UT-BATTELLE

Computing and Computational Sciences Directorate

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for

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Research Alliance in Math and Science
Faculty/Mentor Workshop

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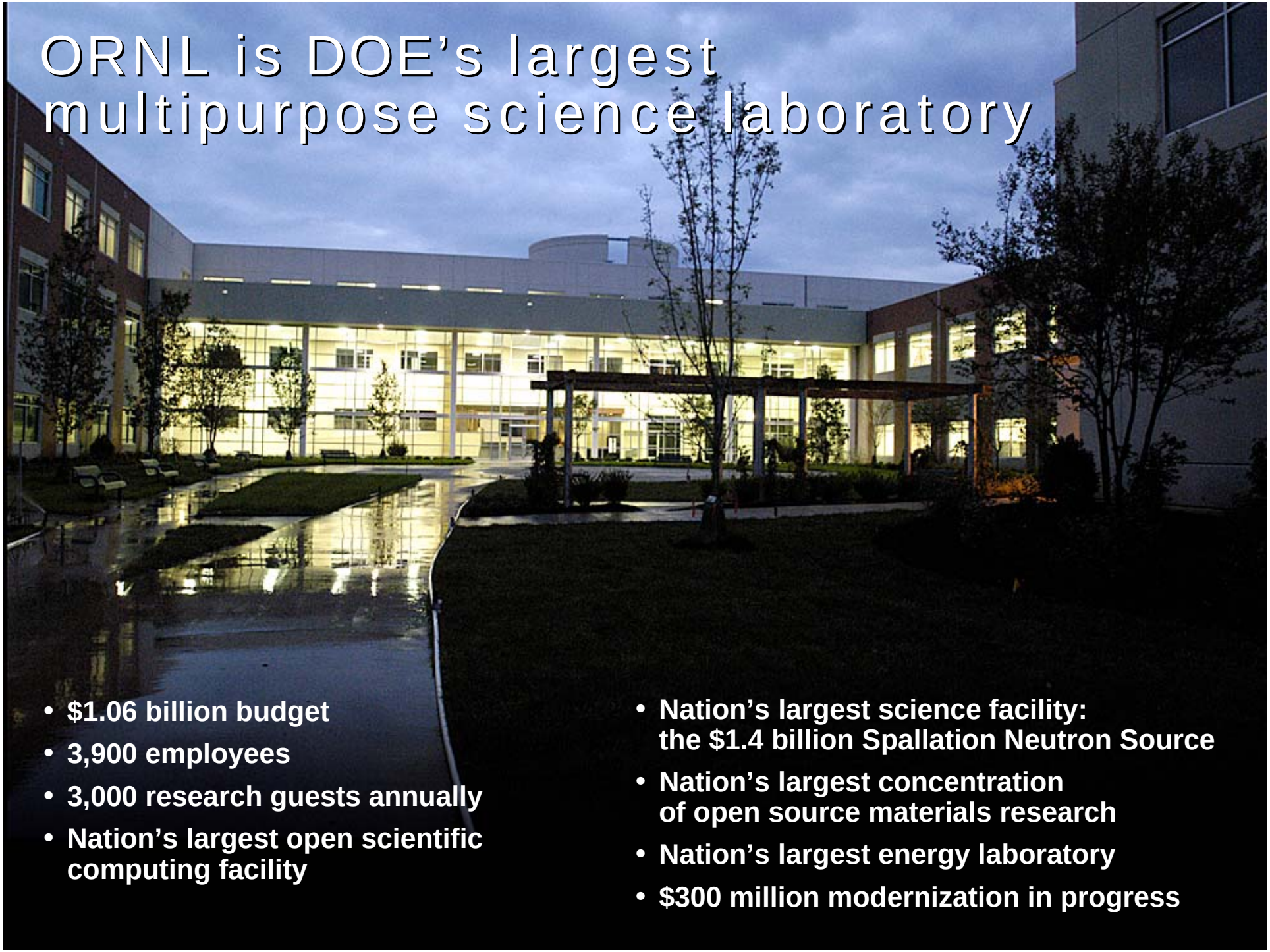
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

ORNL is DOE's largest multipurpose science laboratory



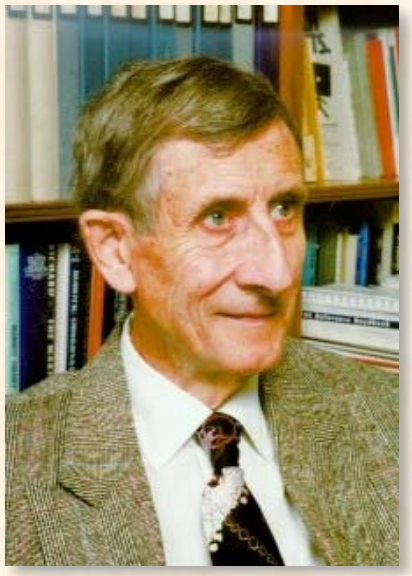
- **$1.06 billion budget**
- **3,900 employees**
- **3,000 research guests annually**
- **Nation's largest open scientific computing facility**
- **Nation's largest science facility: the $1.4 billion Spallation Neutron Source**
- **Nation's largest concentration of open source materials research**
- **Nation's largest energy laboratory**
- **$300 million modernization in progress**

Site of world leading computing and computational sciences

The Department of Energy's national laboratories: A flair for getting after very big and difficult matters

- **Multidisciplinary R&D to solve large-scale, long-term problems of national importance**
  - **National security**
  - **Energy**
  - **Environment**
- **Design, construction, and operation of unique research facilities and equipment**
- **Technology transfer**
- **Education**

Tool-driven revolutions



"There are two kinds of scientific revolutions, those driven by new tools and those driven by new concepts…

The effect of a concept-driven revolution is to explain old things in new ways. The effect of a tool-driven revolution is to discover new things that have to be explained.

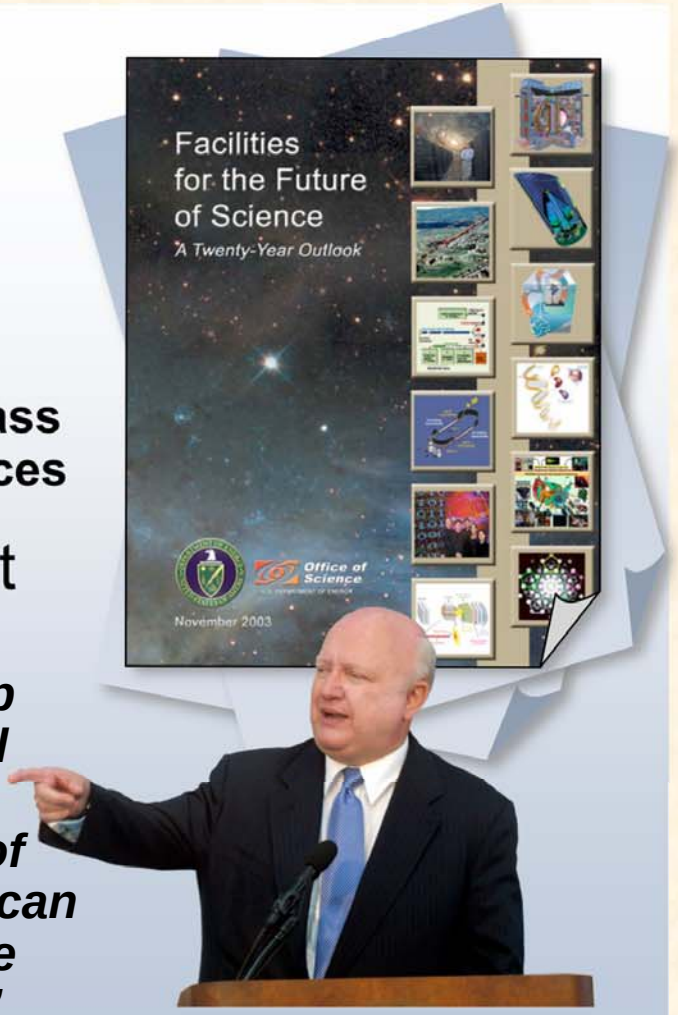
In almost every branch of science, and especially in biology and astronomy, there has been a preponderance of tool-driven revolutions."

Freeman Dyson
***Imagined Worlds* (1997)**

Leadership computing is highest domestic priority for Office of Science

- Ray Orbach has articulated his philosophy for the SC laboratories
  - **Each lab will have world-class capabilities in one or more areas of importance to Office of Science**
  - **ORNL: SNS and NLCF will underpin world-class programs in materials, energy, and life sciences**
- 20-year facilities plan being used to set priorities among projects

"I am committed to the concept of a Leadership Class Computing facility at Oak Ridge National Laboratory.
The facility will be used to meet the missions of the Department and those of other agencies. I can assure you that I understand the important role supercomputing plays in scientific discovery."
Secretary Bodman



Leadership computing is a State of Tennessee priority

- **$9M State of Tennessee Investment in the Joint Institute for Computational Sciences**
- **$10M for National Academy Level Joint Faculty**
- **$35M for high speed networks for research and education**
- **$1M/year for Computational Science Initiative for graduate student training and outreach**

"I have recommended funds …to attract more nationally-recognized faculty members (jointly with ORNL)…. There is an opportunity today…. to rapidly become world class in some areas like supercomputers, materials science, and nanotechnology.

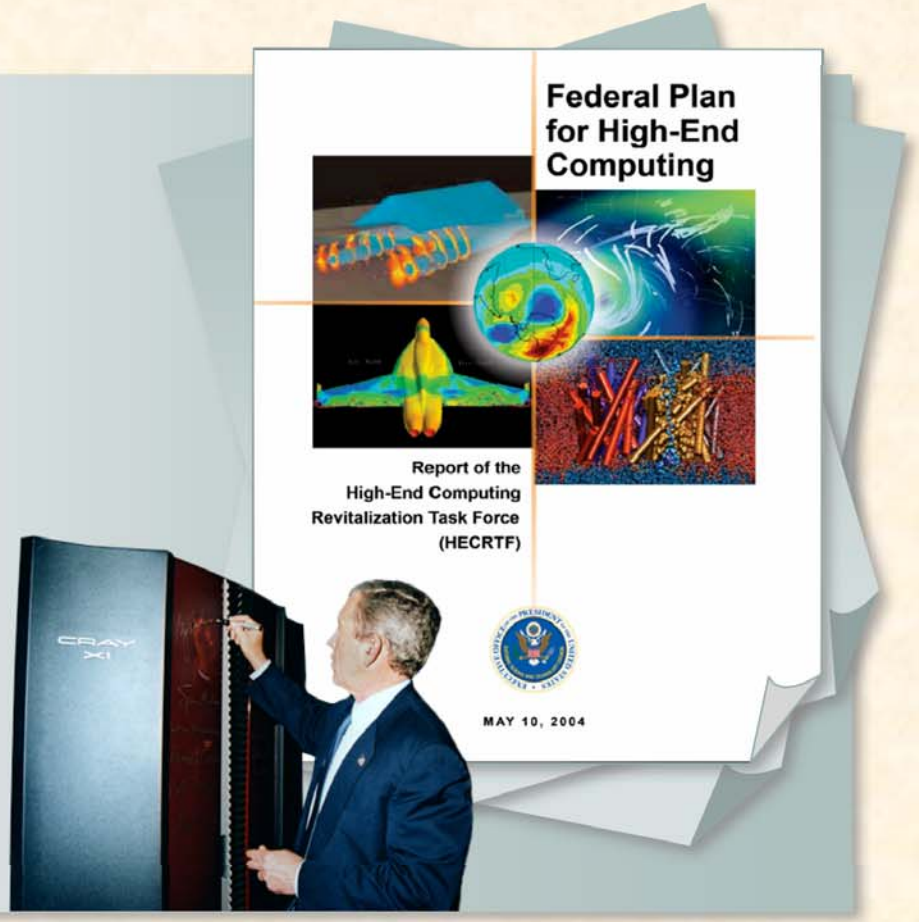
….Our pioneer ancestors wouldn't have known what supercomputers were, but I believe they would have understood our aspirations perfectly."

- Gov. Bredesen, State of the State Speech, January 31, 2005

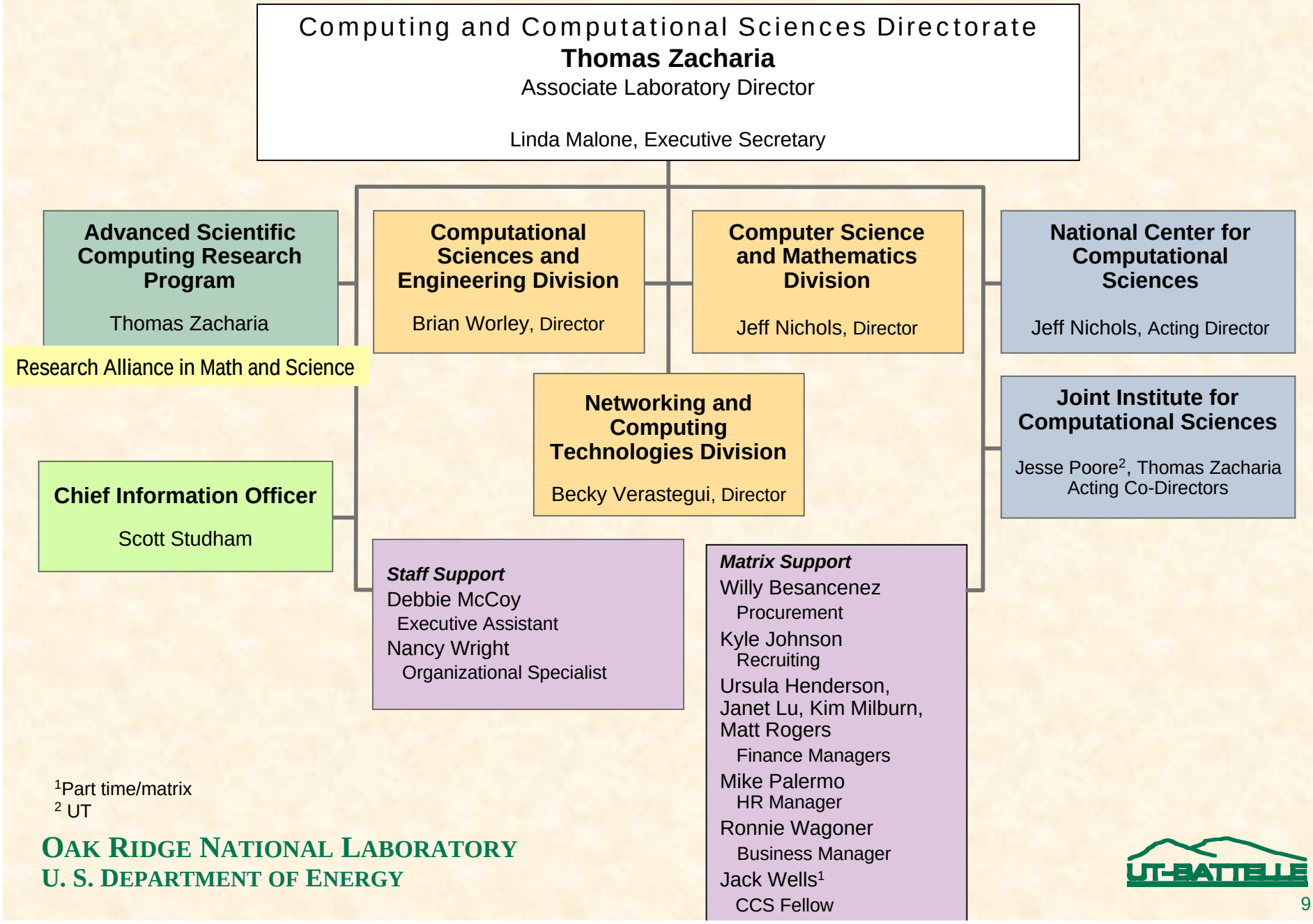
Leadership computing a key enabler of science and engineering

"The goal of such systems [leadership systems] is to provide computational capability that is at least 100 times greater than what is currently available."

"…Leadership Systems are expensive, typically costing in excess of $100 million per year...."



Organized for success



[1]Part time/matrix
[2] UT

New world-class facility capable of housing leadership class computers

- $72M private sector investment in support of leadership computing
- Space and power:
  - **40,000 ft² computer center with 36-in. raised floor, 18 ft. deck-to-deck**
  - **8 MW of power (expandable) @ 5c/kWhr**
- High-ceiling area for visualization lab (Cave, Powerwall, Access Grid, etc.)
- Separate lab areas for computer science and network research

Leadership Computing for Science

Critical for success in key national priorities

Office of Science research priorities

Computational design of innovative nanomaterials

Predictive understanding of microbial molecular and cellular systems

Full carbon cycle in climate prediction, IPCC

Simulation of burning plasma, Fusion Simulation Project

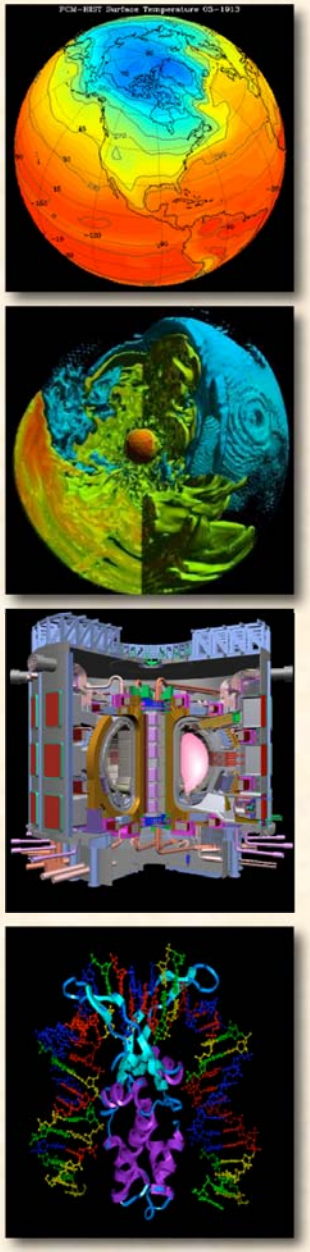
Terascale Supernovae Simulation

Theory, Mathematics, Computer Science

National Leadership-Class Computing Facility for Science

At forefront in computing and simulation

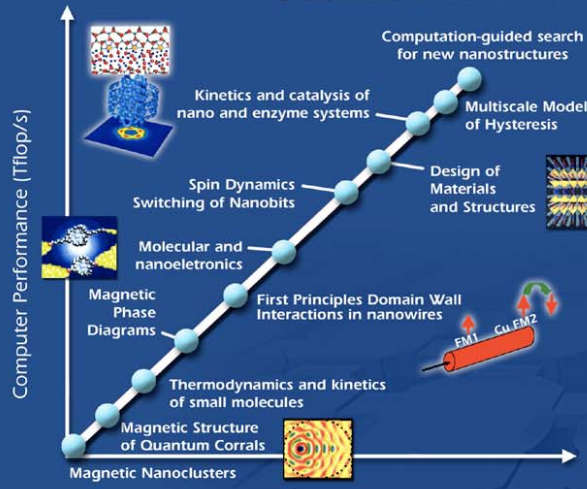
- **Leading partnership in developing the National Leadership Computing Facility**
  - **Leadership-class scientific computing capability**
  - **100 teraflops by 2006; 250 teraflops by 2007**
- **Attacking key computational challenges**
  - **Climate change**
  - **Nuclear astrophysics**
  - **Fusion**
  - **Materials sciences**
  - **Biology**
- **Providing access to our computational resources through high-speed networking**




National Leadership Computing Facility
May 12, 2004
FCW.COM
Oak Ridge gets super win
"Feds spark high-end computing resurgence"
CNN
Wednesday, May 12, 2004
U.S. Moves to Build Top Supercomputer
ITmedia News
ニュース
ComputerWeekly
U.S. Energy Dept. Awards $25M Grant for Supercomputer Build
COMPUTERWORLD
Energy Department Grant Spurs Work on Supercompute
The $25M grant went to the Oak Ridge National Laborator
BusinessWeek
Where No Computer Has Gone B
CBS 2
WCBS-TV NEW YORK
cbsnewyork.com
Uncle Sam Wants World's Fastest Computer
Want To Surpass Japanese Supercomputer
TechWeb
The Business Technology Network
Tennessee is a Rising Star in Supercomputing
The Atlanta Journal-Constitution
Computer to be more than a bit faster
Supercomputer-generated "power wall" at Oak Ridge, Tenn., National Laboratory illuminates climate change
cnews
Tech News
U.S. to Build Civilian Supercomputer
The Oak Ridger
ORNL Nabs Supercomputer Deal
LAB CHIEF: 'Oak Ridge will help lay the foundation for our country's next generation of scientific discovery.'
WASHINGTON TECHNOLOGY
DOE Orders World's Fastest Supercomputer
San Francisco Chronicle
SFGate
U.S. Government Moves to Build World's Fastest Civilian Computer
矽谷科技
全球最快速民用科研電腦
能源部將在田納西州的美國橡樹嶺國家實驗室(Oak Ridge National Laboratory)興建全球最快速的民用科研電腦，這套電腦將會置在田萬平方呎的運算科學中心內，這系統每秒運算能力高達50兆次，這台電腦將於2006年開始運作。
(美聯社)
CENTER FOR COMPUTATIONAL SCIENCES
OAK RIDGE NATIONAL LABORATORY
GLOBEANDMAIL.COM
U.S. Aims to Regain Computer Speed Lead
DOE Leadership-Class Computing Capability for Science will be Developed at Oak Ridge National Laboratory
Office of Science
U.S. DEPARTMENT OF ENERGY

Delivering Science and Leadership in High-end Computing

Nanoscience



Expected Outcomes

5 years

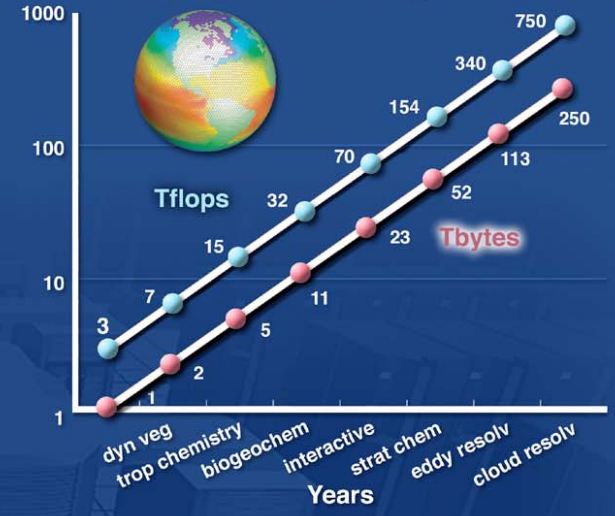
- Realistic simulation of self-assembly and single-molecule electron transport
- Finite temperature properties of nanoparticles/quantum corrals

10 years

- Multi-scale modeling of molecular electronic devices
- Computation-guided search for new materials/nanostructures

Climate

Machine and Data Requirements



Expected Outcomes

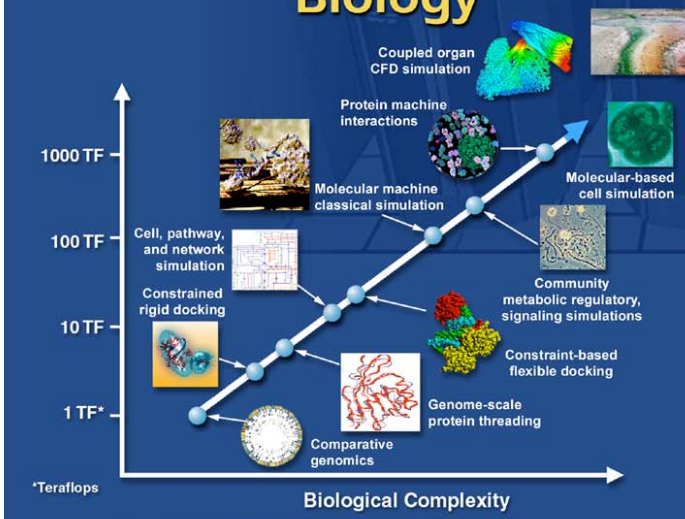
5 years

- 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



High-performance computing is essential to the high-throughput experimental approach.

Expected Outcomes

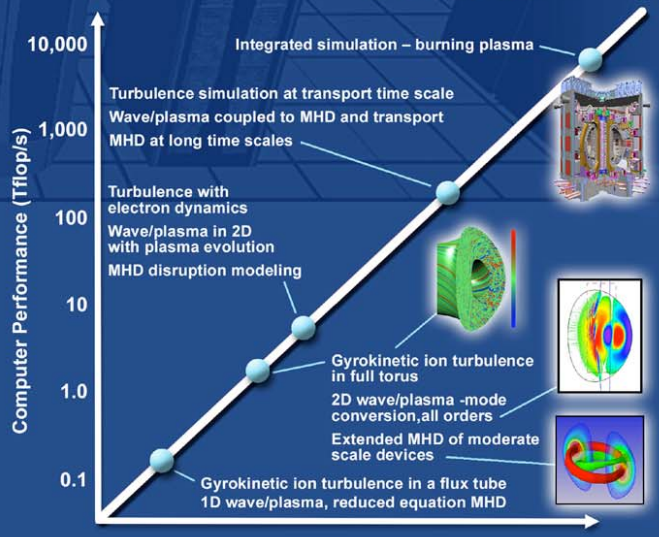
5 years

- 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

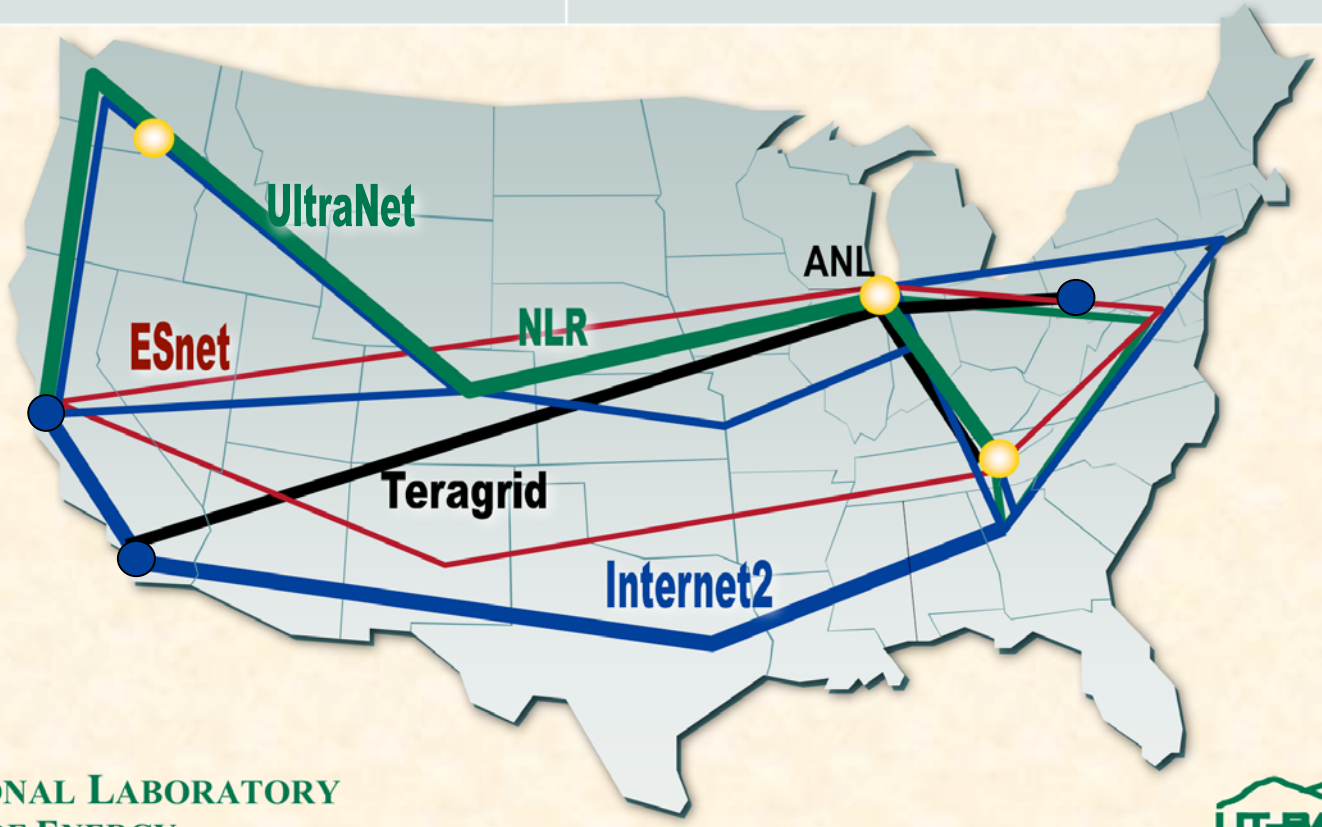
- Develop quantitative, predictive understanding of disruption events in large tokamaks
- Begin integrated simulation of burning plasma devices - multi-physics predictions for ITER

Center for Computational Sciences
Oak Ridge National Laboratory

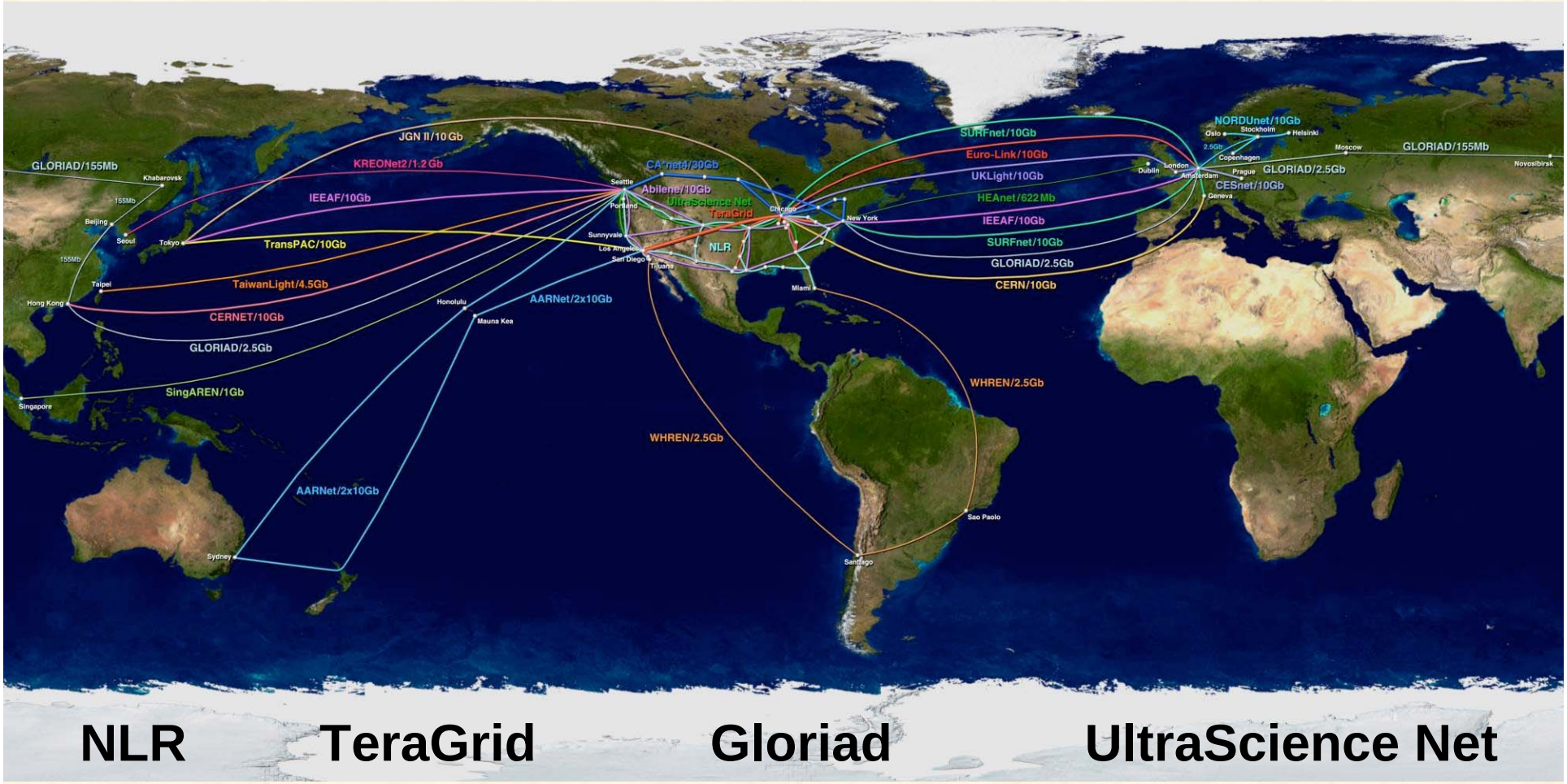
Office of Science
U.S. Department of Energy

Leadership in Networking

Connected to major science networks	
OC48 to ESNET (provisioned by ESNET)	1 - 4 x 10Gb to NSF Teragrid
10Gb to Internet2	2 x 10Gb Ultranet
4 x 10Gb to National Lambda Rail	180 x 10Gb Futurenet



Imbedded in the grid



NLR **TeraGrid** **Gloriad** **UltraScience Net**

The Spallation Neutron Source

Total cost: $1.4 billion

- **Operational in 2006**
- **World's most powerful pulsed spallation source**
- **With complementary resources at the High Flux Isotope Reactor, Oak Ridge will lead the world in neutron scattering**

Maintain active dialogue with academia, industry, labs, and centers

- **Joint Institute for Computational Sciences**
  - State-of-the-art distance learning center
  - Incubator suites, joint faculty offices, conference facilities
  - Strong student and postdoctoral programs
  - Summer institutes for interdisciplinary research
  - Annual conference in computational sciences
- **Educational outreach through Research Alliance in Math and Science program**
- **Industrial outreach through Computational Center for Industrial Innovation**
- **International collaborations in computational sciences**
  - Guest scientists and visiting scholars

Committed to strong university partnerships

ORAU
Duke University
Battelle
NC State University
Florida State University
Georgia Tech
University of Virginia
Virginia Tech

Oak Ridge Center for Advanced Studies
- 21st century think tank
- Focused on complex interdisciplinary problems

Collaborative research
- More than 100 universities

Joint hiring
- Governor's Chairs
- 45 joint faculty with 6 universities

Joint institutes
- Heavy ion research
- Neutron sciences
- Biological sciences
- Computational sciences

User facilities
- 18 at ORNL
- Thousands of university users

OAK RIDGE NATIONAL LABORATORY

Questions?