



U.S. DEPARTMENT OF
ENERGY

ASCR ARRA Update

March 30, 2010

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Advanced Scientific Computing Research



American Recovery and Reinvestment Act (Recovery Act)

ASCR's Recovery Act Projects (\$154.9M)

- Advanced Networking Initiative (\$66.8M)
 - Testbed to demonstrate and build tools for 100Gbps optical networking technologies
- Leadership Computing Facility Upgrades (\$19.9M)
 - Six-core upgrade to Oak Ridge LCF machine delivered 2.2 Petaflops
- Advanced Computer Architectures (\$5.2M)
 - Research on next generation technologies
- Magellan (\$33M)
 - Research to demonstrate and build tools to enable scientists to utilize cloud computing resources for mid-range computing needs
- SciDAC-e (\$30M)
 - 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.



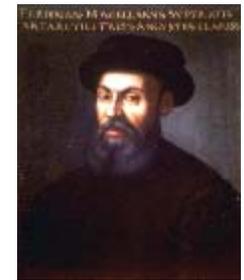
■ ASCR Magellan Project Summary

- \$32M 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 procured and installed compute and first stage of data hardware
- Identified experts to review integrated research demonstration topics (Q1)
- Joint Magellan-ANI PI meeting was conducted at SC09
- Coordination with ANI on-going
- First cycles now available



■ Cloud questions to explore on Magellan:

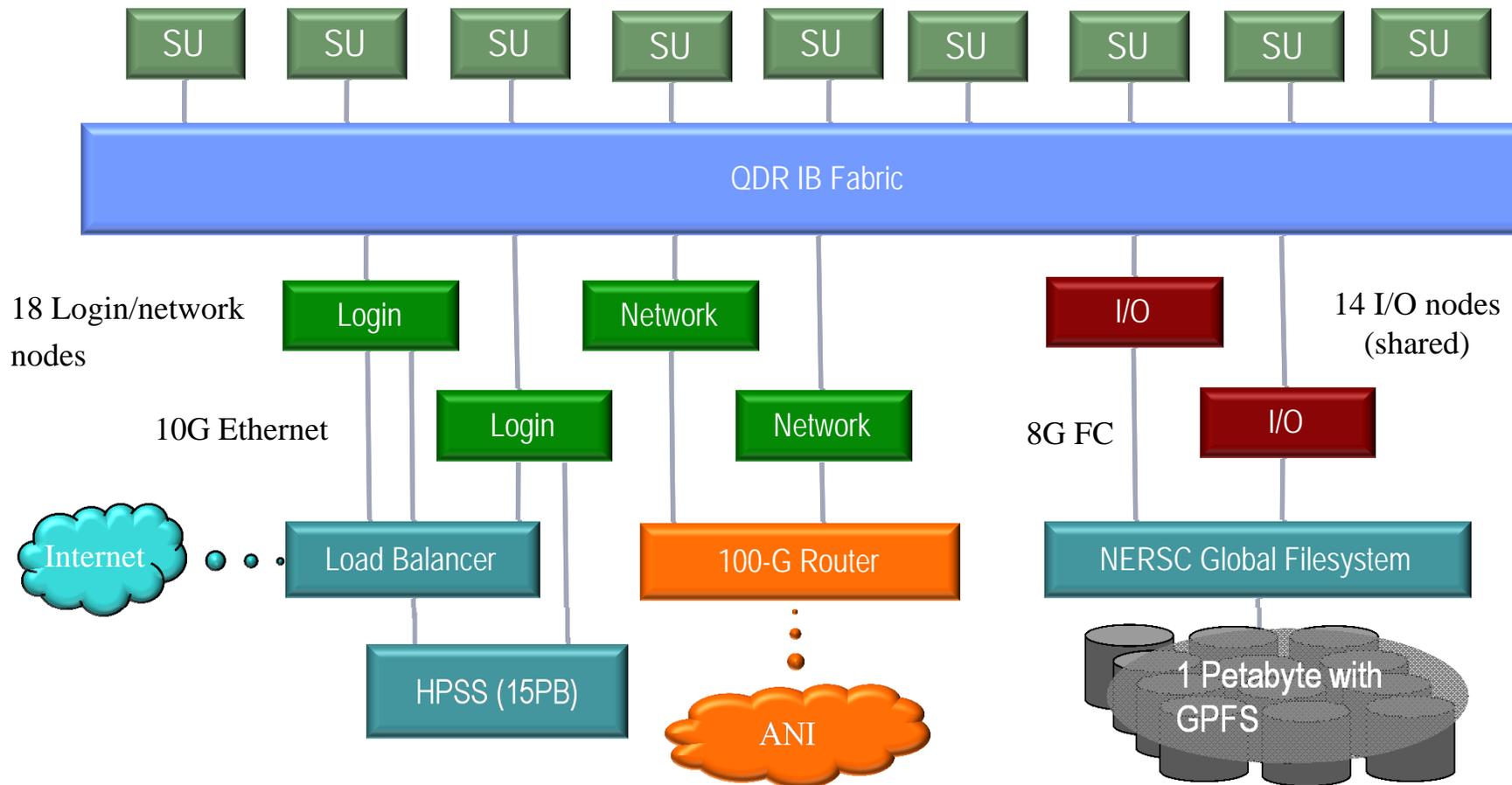
- Can a cloud serve DOE's mid-range computing needs?
 - More efficient than cluster-per-PI model
- What part of the workload can be served on a cloud?
- What features (hardware and software) are needed of a "Science Cloud"? (Eucalyptus at ALCF; Linux at NERSC)
- How does this differ, if at all, from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



NERSC Magellan Cloud Hardware

720 nodes, 5760 cores in 9 Scalable Units (SUs) → 61.9 Teraflops

SU = IBM iDataplex rack with 640 Intel Nehalem cores



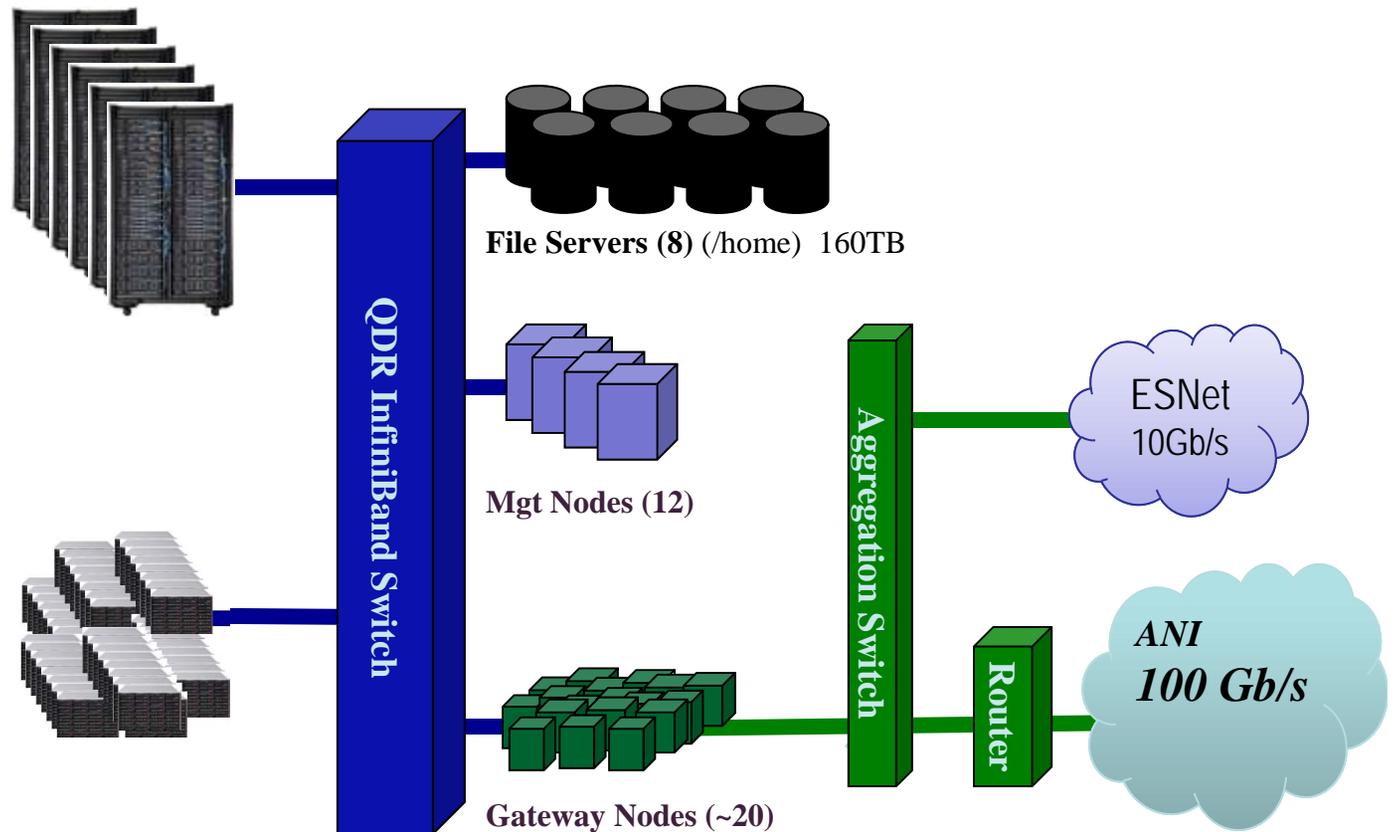


Compute

504 Compute Nodes
Nehalem Dual quad-core 2.66GHz
24GB RAM, 500GB Disk
QDR IB link
Totals
4032 Cores, 40TF Peak
12TB RAM, 250TB Disk

Active Storage

~100 Compute/Storage Nodes
~10TB FLASH/SSD Storage
~500TB Disk Storage





Key is flexible and dynamic scheduling of resources



- Runtime provisioning of software images
- Rolling upgrades can improve availability
- Ability to schedule to local or remote cloud for most cost effective cycles

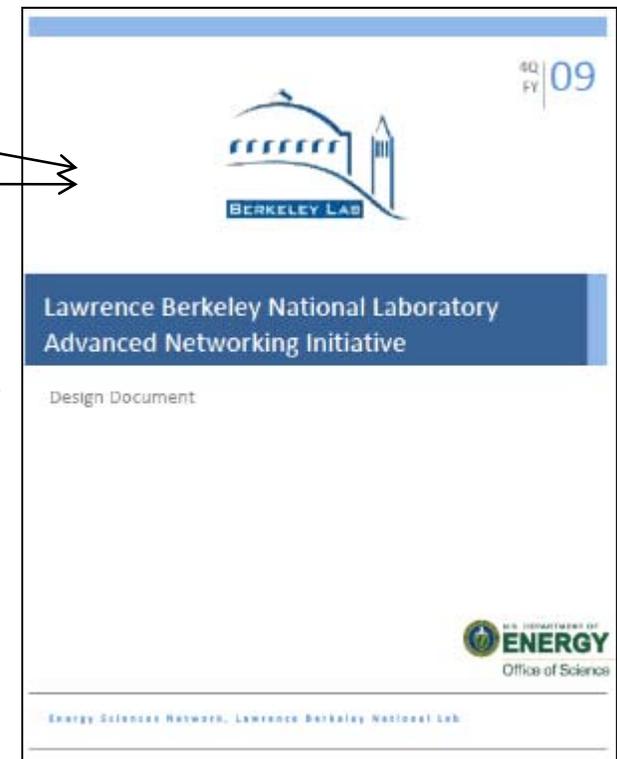


ANI: Advanced Network Initiative

The goal of the ANI project is two-fold:

- Accelerate the commercialization of 100 Gigabit per second (Gbps) networking technologies by deploying a national-scale prototype network that will span four distinct geographic regions, connecting the three major ASCR computing facilities and the New York multi-agency peering point providing transatlantic Research and Education (R&E) connectivity at 100 Gbps.
- Complement the prototype 100 Gbps network with a testbed providing an experimental network research environment at sufficient scale to usefully test experimental approaches to next generation networks and applications.

- Funds sent to all contractors and grant recipients
- Program review of preliminary design for ChiExpress and design posted on ASCR website: <http://www.sc.doe.gov/ascr/Misc/ASCRRecovery.html>
- Project Plan (design document) posted on ASCR website:
 - <http://www.sc.doe.gov/ascr/Misc/ASCRRecovery.html>
- Testbed Timeline
 - Feb 2010: Initial 'table top' node hardware setup at LBNL
 - Sept 2010: 10 Gbps 'table top' testbed available to researchers
 - April 2011: 10/100 Gbps WAN testbed available to researchers
 - Jan 2012: full 100 Gbps WAN testbed available to researchers.
- Upcoming
 - Solicitation for second round of research topics for use of test bed (Q3-Q4).



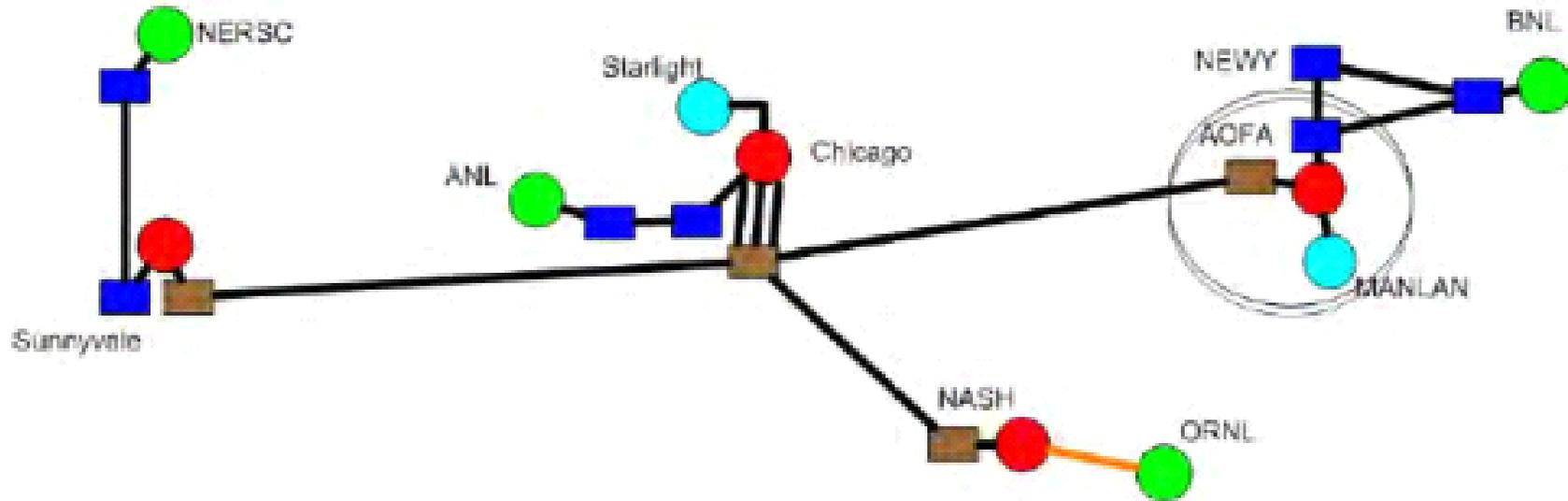


Advanced Network Initiative Topology





ANI: 100 Gbps Prototype Network Preliminary Baseline Design



Key

-  Carrier Layer 1 device
-  ESnet co-managed Layer 1 device
-  Site Router
-  ANI Router
-  Exchange Point Router
-  ESnet co-managed 100G
-  Site managed fiber

Assumptions:

- co-managed IRU dark fiber for the following paths
- SUNN to NERSC
- Chicago to ANL
- AOFA to BNL

Carriers will provide 100G ethernet circuit

This network provides:

- L3 (routed) service between sites and 100G ANI routers
- L2 (VC) service between sites
- Backbone VCs are hybrid:
 - L2.5 on carrier Link (MPLS)
 - L1 on dark fiber (GMPLS)



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Leadership Computing Upgrade

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

- ASCR reviewed LCF's upgrade implementation plan to ensure upgrade activities result in less than 10% unscheduled downtime for current users. (2009)
- ASCR reviewed and approved acceptance test plan including applications to be used in acceptance test. (2009)
- OLCF Completed acceptance test for quad-core to six-core upgrade of Cray XT5 at Oak Ridge (Q1).
 - ASCR reviewed acceptance test results and approved start of operations.





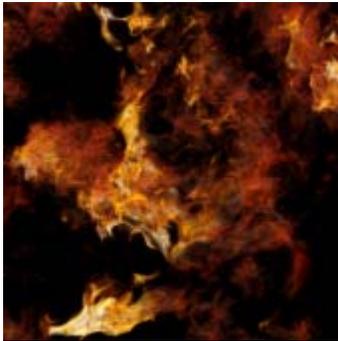
OLCF worked with users to produce scalable, high-performance apps for the petascale

Science Area	Code	Contact	Cores	Total Performance	Notes
Materials	DCA++	Schulthess	213,120	1.9 PF*	2008 Gordon Bell Winner
Materials	WL-LSMS	Eisenbach	223,232	1.8 PF	2009 Gordon Bell Winner
Chemistry	NWChem	Apra	224,196	1.4 PF	2009 Gordon Bell Finalist
Nano Materials	OMEN	Klimeck	222,720	860 TF	
				165 TF	2008 Gordon Bell Finalist
Weather	WRF	Michalakes	150,000	50 TF	
Combustion	S3D	Chen	144,000	83 TF	
Fusion	GTC	PPPL	102,000	20 billion Particles / sec	
Materials	LS3DF	Lin-Wang Wang	147,456	442 TF	2008 Gordon Bell Winner
Chemistry	MADNESS	Harrison	140,000	550+ TF	



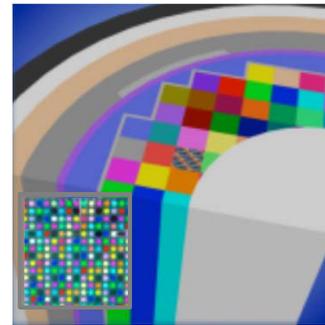


Scientific Progress Resulting from OLCF Upgrade



Turbulence

Understanding the statistical geometry of turbulent dispersion of pollutants in the environment.

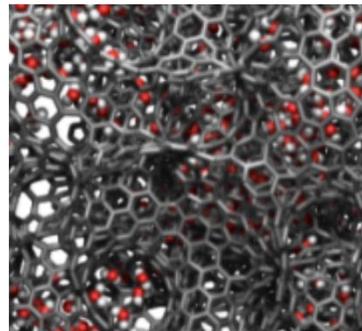


Nuclear Energy

High-fidelity predictive simulation tools for the design of next-generation nuclear reactors to safely increase operating margins.

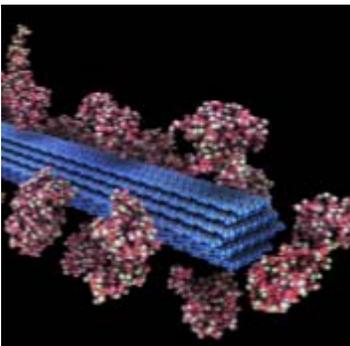
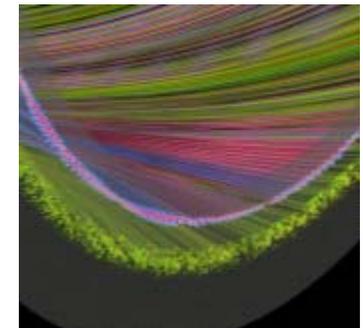
Energy Storage

Understanding the storage and flow of energy in next-generation nanostructured carbon tube supercapacitors



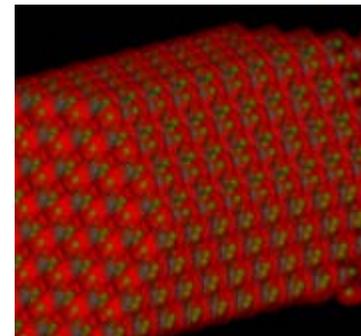
Fusion Energy

Substantial progress in the understanding of anomalous electron energy loss in the National Spherical Torus Experiment (NSTX).



Biofuels

A comprehensive simulation model of lignocellulosic biomass to understand the bottleneck to sustainable and economical ethanol production.



Nano Science

Understanding the atomic and electronic properties of nanostructures in next-generation photovoltaic solar cell materials.

- **What it is:**

- New effort to provide early access to DOE researchers of emerging.
- 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.

- **Goal:**

- By September 30, 2010, complete initial definition of architectural features and performance levels for a system that will meet the needs of at least one science application that requires extreme scale computing while using energy efficiency.

- **Progress:**

- Funding in place at ORNL for IBM PERCS effort
 - Negotiations underway for prototype testbed
- Grant for RAMP Awarded March 19, 2010

- **Review:**

- Established the Charge for Expert Panel peer review with definitions of ratings(Q1).
- Identify Expert Panel Chair and reviewers (Q3).

- **Applied mathematics research in support of DOE electricity grid efforts.**
 - *Robust Optimization for Connectivity and Flows in Dynamic Complex Networks*, Lead PI: Balasundaram (Oklahoma State)
 - *Reconfiguring Power Systems to Minimize Cascading Failures: Models and Algorithms*, Co-PIs: Bienstock (Columbia), Wright (UW-Madison)
 - *Approaches for Rare-event Simulation and Decision Making*, Lead PI: Shortle (GMU)
 - *Analysis and Reduction of Complex Networks under Uncertainty*, Marzouk (MIT), Knio (JHU), Ghanem (USC), Najm (SNL)
 - *Optimization and Control of the Electric Power Systems*, Co-PIs: Meza (LBNL), Thomas (Cornell), Lesieutre (UW-Madison)
 - *Advanced Kalman Filter for Real-Time Responsiveness in Complex Systems*, Co-PIs: Huang (PNNL), Welch (UNC-Chapel Hill)
 - *Extending the Realm of Optimization for Complex Systems: Uncertainty, Competition and Dynamics*, Lead PI: Shanbhag (UIUC)

- **All awards made and work has begun.**

- **Plan to conduct programmatic and expert review of progress and results.**

Progress (10/28/2010)

NERSC (Goal: 8 total)

- 5 hired/accepted, 3 of those started work
- 3 new candidates contacted and in pipeline to be interviewed

ALCF (Goal: 10-11 total)

- 5 hired (3 have already started work)
- 1 in process
- 4 candidates identified for interviews

OLCF (Goal: 10 total)

- 2 hired/accepted
- 4 in process
- 4 candidates interviewed/to be interviewed
- Looking for additional candidates

Overview

- Post Doctoral Fellows to provide extra user support for Extra Energy related projects at the Leadership Computing and NERSC facilities
- Funds became available at the end of FY09

