



U.S. DEPARTMENT OF  
**ENERGY**

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# ASCR ARRA Update

November 4, 2009

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# American Recovery and Reinvestment Act (Recovery Act)

## ASCR's Recovery Act Projects (\$153.9M)

- Advanced Networking Initiative (\$66.8M)
  - Testbed to demonstrate for 100Gbps optical networking technologies
  - Research to develop tools for 100Gbps optical networks
- Leadership Computing Facility Upgrades (\$19.9M)
  - Six-core upgrade to Oak Ridge LCF machine to take the OLCF to ~2 Petaflops
- Advanced Computer Architectures (\$5.2M)
  - Research on next generation technologies
- Magellan (\$32.8M)
  - Research to demonstrate viability of cloud computing for mid-range computational science
- SciDAC-e (\$29.2M)
  - Supplement and leverage existing SciDAC investments to advance the high performance computational capabilities of the BES - Energy Frontier Research Centers; Extra user support for Energy related projects at the Leadership Computing and NERSC facilities; Applied mathematics research in support of DOE electricity grid efforts.



## ■ ASCR Magellan Project Summary

- \$32.8M project at NERSC and ALCF
- ~100 TF/s compute cloud testbed (across sites)
- Petabyte-scale storage cloud testbed

## ■ Project Progress

- Funding distributed to ANL and LBNL based on peer reviewed proposal;
- ANL and LBNL have issued contracts to procure compute and first stage of data hardware;
- Coordination with ANI has begun
- First availability of cycles expected January 2010
- Joint Magellan-ANI PI meeting scheduled at SC09

## ■ Cloud questions to explore on Magellan:

- Can a cloud serve DOE's mid-range computing needs?  
→ More efficient than cluster-per-PI model
- What part of the workload can be served on a cloud?
- What features (hardware and software) are needed of a "Science Cloud"? (Eucalyptus at ALCF; Linux at NERSC)
- How does this differ, if at all, from commercial clouds?

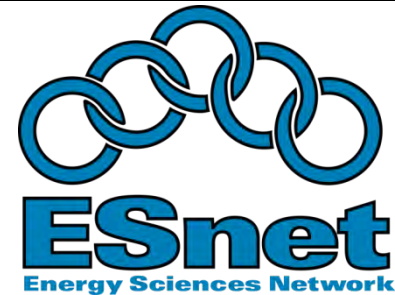




# ANI: Advanced Network Initiative

## DOE Science Network challenges:

- 72% annual growth in traffic since 1990 compared to 45% at AT&T
- Growth is accelerating, rather than moderating
- Scientific collaborations were becoming more international, e.g. CERN, ITER, EAST Tokamak, etc.



## Advanced Networking Initiative (ANI):

- Evaluate transport technologies for optical fiber backbone
- Deploy prototype 100Gbps capable network connected to NERSC, ALCF, OLCF and transatlantic peering point in New York
- Develop and support an experimental network environment allowing researchers to test new concepts in networking



# Advanced Network Initiative Topology





# Leadership Computing Upgrade

## ASCR Deploys World's Most Powerful Computer for Open Science at ORNL

- ORNL's Cray XT5 was upgraded from 2.3 GHz quad-core processors to 2.6 GHz 6-core processors.
- Increases system peak performance to 2.3 Petaflops
- Increases allocatable hours by 50% (from 1 billion to 1.5 billion hours)
- Upgrade was done in steps, keeping part of the system available
- System undergoing acceptance testing now



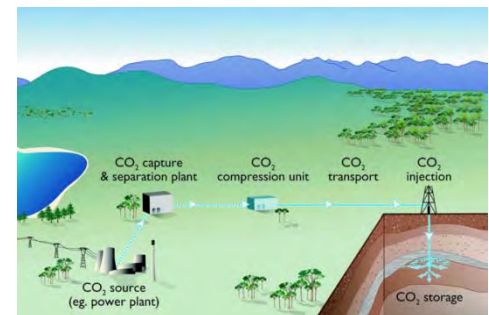
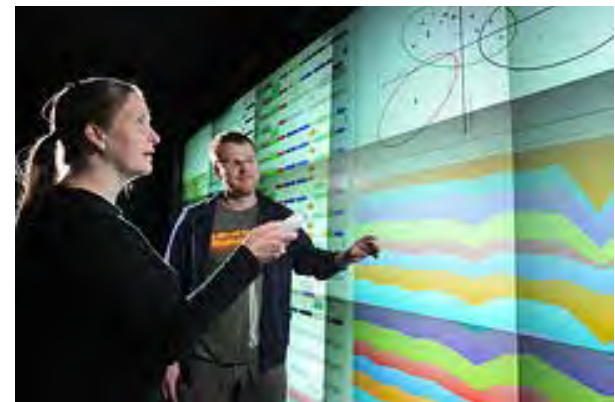
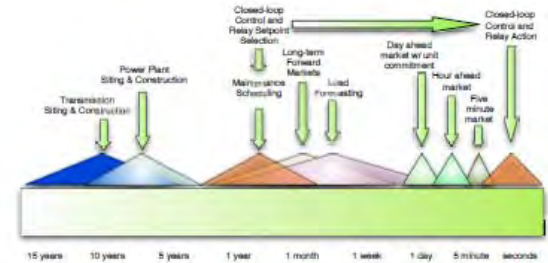


- **What it is:**
  - New effort to provide early access to DOE researchers of technologies emerging from IBM PERCS effort.
  - Enhancement of University of California, Berkeley RAMP effort to provide focused research on flexible simulations of performance of scientific applications on next generation microprocessors.
  - Both proposals were in hand and were peer reviewed.
- **Progress:**
  - Funding in place at ORNL for IBM PERCS effort
  - Grant Paperwork for RAMP effort submitted to Chicago for processing



# SciDAC-e Overview

- **Research grants and national laboratory projects to develop mathematical techniques and algorithms to enable a bigger, better, and a smarter electric grid (\$8.3M)**
  - 7 applied mathematics projects awarded.
- **Approximately new 30 postdoctoral at ASCR facilities to offer assistance to SciDAC-e projects and other energy users awarded. (\$10M)**
- **Supplemental awards to existing SciDAC efforts to support BES EFRCs to develop a high-performance computing capability relevant to the goals of the EFRC (\$10.86M)**
  - In progress







- “Robust Optimization for Connectivity and Flows in Dynamic Complex Networks”; Balasundaram- Oklahoma State; Butenko- Texas A&M; Boginski, Uryasev- University of Florida
- “Reconfiguring Power Systems to Minimize Cascading Failures: Models and Algorithms”; Bienstock- Columbia; Wright, Dobson, Hiskens, Linderoth- Wisconsin
- “New Approaches for Rare-event Simulation and Decision Making”; Shortle, Chen, Noblis, Fischer, Masi- George Mason
- “Analysis and Reduction of Complex Networks under Uncertainty”; Marzouk- MIT; Debusschere, Najm- Sandia; Knio- Johns Hopkins; Ghanem- USC
- “Optimization and Control of the Electric Power Systems”; Meza, Pinar- LBNL; Thomas, Zimmerman- Cornell
- “Advanced Kalman Filter for Real-Time Responsiveness in Complex Systems”; Huang, Nieplocha, Schneider- PNNL; Welch, Bishop- University of North Carolina
- “Extending the Realm of Optimization for Complex Systems: Uncertainty, Competition and Dynamics”; Shanbhag, Basar, Mehta, Meyn- UIUC

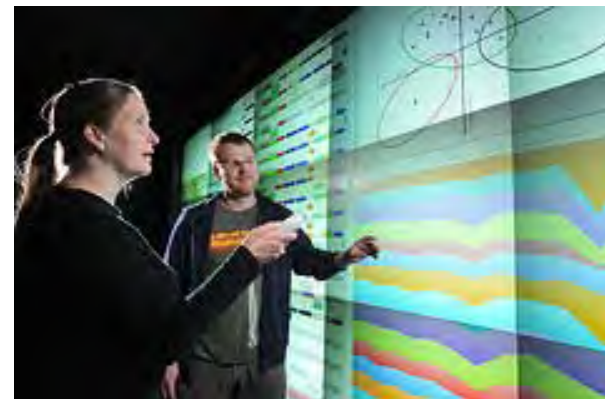


### Overview

- Based on Argonne's existing *Directors Postdoc Program*  
([www.dep.anl.gov/postdocs/Directorpostdoc.htm](http://www.dep.anl.gov/postdocs/Directorpostdoc.htm))
- 10 member search committee
  - Representation from all of the Argonne's research directorates
  - Representation from each of the Argonne led Energy Frontier Research Centers
- Requirements
  - Curriculum vitae
  - Research proposal (< 2 pages)
  - List of publications and significant presentations
- \$3.125M became available 9/28/09 for approximately 11 Postdocs

### Progress (10/28/2010)

- 80 applications received
- 4 have interviewed
- 1 offer made and accepted
  - Center for Nanoscale Material's Theory and Modeling Group under the supervision of Dr. Stephen Gray, within the ALCF mentored by Graham Fletcher – January 2010



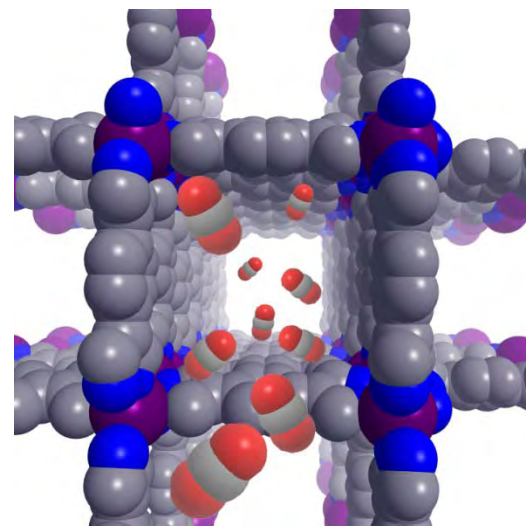


- NERSC received \$3.125M in stimulus money for this initiative in late September
- Funds 8 post-docs for ~25 months each and their costs (travel and computers)
- Goal is to provide computational capability directly to key areas of energy-related research
- Most of the post-docs will be directly embedded in a specific application area, while also spending approximately half of their time at the NERSC facility, to directly interact with NERSC staff to ensure there is communication of new ideas and “what works”



- Project is aimed at parallelization and performance improvement
- Jihan Kim has started work with the Berkeley EFRC's
- Computational intensive algorithms identified in Q-Chem
- Implementing parallelization of analytical gradient evaluation in resolution-of-the-identity second-order Møller-Plesset perturbation theory (RI-MP2)
- Some MPI exists, however several steps require parallelization
- Prospects for OpenMP/hybrid parallelization are available and may be considered

- Capture of CO<sub>2</sub> from gas mixtures requires molecular modeling and control
- Q-Chem provides valuable input for EFRC studies





- Oak Ridge Leadership Computing Facility (OLCF) received 3.75M in stimulus money September to
  - Support approximately 10 SciDAC-e PostDocs and
  - Host a Summer Institute on focused on utilization of computational capability at large high performance computing centers
- Progress
  - Rooms reserved for Summer Institute to be held August, 2010
  - Identified climate, chemistry, materials science, biology, combustion, fusion, nuclear energy and computer science as areas for targeted recruitment of PostDocs