U.S. DEPARTMENT OF ENERGY | Office of Science

Recovery Act Projects

-- Update --

ASCAC Meeting
March 22-23, 2011
Washington, DC

Walter M. Polansky
Advanced Scientific Computing Research

ASCR's Recovery Act Projects ($153.9M)

- Leadership Computing Facility Upgrades ($19.9M) Six-core upgrade to Oak Ridge LCF machine to take the OLCF to ~2 Petaflops peak -- **COMPLETED**
- Advanced Networking Initiative ($66.8M) 100Gbps optical networking demonstration prototype, research testbed, and tools
  - **Proposals for the second round of research on the testbed due April 1, 2011**
- Advanced Computer Architectures ($5.2M) Research on next generation technologies
  - **P7 Board delivered; Planning underway for incorporating into OLCF**
- Magellan ($32.8M) Research to demonstrate viability of cloud computing for mid-range computational science
  - **See presentation by Susan Coghlan to ASCAC on March 22, 2011 at 2pm**
- SciDAC-e ($29.2M)
  - Supplement and leverage existing SciDAC investments to advance the high performance computational capabilities of the BES - Energy Frontier Research Centers (EFRCs)
  - Applied math research on electric grids
  - Post docs at NERSC, ALCF and OLCF

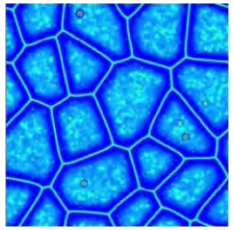
SciDAC-e

Progress since August 2010:

- Supplemental awards to SciDAC Centers and Institutes: to support BES Energy Frontier Research Centers (EFRCs) to develop a high-performance computing capability relevant to the goals of the EFRC
  - 14 projects awarded in FY2010; funds arrived at the end of August
  - Start-up activities: postdocs hired at TOPS (1), VACET (1)
- Applied Math projects: to advanced the Department's goals for smart grid.
  - research ongoing and early research results reported
- Postdocs at ALCF, OLCF, and NERSC: to hire post-doctoral researchers for a ~24 month period to work on key areas supporting DOE's energy mission including energy-related research and ARRA funded projects EFRCs
  - 9 hired at NERSC (goal: 8 PDs)
    - 7 have started working, number 8 is due to start April 4, number 9 in May
  - 6 PDs on board at OLCF (goal: 10 PDs)
    - 1 to start in August, 1 offer in process (interviewing one more)
    - Also held a workshop in August 2010 to broaden community
  - 11 PDs on board at ALCF (goal: 10 PDs)

Next Steps:

- Joint ASCR-BES programmatic review of SciDAC-e by end of FY11



Applied Mathematics Research to Enable Smart Grids

- **ARRA SciDAC-e Applied Mathematics projects selected from Multiscale Mathematics and Optimization of Complex Systems solicitation (DE-PS02-08ER08-13 and Lab 08-13)**
  - 7 ARRA projects awarded (Sept 2009 timeframe)
    - Next-tier of highly competitive proposals
    - Applied Mathematics research related to future power grid / smart grid including:
      - Optimization and Control
      - Rare Event Simulation and Decision-Making
      - Complex Networks under Uncertainty

ANI Testbed Overview

- **Three Phases**
  - Tabletop testbed at LBNL (June 2010 to March 2011)
  - Move to Long Island MAN when dark fiber is available (April 2011 to September 2011)
  - Extend to WAN when 100Gbps available (late 2011)

- **Capabilities**
  - Ability to support end-to-end networking, middleware and application experiments, including interoperability testing of multi-vendor 100Gbps network components
  - Researchers get “root” access to all devices
  - Use Virtual Machine technology to support custom environments
  - Detailed monitoring capabilities

ANI Testbed Access…

.. Granted through merit review

- **Proposal submission process:**

  https://sites.google.com/a/lbl.gov/ani-testbed/

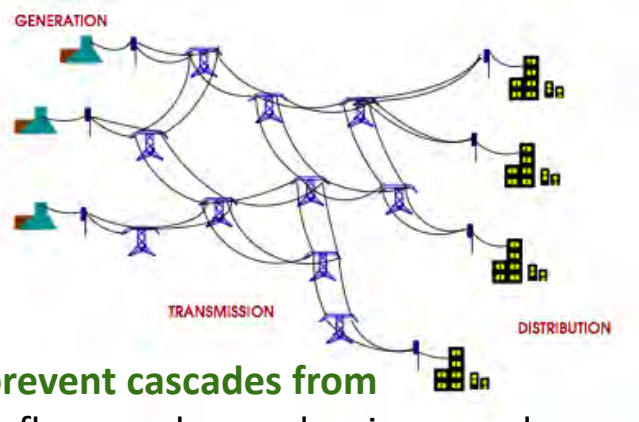
- **Eligibility**
  - **Researchers funded by DOE or other Federal Agencies**
  - **Industry**

- **Bi-annual cycle**
  - **Next round of proposals due April 1, 2011**

Sample ANI Testbed Project:
Hybrid Network Traffic Engineering Software (HNTES)

- **PI: Malathi Veeraraghavan, University of Virginia**
  - Investigating the role of hybrid networking at 100Gbps
- **Project goal:**
  - To learn how to optimize a hybrid network comprised of an IP datagram network and a high-speed optical dynamic circuit network
    - Because large-sized flows adversely effect small-sized flows, use machine learning techniques to identify large-sized flows based on size and duration
    - Upon detecting such a flow, HNTES reconfigures the router to redirect packets from this flow to a circuit on a different path
- **Current status: completed initial phase of software implementation; demonstrated capability in October, 2010**

Reconfiguring Power Systems to Minimize Cascading Failures



Background: Failures of a few components of a power grid can stress the grid and cause other components to fail, setting off a cascade of failures that may produce a large blackout.

Goal: Devise strategies for reacting to component failures, to prevent cascades from developing. Need improved modeling and formulation of power flows and cascades, improved algorithms for optimization (discrete, nonlinear-continuous, simulation-based, nondifferentiable, stochastic, parameterized nonlinear equations), advanced computing.

Long-Term Impact: Better understanding of grid behavior under various failure scenarios. Better advice to grid operators.

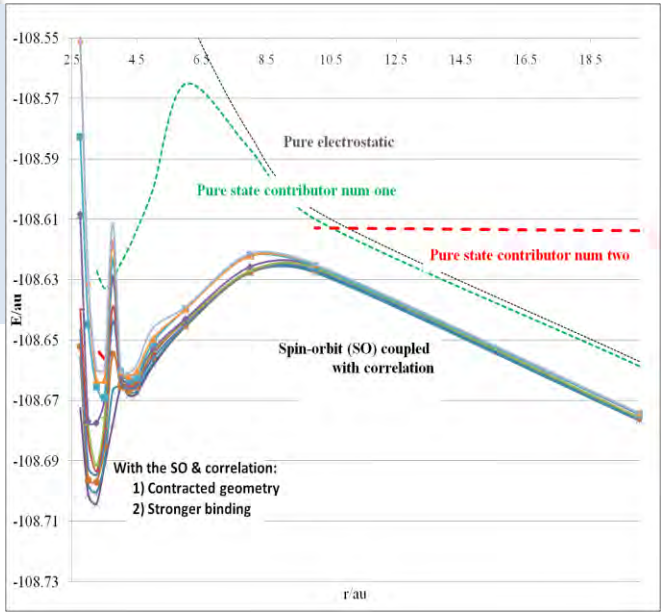
Y1 Progress:

- Integer programming to devise control strategy (limited load-shedding) to mitigate cascades – maximize fraction of power demand satisfied.
- Improved cascade models obtained by testing against real blackout data.
- Modeling energy hubs, i.e. interface between different infrastructures and loads, via energy converters, direct connections, and storage devices
- Robust optimization algorithms solving AC power flow equations.

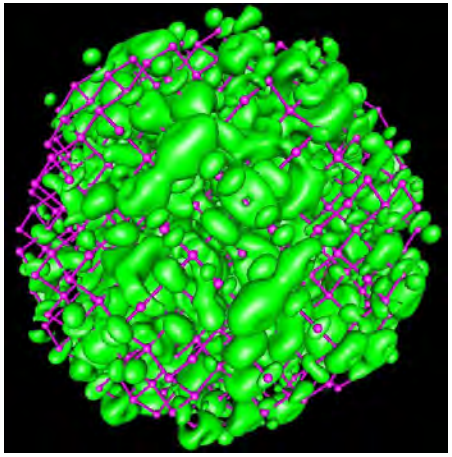
Dan Bienstock (Columbia), Ian Dobson (UW-Madison), Ian Hiskens (Michigan), Jeff Linderoth (UW-Madison), Steve Wright (UW-Madison)

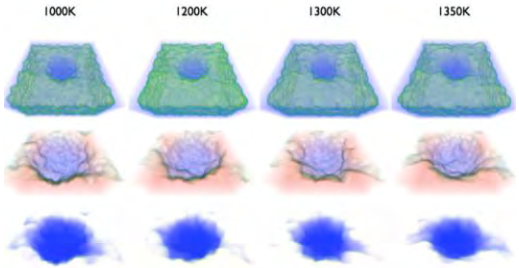
SciDAC-e Illustrative Example
-- Solar Materials Discovery --

New parallel software enables analysis enables analysis of solar driven catalysts, and recognition of need to include additional chemistry in models. (Fowler/Meyer)



Improved conjugate gradient method and MPI+OpenMP programming for large-scale electronic structure calculations for carrier dynamics in a quantum dot based solar cell (Ng/Zunger)





Visualization of Evolution of 15 angstrom nanobowls at different temperatures, that captures material interfaces (Ross/Peterka/Thackery)