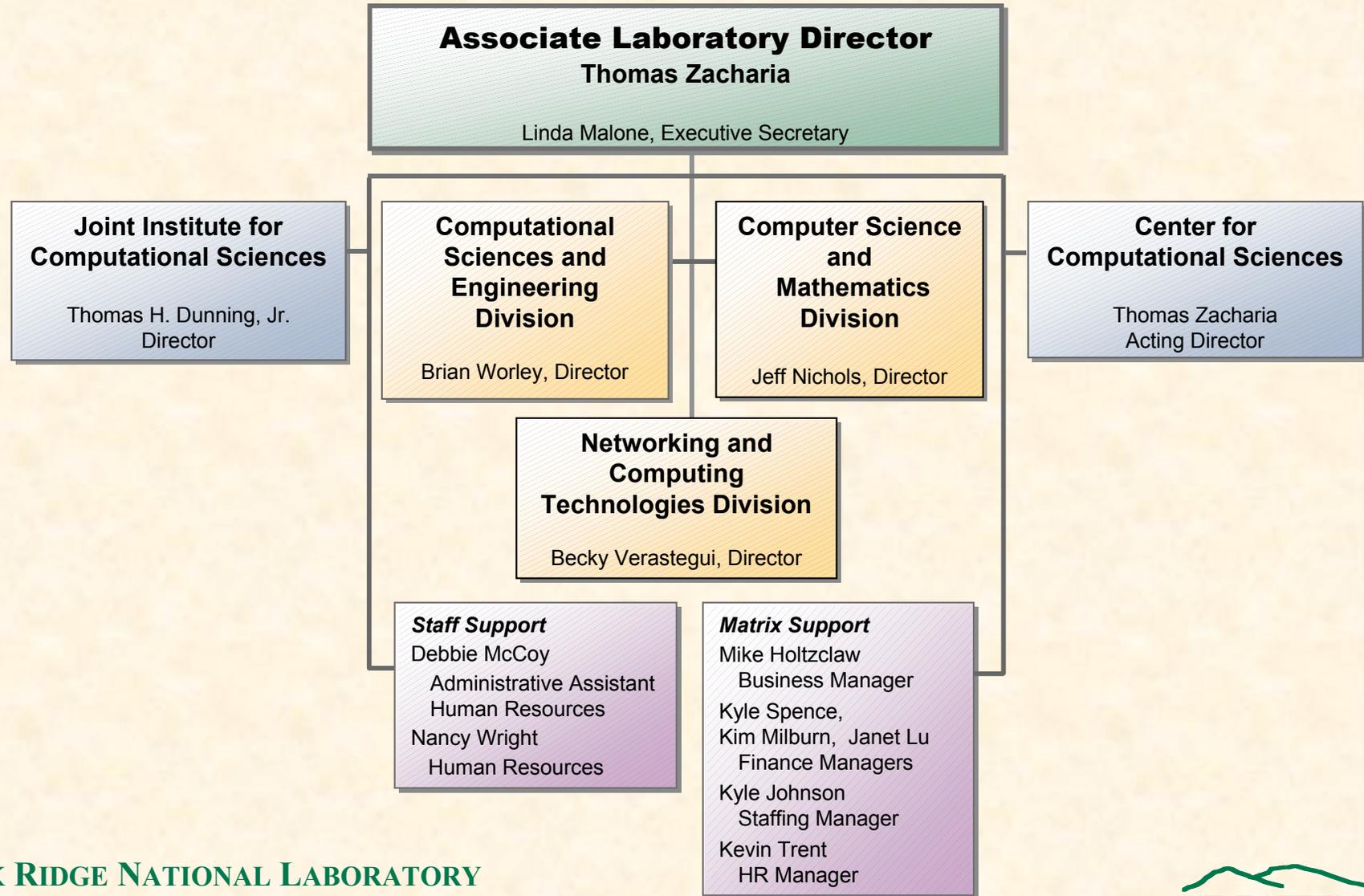


- ▶ **\$1 billion budget**
- ▶ **DOE's largest multiprogram science laboratory**
- ▶ **Nation's largest energy R&D laboratory**
- ▶ **Nation's largest concentration of open source materials research**
- ▶ **Building the \$1.4 billion Spallation Neutron Source**
- ▶ **3700 employees**
- ▶ **3000 research guests annually**
- ▶ **18 user facilities**
- ▶ **Very strong university partners**
- ▶ **\$300 million modernization program in progress**

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**UT-BATTELLE**

# Computing and Computational Sciences Directorate



# Advanced scientific computing is an Administration priority for FY05

- **Develop**
  - An interagency R&D roadmap for high-end computing core technologies
  - A federal high-end computing capacity and accessibility improvement plan
  - A discussion of issues (with recommendations where applicable) relating to federal procurement of high-end computing systems
- **Produce a coordinated, multi-year, interagency plan to guide future Federal investments in high-end computing for scientific R&D**
- **“...Task Force recommendations will be considered in preparing the President’s budget for FY 2005 and beyond”**
- **PITAC extended “...PITAC will help guide the administrations efforts to accelerate the development and adaptation of information technologies vital for American prosperity in the 21<sup>st</sup> century”**

## **NSTC High-End Computing Revitalization Task Force**

*Co-chairs:*  
Alan Laub (DOE-SC),  
John Grosh (DOD)

# ORNL: DOE's best opportunity for a high-end computing initiative

## Center for Computational Sciences

- World-class facility on schedule for summer occupancy
- Internet 2/Abilene membership enhances connectivity to academia

## Leadership in math and computer science

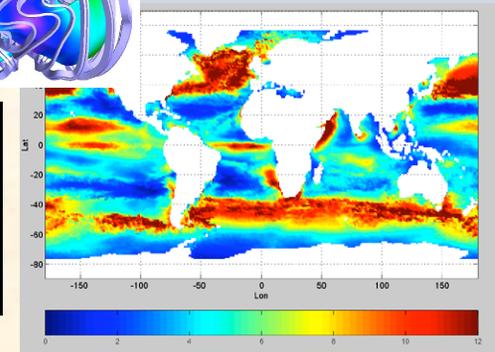
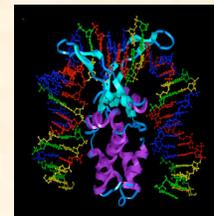
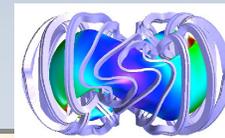
- Robert Harrison: Fernbach Award
- Common Component Architecture (CCA): one of top 10 DOE science achievements for 2002

## Next-generation Cray X1 architecture

- First tutorial drew >100 participants
- \$14M in FY04 budget request

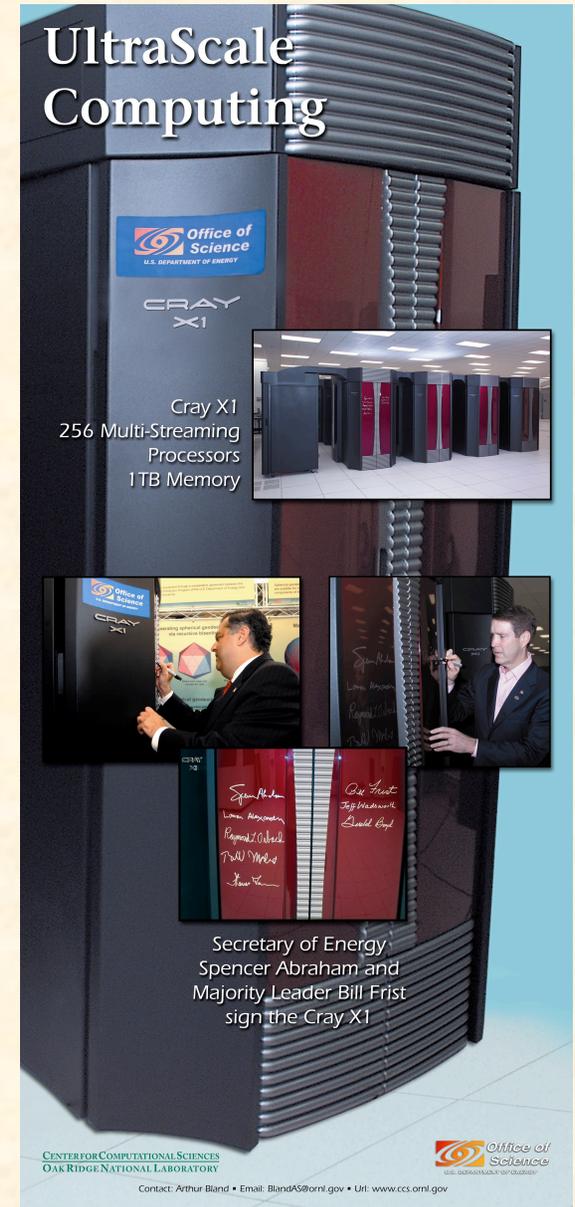
## Leadership in SciDAC

- Enabling scientific discovery in biology, climate, fusion, materials



# Vision

- New capability for science for the Nation
- Focal point for the scientific research community as it embraces computing as a peer to experiment and theory
- Providing the leadership and organizational framework needed for multidisciplinary research
- Focused on critical national scientific priorities

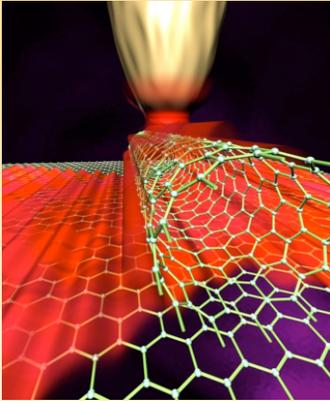


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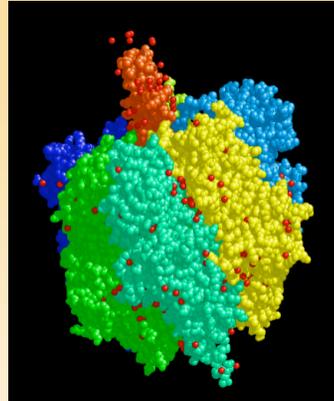
# Computational science is critical for success in key national priorities

## Nano



Computational design of innovative nanomaterials

## Bio



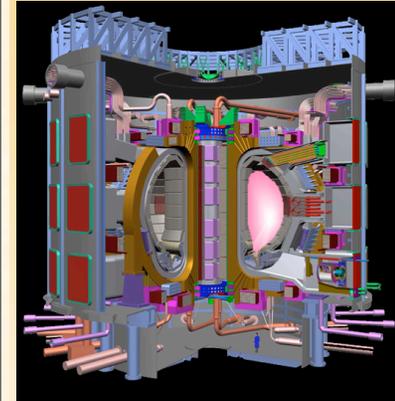
Predictive understanding of microbial molecular and cellular systems

## Climate



Full carbon cycle in climate prediction

## Fusion



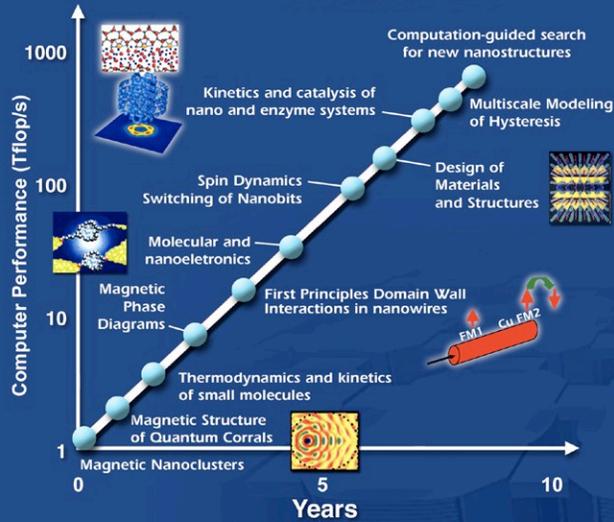
Simulation of burning plasma (ITER)

Theory, Math, Computer Science

Leadership-Class Computing Facility for Science

# Delivering Science and Leadership in High-end Computing

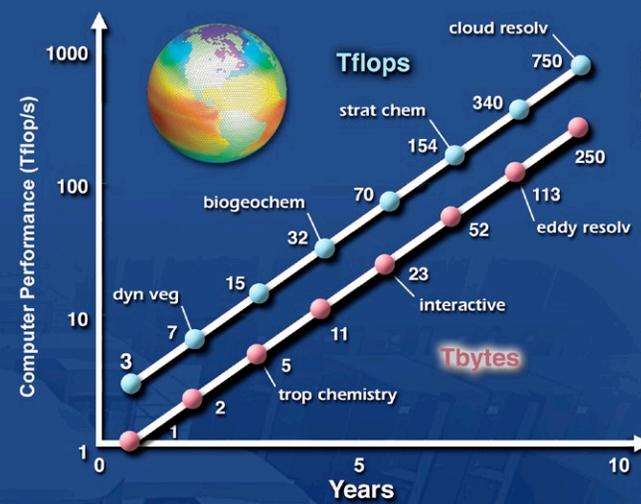
## Nanoscience



### Expected Outcomes

- 5 years**
- Realistic simulation of self-assembly and single-molecule electron transport
  - Finite temperature properties of nanoparticles/quantum corrals
- 10 years**
- Multi-scale modeling of molecular electronic devices
  - Computation-guided search for new materials/nanostructures

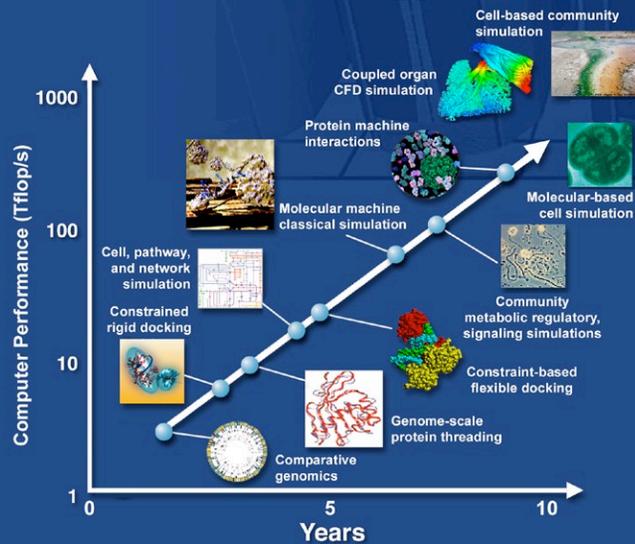
## Climate



### Expected Outcomes

- 5 years**
- Fully coupled carbon-climate simulation
  - Fully coupled sulfur-atmospheric chemistry simulation
- 10 years**
- Cloud-resolving 30-km spatial resolution atmosphere climate simulation
  - Fully coupled, physics, chemistry, biology Earth system model

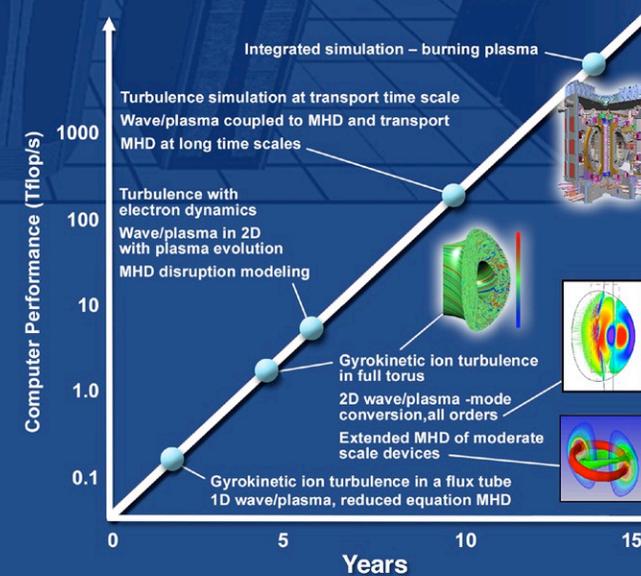
## Biology



### Expected Outcomes

- 5 years**
- Metabolic flux modeling for Hydrogen and Carbon fixation pathways
  - Constrained flexible docking simulations of interacting proteins
- 10 years**
- Multi-scale stochastic simulations of combined microbial metabolic, regulatory and protein interaction networks
  - Dynamics simulations of complex molecular machines

## Fusion

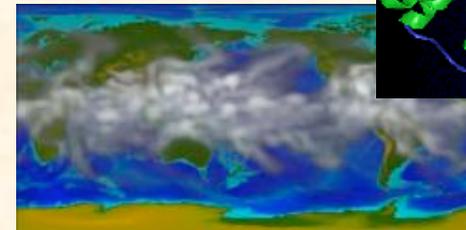
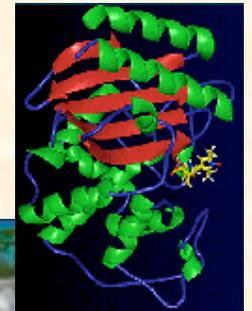
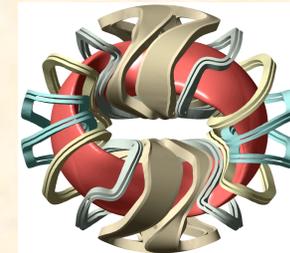


### Expected Outcomes

- 5 years**
- Full-torus, electromagnetic simulation of turbulent transport with kinetic electrons for simulation times approaching transport time-scale
  - Develop understanding of internal reconnection events in extended MHD, with assessment of RF heating and current drive techniques for mitigation
- 10 years**
- Develop quantitative, predictive understanding of disruption events in large tokamaks
  - Begin integrated simulation of burning plasma devices - multi-physics predictions for ITER

# Our strategy brings resources together to enable the vision

- Provision ORNL Center for Computational Sciences as a national user facility for leadership-class scientific computing
- Create resident world-class computational science teams to serve as focal point for key grand challenges for the Nation, ensuring the Center's scientific impact
- Work closely with industry in design of next-generation and experimental architectures for science
- Build strong collaborations with academia, industry, and other agencies in research, education, and training
- Recruit and attract the world's best researchers

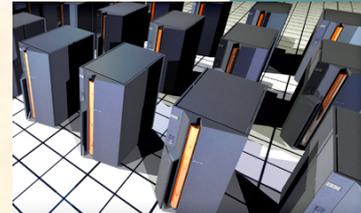


# Center for Computational Sciences

- Focus on grand challenge science and engineering applications
- Evaluate new hardware for science
  - Develop and evaluate emerging and unproven systems and experimental computers
- Deliver leadership-class computing for DOE science
  - Specialized services to the scientific community: biology, climate, nanoscale science, fusion
  - Principal resource for SciDAC
  - Performance improvement for major scientific simulations (50x by 2005, 1000x by 2008)
- Educate and train the next generation of computational scientists



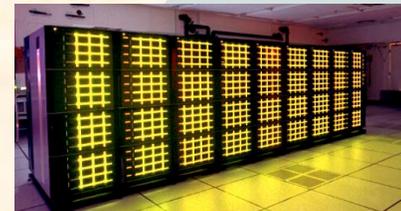
**Cray X1/X2:**  
Leadership class  
computer for  
science



**IBM Power4:**  
8th in the world



**IBM Power3:**  
DOE-SC's first  
terascale system

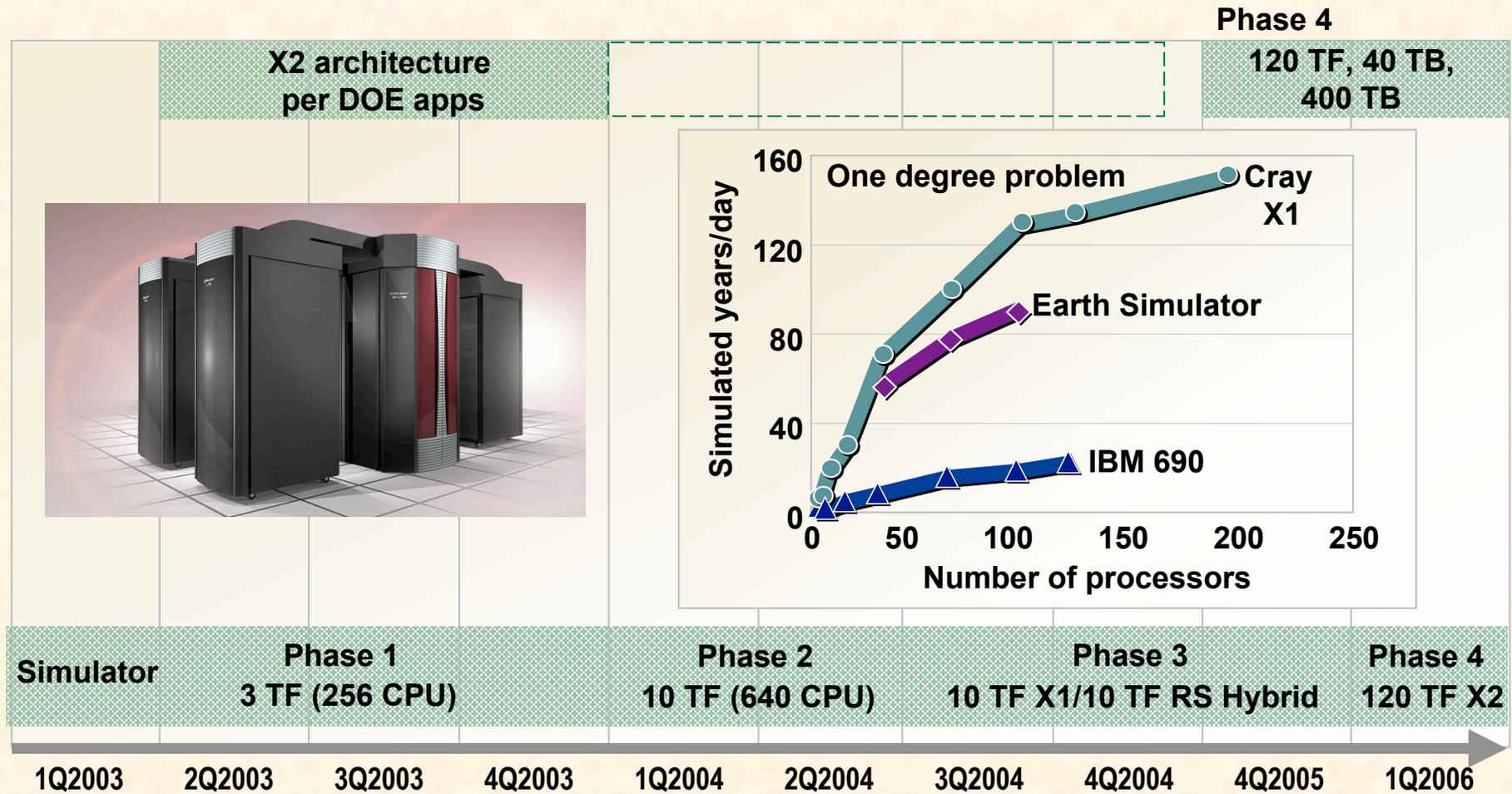


**Intel Paragon:**  
World's fastest computer

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# On track to deliver leadership-class Cray system for science



# A Decade of Firsts (1992-2002)

**1992**

First Paragon XP/S 35  
KSR1-64  
CCS formed

**1995**

Install Paragon XP/S 150  
World's fastest computer  
Connected by fastest  
network OC-12 to Sandia



Facilities modernization



**1993**

PVM used to create  
first International  
grid

**1994**

PVM wins R&D 100



First OSC TeraFLOP  
peak system

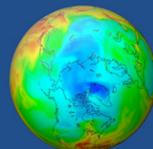
**2003**

OC-192  
connectivity  
implementation



**1996**

ORNL-SNL create first  
high-performance  
computational grid



**2000**

Climate simulation  
throughput of  
5 years/day

**2001**



First IBM Power 4  
SciDAC leadership  
Human Genome

Construction  
starts on new  
CCS building—  
a world-class  
DOE facility

**1997**

R&D 100 Award for  
successful development  
and deployment of HPSS

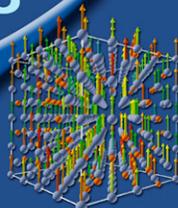


Developed first  
application to  
sustain 1 TF

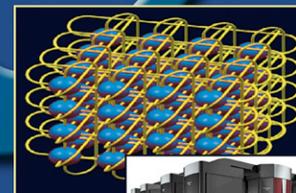
**1999**

NetSolve wins  
R&D 100  
ATLAS wins  
R&D 100

**1998**



PROSPECT  
wins R&D 100



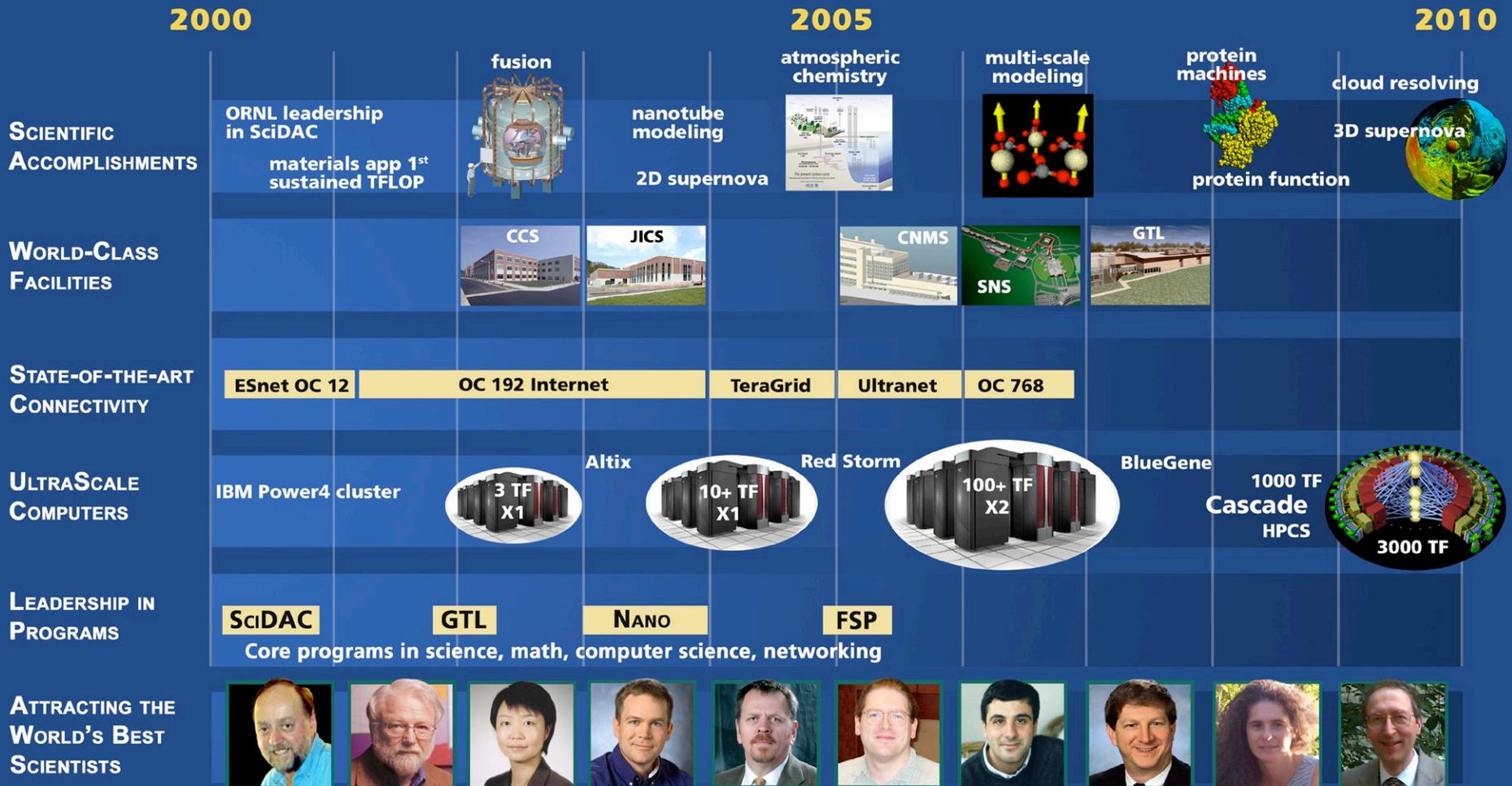
**2002**

IBM Blue Gene  
CRADA to develop  
super scalar  
algorithms begins

Partnership with  
Cray on X1 begins



# Roadmap 2000-2010



Opportunity for Extraordinary Advances through Effective Integration

# People and partnerships

## Attracting the best scientists

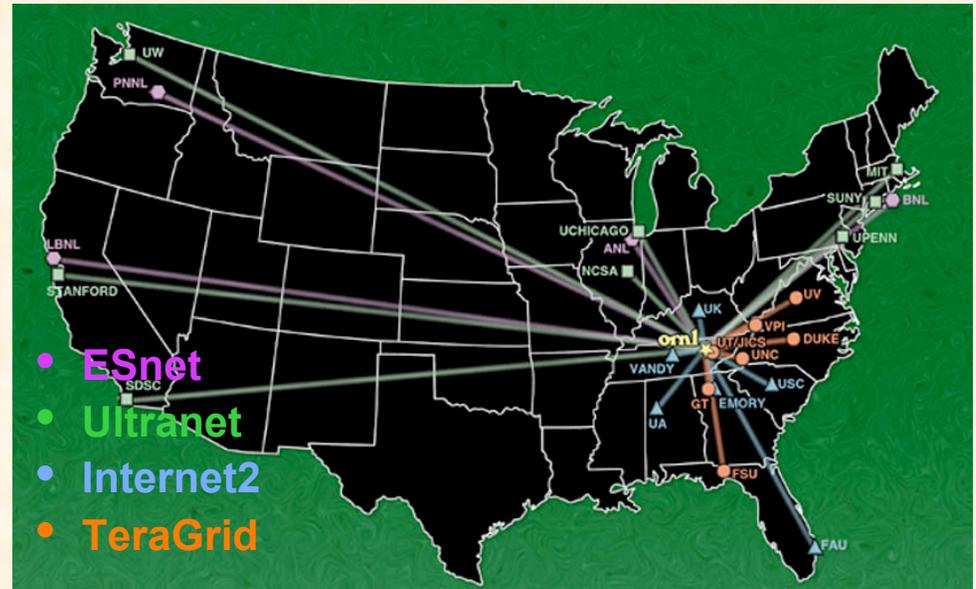


**Thomas Maier**  
Wigner Fellow



**Jennifer Ryan**  
Householder Fellow

Staffing	'01	'02	'03
S&T	15	21	31
Postdocs	58	40	56
Students	34	41	46



## State-of-the-art connectivity

## Building enduring partnerships

- Interagency partnerships with NSF, NSA, NNSA, NASA, DHS
  - Key resource for Intergovernmental Panel on Climate Change (IPCC)
- Joint Institute for Computational Sciences/core universities
- Research Alliance for Minorities
- Strong industrial partnerships with Cray, SGI, IBM
- International collaborations

# Questions?

<http://www.csm.ornl.gov/Internships/RAM>

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