ASCR ARRA Update
March 30, 2010

Walt Polansky and Dan Hitchcock
Advanced Scientific Computing Research
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.
DOE Explores Cloud Computing

- **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) \(\Rightarrow\) 61.9 Teraflops
SU = IBM iDataplex rack with 640 Intel Nehalem cores

- 18 Login/network nodes
- 10G Ethernet
- 14 I/O nodes (shared)
- 8G FC
- NERSC Global Filesystem
- 1 Petabyte with GPFS
- HPSS (15PB)
- Load Balancer
- 100-G Router
- ANI

ASCAC March 30, 2010
Argonne Magellan Cloud Hardware

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

File Servers (8) (/home) 160TB
Gateway Nodes (~20)
Mgt Nodes (12)
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.
ANI: Status

- 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](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](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

NERSC / LBNL
Sunnyvale

ALCF / ANL
Chicago

OLCF / ORNL
Nashville

NYC
ANI: 100 Gbps Prototype Network
Preliminary Baseline Design
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.

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<th>Science Area</th>
<th>Code</th>
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<td>Harrison</td>
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Scientific Progress Resulting from OLCF Upgrade

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

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

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

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

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

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

- **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)
- **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.
SciDAC-e
Computational Postdoctoral Fellows

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