

Training the Scientific Workforce of the 21st Century at Oak Ridge National Laboratory

Presented to

ACSESS

Applied Computational Science & Engineering Student
Computational Science Curriculum Development

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Oak Ridge Leadership Computing Facility

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Today, ORNL is DOE's largest science and energy laboratory



- \$1.5B budget
- 4,650 employees
- 4,000 research guests annually
- \$500 million invested in modernization
- United States most powerful open scientific computing facility
- Nation's largest concentration of open source materials research
- Nation's most diverse energy portfolio
- Operating the world's most intense pulsed neutron source
- Managing the billion-dollar U.S. ITER project

ORNL is well positioned to deliver science and technology for energy

We have an extraordinary set of assets

- Outstanding tools for materials R&D
- World-leading systems for open scientific computing
- BioEnergy Science Center
- Growing strength in climate change impact R&D
- The nation's broadest portfolio of energy programs
- Unique resources for nuclear technology
- Robust national security programs

Our challenge:
Use these assets to
enable science and
technology
breakthroughs that
transform our
energy future



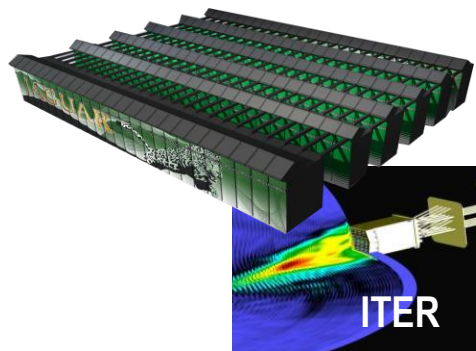
Delivering science and technology:

We lead major R&D programs for DOE and other customers

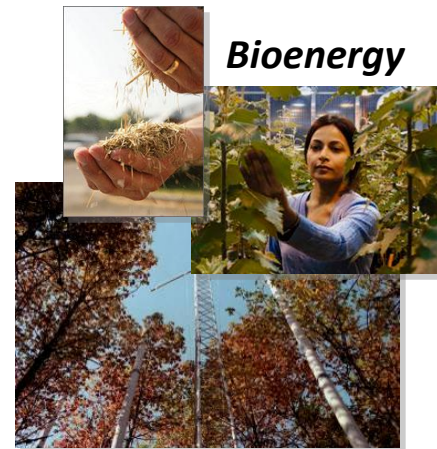
Energy Technologies



Ultrascale Computing

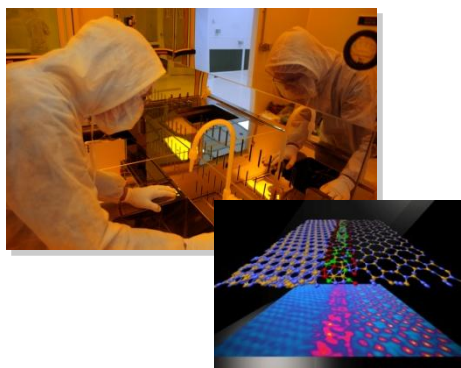


Bioenergy



Climate

Materials at the Nanoscale



Neutron Sciences



Nuclear Energy

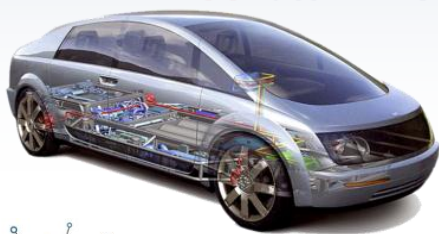


National Security



We partner with industry to put our energy innovations to work

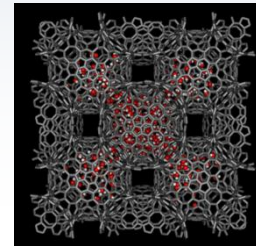
Transformational transportation technologies



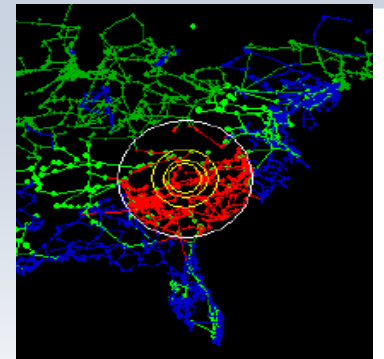
High-efficiency green buildings



Advanced materials for energy applications



Electric grid reliability and resilience



Leading the development of ultrascale scientific computing

- Leadership Computing Facility:

- United State's most powerful open scientific computing facility
- Jaguar XT operating at 2.33 petaflops
- Exascale system by the end of the next decade
- Focus on computationally intensive projects of large scale and high scientific impact

- Addressing key science and technology issues

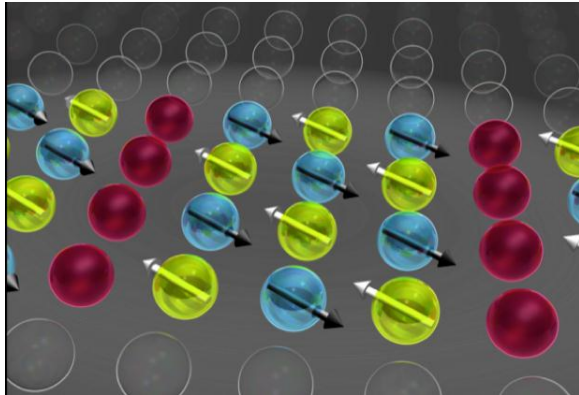
- Climate
- Fusion
- Materials
- Bioenergy



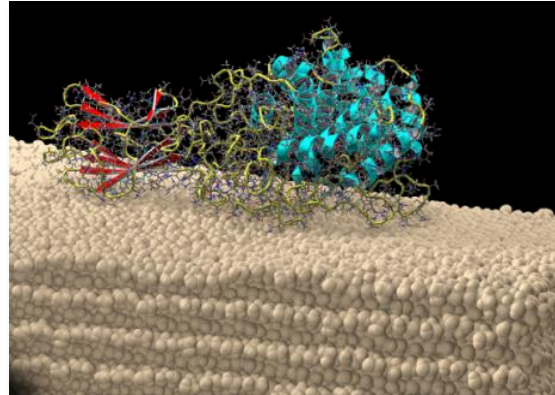
The world's most powerful system for open science

High-performance computing is opening new research frontiers

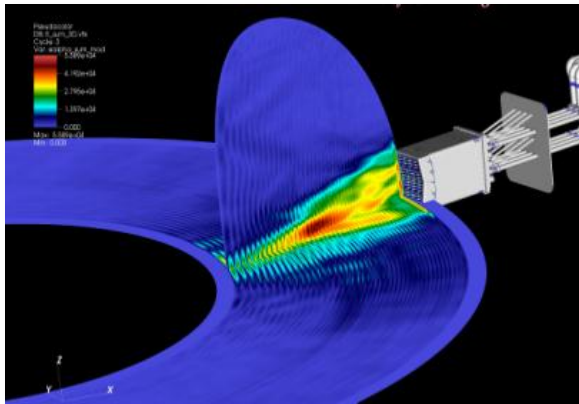
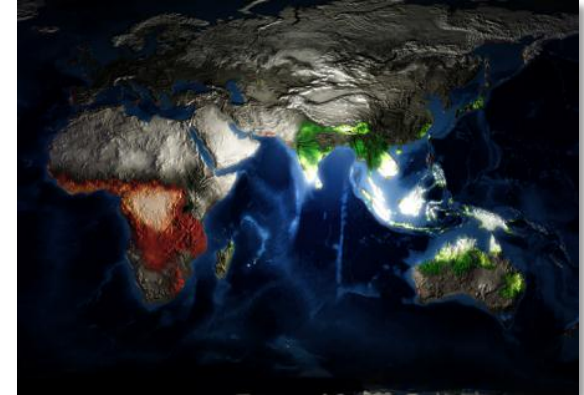
Physics of high-temperature superconducting cuprates



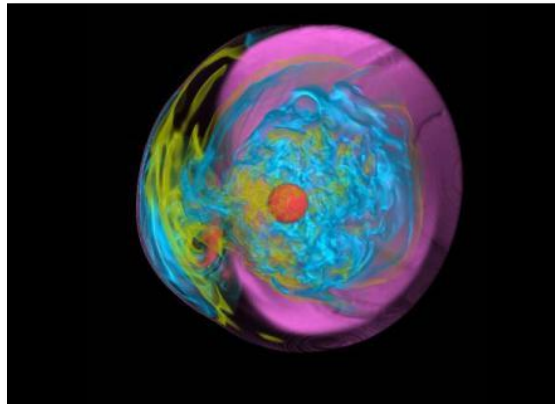
Protein structure and function for cellulose-to-ethanol conversion



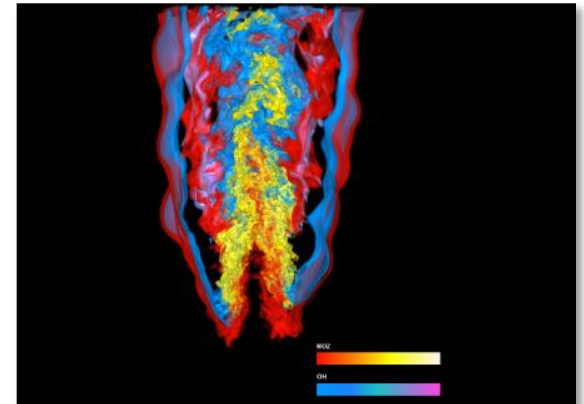
Global simulation of CO₂ dynamics



Optimization of plasma heating systems for fusion experiments



Fundamental instability of supernova shocks



Next-generation combustion devices burning alternative fuels

Curriculum development

- **What skills/topics academia should include in its curriculum design for computational science to make students more competitive in the workforce?**
 - **Why is architecture/hardware important to scientific computing**
 - **What is the big and broad picture**
 - **Relevance to national mission, industry, customer**
 - **Relationship between simulation and experiment/applications**
 - **Ability to see how techniques can be applied to various domains**
 - **What are new areas of research that will be relevant when I graduate**
 - **Prepare students for new focus areas**

Importance of architecture

ORNL Completes First Phase of Jaguar Upgrade

US's fastest computer gets upgrade to extend Leadership Computing for DOE/SC

- Oak Ridge Leadership Computing Facility (OLCF) has completed the upgrade of the Jaguar supercomputer from a Cray XT5 to Cray's latest XK6 technology
- Jaguar has new AMD 16-core processor, double the memory, and a faster, more scalable network
- Jaguar now has available slots for over 18,000 of NVIDIA next generation of computational accelerators
 - Next generation accelerators will be available to ORNL in Fall 2012.
 - Fully populated system capable of 28.8 petaflops
- Energy Secretary Chu was briefed by OLCF's Project Director Buddy Bland on progress made on Jaguar's upgrade to Titan during a recent visit to ORNL
- The upgraded system is already doing work that couldn't be done before the upgrade
 - Ramgen Power Systems accelerate their design of shock wave turbo compressors for carbon capture and sequestration
 - Molecular Dynamics codes are using the faster network to address problems that were too complex before the upgrade



U.S. Energy Secretary Steven Chu examines an NVIDIA accelerator that is part of the recently completed upgrade of the Jaguar supercomputer

Today's Jaguar Supercomputer	
AMD Processing Cores	299,008
System Memory	600 TB
Computational Accelerators Today (Current Generation)	960
Available slots for Accelerators (Awaiting Next Gen Accelerators)	18,688

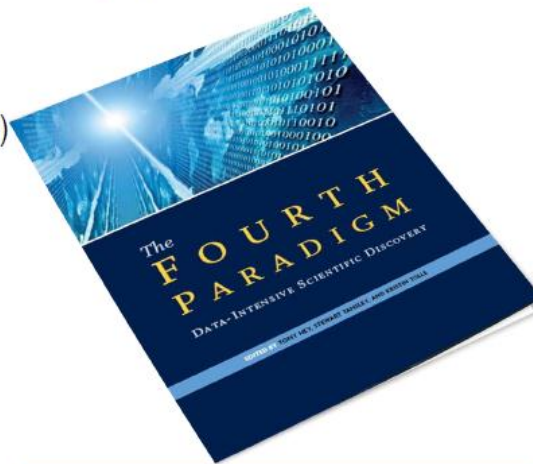
New areas of research

**External speakers,
conferences, workshops,
paper seminars**

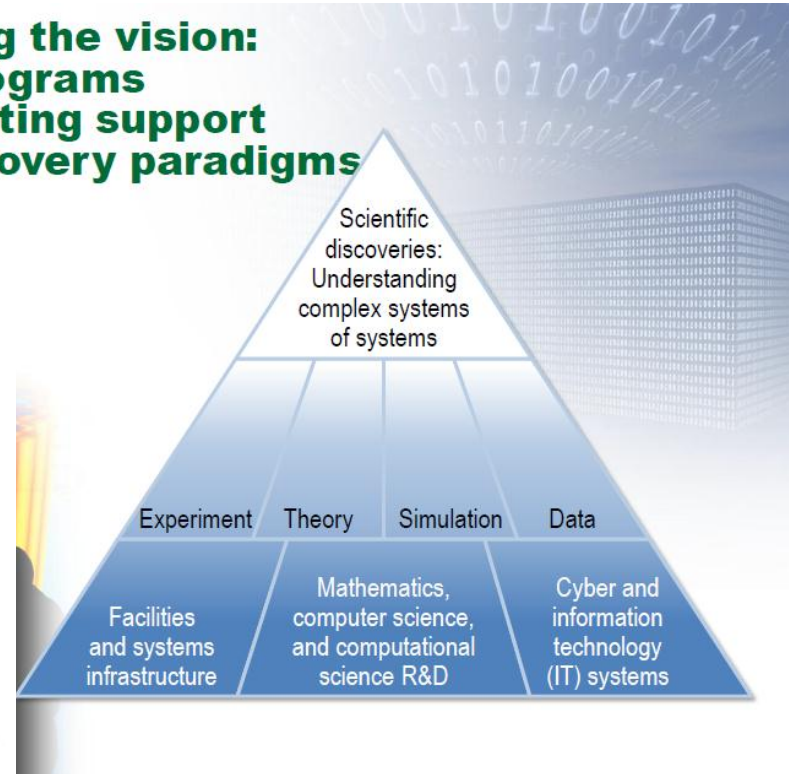
**Executing the vision:
ORNL programs
in computing support
all 4 discovery paradigms**

**Data joins experiment, theory, and
simulation in the discovery process**

- Sources
 - Experiments (e.g., science facilities)
 - Output from simulations
 - Human activity (e.g., social media)
 - Sensors (e.g., satellite data)
- Potential applications
 - Medicine
 - Economics
 - Science
 - Disaster recovery
 - National security



**Bringing many types of disparate data
to bear on a particular discovery
process or mission outcome is one of
the new frontiers of science and
technology.**



Opportunities at ORNL

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- The screenshot shows the Oak Ridge National Laboratory website. On the left is a vertical navigation menu with links: Home, About ORNL, ORNL History, ORNL News, ORNL Research, ORNL Facilities, ORNL Education, ORNL Outreach, ORNL Employment, ORNL Security, ORNL Legal, ORNL Privacy, ORNL Accessibility, ORNL Contact Us, and ORNL Search. The main content area features a banner with the text 'Real Science, Real Life.' and a sub-header 'A new look for ORNL in different angle'. Below this is a section titled 'New Real Science' with a grid of links: Advanced Materials, Biological Sciences, Chemical Sciences, Computer Sciences, Earth and Environmental Sciences, and Engineering Sciences. To the right of the grid is a sidebar with links: ORNL Research, ORNL Facilities, ORNL Education, ORNL Outreach, ORNL Employment, ORNL Security, ORNL Legal, ORNL Privacy, ORNL Accessibility, ORNL Contact Us, and ORNL Search. Below the grid is a section titled 'Oak Ridge National Laboratory' with a photo of a woman and a man. To the right of the photo is a section titled 'New Real Science' with a list of links: Advanced Materials, Biological Sciences, Chemical Sciences, Computer Sciences, Earth and Environmental Sciences, and Engineering Sciences. Below the list is a section titled 'ORNL Research' with a list of links: ORNL Research, ORNL Facilities, ORNL Education, ORNL Outreach, ORNL Employment, ORNL Security, ORNL Legal, ORNL Privacy, ORNL Accessibility, ORNL Contact Us, and ORNL Search.

At a Glance: Student, Postdoctoral, and Fellow Programs

Undergraduate	Graduate	Postdoctoral	Faculty	Fellows*
• DHS HS-STEM Internship • HERE@ORNL • Laboratory Technology Program • Nuclear Engineering Science Laboratory Synthesis Internship • Research Alliance in Math and Science • Science Undergraduate Laboratory Internship	• Advanced Short-Term Research Opportunity • HERE@ORNL • Nuclear Engineering Science Laboratory Synthesis Internship • Research Alliance in Math and Science • Post-Master's Research Participation	• Advanced Short-Term Research Opportunity • Instrument Development Fellows • Postdoctoral research associates	• DHS Summer Research Team • Visiting Faculty Program • HERE@ORNL • NRC Faculty Research Participation • Sabbaticals and summer research	• Eugene Wigner Fellows • Alvin M. Weinberg Fellows • Clifford Shull Fellows: Neutron science • Alston Householder Fellows: Scientific computing

* ORNL employment program

<http://jobs.ornl.gov>

Oak Ridge National Laboratory:

Meeting the Challenges of the 21st Century

