View from Washington and Germantown

Michael Strayer, Director
Office of Advanced Scientific Computing
Office of Science
Department of Energy

Office of Science
"New Working Relationships"

Office of Science

Office of the Director

Staff

Deputy Director for Field Operations

George Malosh

Deputy Director for Science Programs

Patricia Dehmer

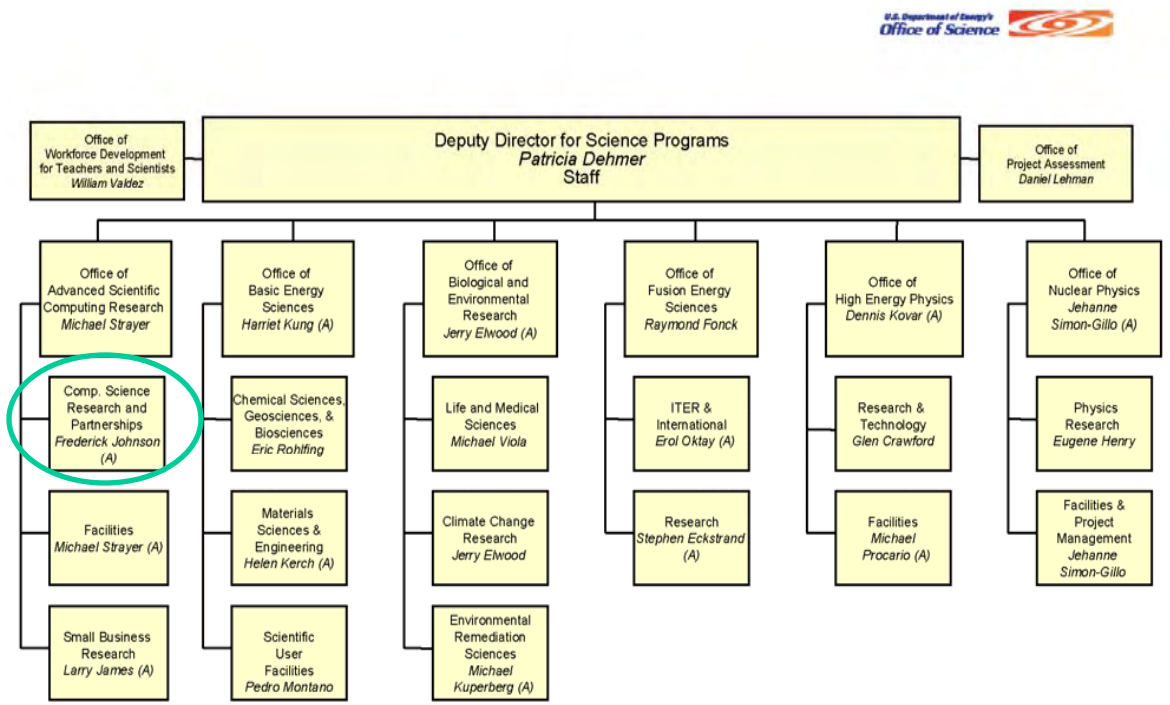
Deputy Director for Resource Management

John Alleva (A)

Deputy for Science Programs

- Provide scientific and management oversight for the six program offices by ensuring program activities are strategically conceived and executed;
- Formulate and defend the Office of Science budget request;
- Establish policies, plans, and procedures related to the management of the program offices;
- Ensure the research portfolio is integrated across the program offices with other DOE program offices and other Federal agencies;
- Represent the organization and make commitments for the Department in discussions and meetings with high-level government and private sector officials:
- Serve as the Acting Director of the Office of Science whenever that position is vacant during changes in Administration or leadership

ASCR Staff Changes



Office of Science and National Nuclear Security Administration

"Working Together"

Successful Partnership

- Acquisition of the Cray XT3 computer at the ORNL was result of a partnership between NNSA-ASC and the Office of Science;
- Lawrence Livermore National Laboratory, Argonne National Laboratory and IBM have entered a Research and Development contract to develop the next generation of Blue Gene-based products.
- Achitecture of the compute node in ASC-Purple at LLNL is a result of direct NNSA-ASC and Office of Science collaborations involving the Livermore and Berkeley national laboratories.
- NNSA and SC Jointly support an $8.6M (annual) research portfolio in Turbulence, Materials, Astrophysics, and Nuclear Structure.
- SC participation in the NNSA workshop on their TriLab L2 petascale user environment milestone that was held after the 2007 ASC PI meeting.
- SC and NNSA cosponsored a workshop on petascale tools in Washington, DC in August 2007.
- SC and NNSA jointly support the highly successful Computational Science Graduate Fellowship to develop the next generation of computational science leaders.

U.S. Department of Energy

Office of Science

FY 2008 Budget Status

Advanced Scientific Computing Research Program

(dollars in thousands)

FY 2006 Appropriation	FY 2007 Request	FY 2007 Current Appropriation	FY 2008 Request	FY 2008 House Mark	FY 2008 Senate Mark
228,382[a]	318,654	283,415	340,198	340,198	334,898

- Senate Appropriations Energy and Water Development (SEWD) Subcommittee Report (110-127)
  - Increase of $7,700,000 is for the Oak Ridge leadership Computing Facility to maintain budget and cost schedule.
  - Shifted $13,000,000 from the Office of Science to the NNSA Advanced Computing and Simulation program to reestablish the Department leadership role in high performance computing.
- Current Continuing Resolution until November 16, 2007

[a] Total is reduced by $2,371,000 for a rescission in accordance with P.L. 109-148, the Emergency Supplemental Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006; $5,627,000, which was transferred to the SBIR program; and $675,000, which was transferred to the STTR program.

SEWD Subcommittee Report 110-127: NNSA

- Reallocated $19M targeted for DOD to support a joint NNSA and Office of Science high performance computing effort to revitalize Departments own R&D capability

- Department directed to establish a joint program office lead by NNSA Administrator and the Under Secretary for Science with responsibility "to ensure sustained availability of a well balanced and hence productive and highly scalable computing platfors for the DOE and the Nation and will serve the missions of NNSA, the Office of Science and emerging economic competitiveness initiatives."

2008 Defense Authorization Bill

SEC. 3126. EVALUATION OF NATIONAL NUCLEAR SECURITY ADMINISTRATION STRATEGIC PLAN FOR ADVANCED COMPUTING.

(a) *In General*.--The Secretary of Energy shall--

(1) enter into an agreement with an **independent entity to conduct an evaluation of the strategic plan for advanced computing of the National Nuclear Security Administration**; and

(2) not later than **180 days after the date of the enactment of this Act**, submit to the congressional defense committees a report containing the results of evaluation described in paragraph (1).

2008 Defense Authorization (cont.)

(b) *Elements*.--The evaluation described in subsection (a)(1) shall include the following:

(1) An assessment of--

(A) **the role of research into, and development of, high-performance computing supported by the National Nuclear Security Administration** in maintaining the leadership of the United States in high-performance computing; and

(B) **any impact of reduced investment** by the National Nuclear Security Administration in such research and development.

(2) An assessment of the **ability of the National Nuclear Security Administration to utilize the high-performance computing capability of the Department of Energy and National Nuclear Security Administration national laboratories** to support the Stockpile Stewardship Program and nonweapons modeling and calculations.

(3) An assessment of the **effectiveness of the Department of Energy and the National Nuclear Security Administration in sharing high-performance computing developments with private industry** and capitalizing on innovations in private industry in high-performance computing.

(4) A description of **the strategy of the Department of Energy for developing an extaflop computing capability**.

(5) An assessment of the **efforts of the Department of Energy** to--

(A) **coordinate high-performance computing work within the Department**, in particular among the Office of Science, the National Nuclear Security Administration, and the Office of Energy Efficiency and Renewable Energy; and

(B) **develop joint strategies with other Federal Government agencies** and private industry groups for the development of high-performance computing.

Recent Workshops and Meetings

"Potential Partners"

Updates

- **Computational Research Needs in Alternative and Renewable Energy**
- **Computational Subsurface Sciences**
- **Cyber Security Research Plan**

U.S. Department of Energy

Office of Science

Advanced Scientific Computing Research Program

Computational Research Needs in Alternative and Renewable Energy

Hilton Rockville Executive Meeting Center
19-20 September 2007

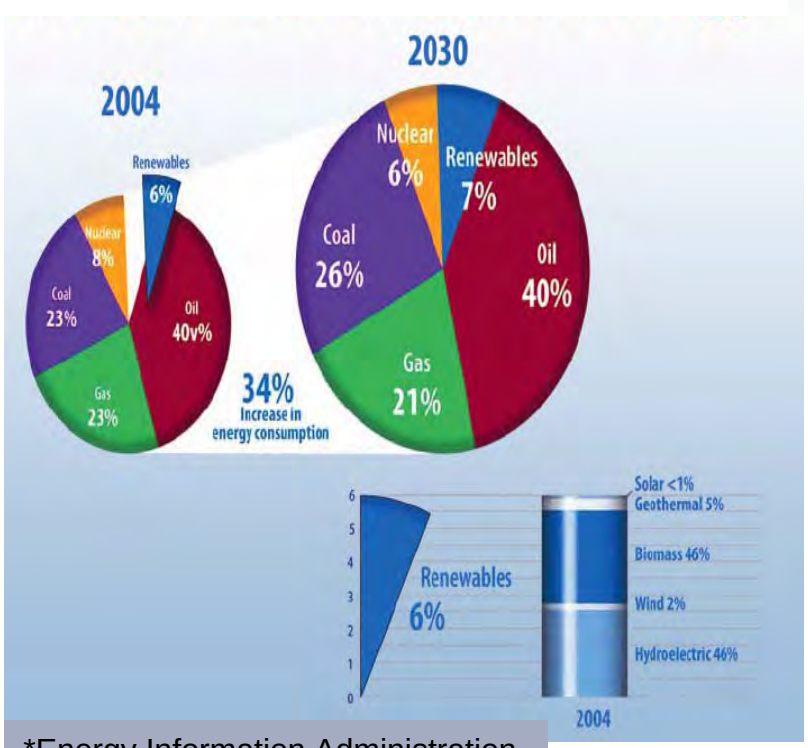
http://www.nrel.gov/crnare_workshop/

Workshop Charge

- Identify computational research needs and opportunities in alternative and renewable energy, with a focus on DOE/Energy Efficiency and Renewable Energy (EE) mission objectives and DOE/Office of Science (SC) capabilities
- Suggest a set of Priority Research Directions for a program of computational research in alternative and renewable energy
- Relate all findings and recommendations to the present and planned alternative and renewable energy research activities of others
- Prepare a preliminary letter report within one week of workshop completion and follow with a full report within 60 days of workshop completion.

Background

- Energy demand is projected to increase 34% in next 25 years*.
- Renewables currently make up ~6% of our U.S. energy supply (most of this is hydroelectric)
- Energy demand is projected to increase 34% in next 25 years*.
- Renewables currently make up ~6% of our U.S. energy supply
  (most of this is hydroelectric)
- Ambitious national goals are being set:
  - Biofuels: reduce gasoline usage by 20% in ten years
  - Solar: market competitive by 2015 for Photovoltaics
  - Wind: 20% of total provided energy by 2030
- Meeting these goals will require:
  - Interdisciplinary collaborative efforts
  - robust and scalable simulation codes
  - robust petascale computational capabilities
  - high speed communication networks



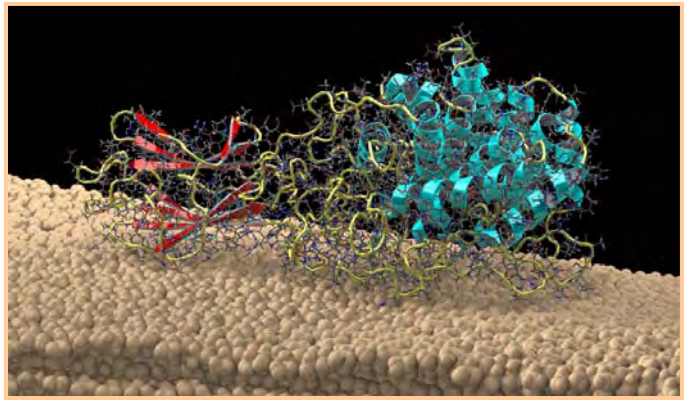
*Energy Information Administration report *Annual Energy Outlook 2006*

Workshop Activities

- 156 Registrants
- 5 Breakout sessions:
  - Renewable Fuels - Hydrogen
  - Renewable Fuels – Biomass Conversion
  - Renewable Electricity – Solar Energy Conversion
  - Renewable Electricity – Wind Energy
  - Energy Distribution – Grid Futures and Reliability
- Letter Report delivered
- Final Report in preparation

Preliminary Priority Research Directions

- Develop effective methodologies and computational tools for rational design of materials with prescribed properties
- Develop methodologies and simulation codes to enable fundamental understanding of the architecture of plant cell walls at the cellular, molecular and atomistic scales
- High fidelity modeling and simulation of fundamental wind turbine aerodynamics and aeroacoustics, at spatial scales extending across nine orders of magnitude
- Accurate, predictive models of the grid to test many different "what if" scenarios (e.g. wind at the 10% level, 20% level, 30% level, millions of solar rooftops, PHEV, etc)



T. fusca Cel9A cellulase enzyme in action on cellulose surface

Computational Subsurface Sciences

Carbon Capture and Storage

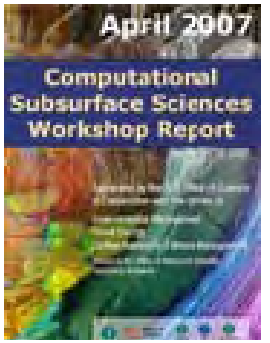
Recent Workshops

Computational Subsurface Sciences

Marriott Bethesda North Conference Center

9-12 January 2007

http://subsurface2007.labworks.org/

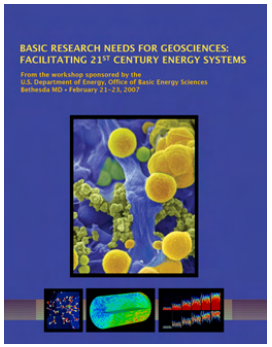


Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems

Marriott Bethesda North Conference Center

21-23 February 2007

http://esd.lbl.gov/BRN-Geosciences2007/index.htm

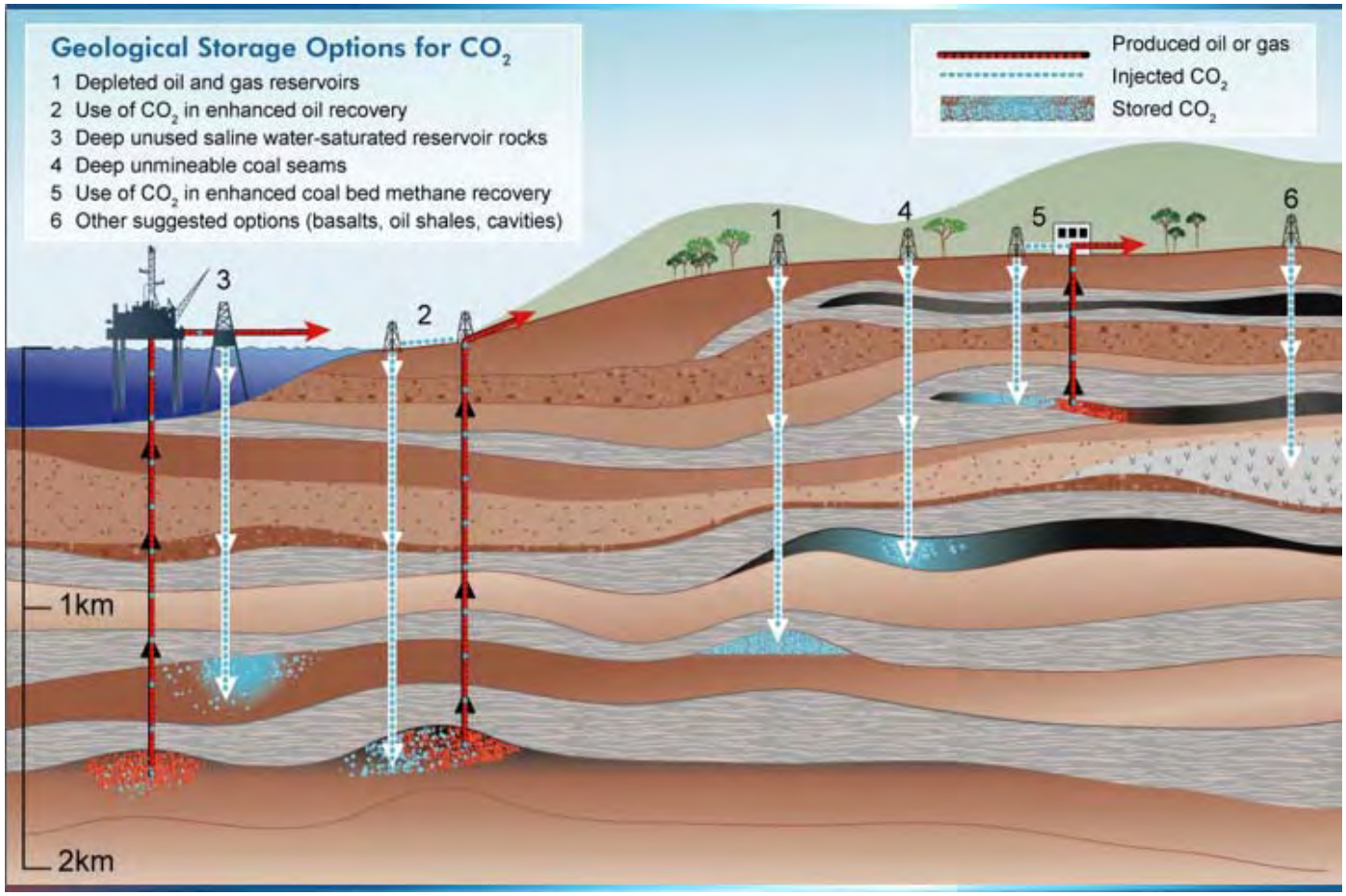


Collaborating DOE Offices

- Office of Fossil Energy (FE)
- Office of Science (SC)
  - Office of Advanced Scientific Computing Research
  - Office of Biological and Environmental Research
  - Office of Basic Energy Sciences

Motivation:

Many CO_2 Sequestration Sites Will Be Required for Future Coal-Fired Power Plants



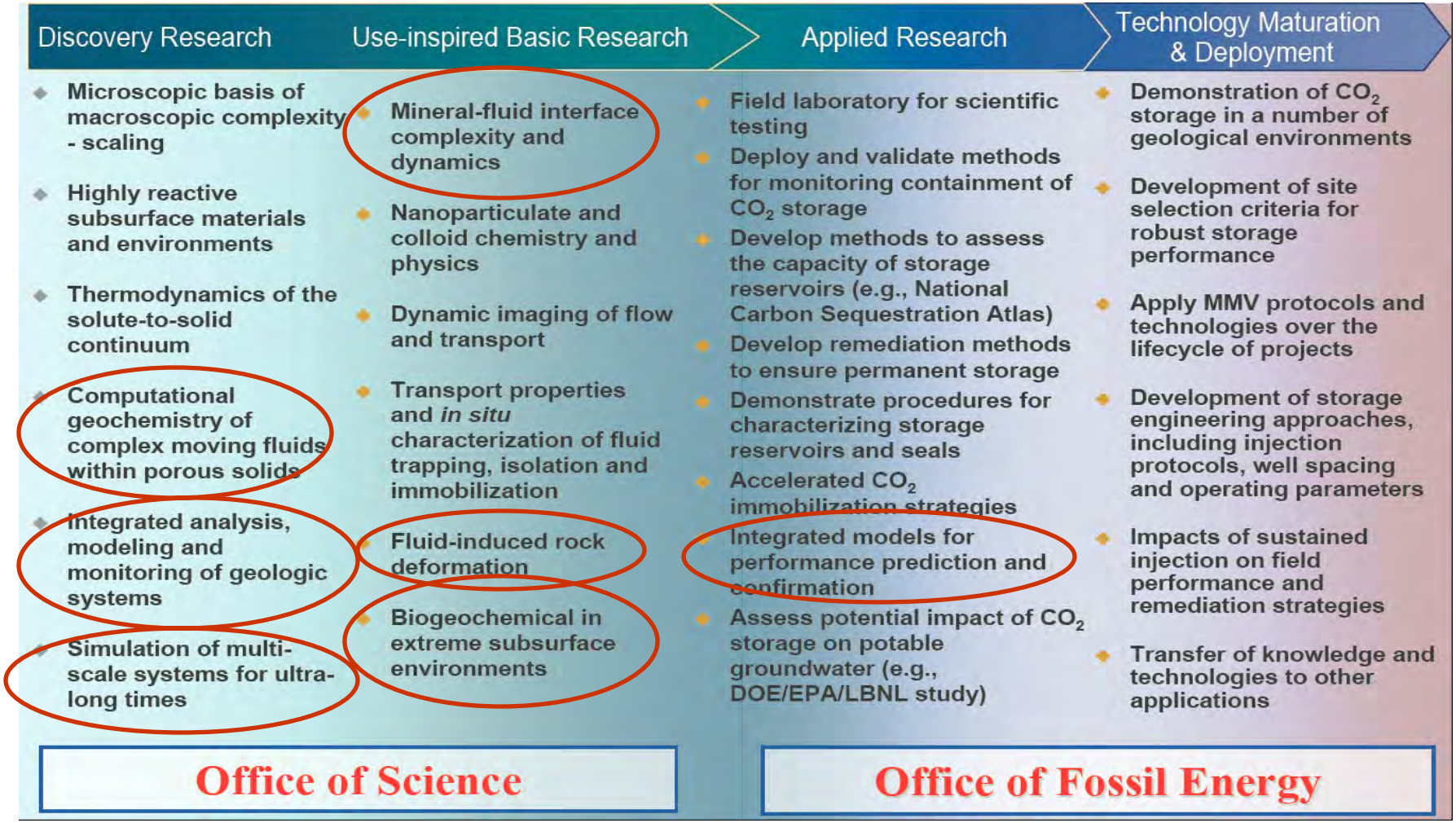
Options for storing CO_2 in underground geological formations for 330,000 MW of electric energy generation. *After Benson and Cook (2005).*

U.S. Department of Energy

Office of Science

Advanced Scientific Computing Research Program

Basic Research Needs for Geosciences: CO_2 Sequestration



Carbon Sequestration R&D Planning

- **December 12-15, 2007**
  - **Regional Carbon Sequestration Partnership Program Annual meeting and Cross-Cutting Working Groups Discussion with Office of Science**
- **March 12-14, 2008**
  - **Joint Office of Science – Office of Fossil Energy Contractor's meeting focusing on Carbon Sequestration Research Programs**

Cybersecurity Research for the Department of Energy

U.S. Department of Energy

Office of Science

Cyber Security

Advanced Scientific Computing Research Program

DOE Senior Leadership Summit on Cyber Security

September 26-27, 2007 Sandia National Laboratories

Outcome: Comprehensive Planning Effort to

Define the Scale of Value
Define the Threat
Define the Protective System
Develop Cyber R&D Plan
Strengthen the Defense
Build a Communications Plan

Office of Science responsibility

Cyber Security Research

Possible Attributes

- Drive transformational changes in cyber security
- Provide near-term benefits to legacy systems
- Be science-based, vision focused
- Create a broad-based community
- Offer potential solutions to all DOE programs (open science, R&D, classified)
- Coordinate efforts throughout the process with those at other Federal agencies

Possible Research Topics

- **Situational Awareness and Response in Federated Systems**
  - ***Mathematics of large datasets, i.e. "Connecting the dots, in real time"***
  - ***Tools and services to thoroughly monitor resources and coordinate with sites to contain cyber incidents***
  - ***Capabilities to quickly distinguish authorized, legitimate activities from unauthorized or illegitimate use.***
- **Management of Trust in Federated Systems**
  - ***Laboratory-wide enterprise to merge data to provide a comprehensive, accurate and up to date view of cyber posture***
  - ***Innovative, secure and authenticated communications to share incident data and to coordinate responses.***
- **Risk Assessment**
  - ***Mathematical methods for evaluating security risks in complex systems such as the internet, power grids, pipelines, transportation systems, and telecommunications infrastructure***

Why DOE?

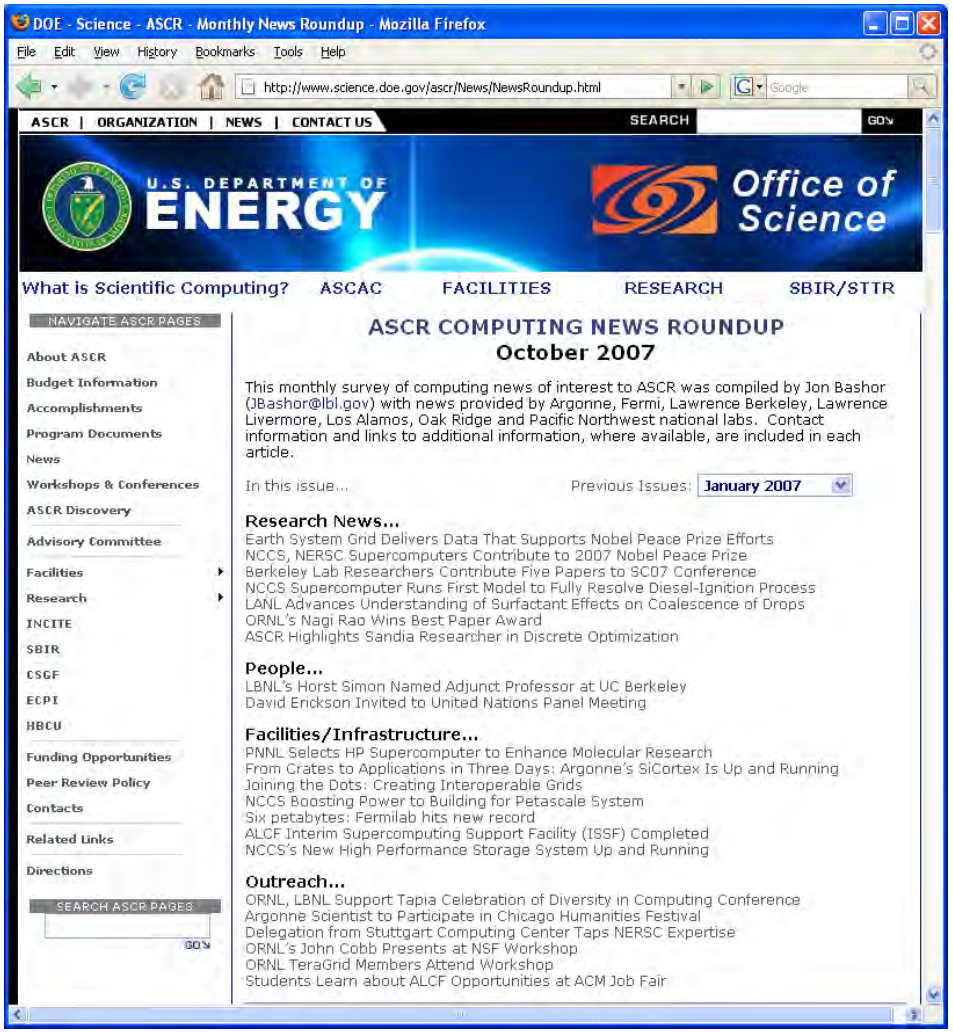
- DOE is responsible for the operations of some of the nation's most advanced research and development user facilities located at national laboratories and universities
  - *Used by more than 18,000 researchers from universities, other government agencies and private industry worldwide*
  - *Many of these researchers rarely, if ever, visit the DOE facility that they are using*
- The DOE mission, which includes unclassified and classified scientific programs, places the agency at the forefront of many of these cyber security issues;
- The Office of Science's widely recognized, outstanding research programs in applied mathematics and computer science research can be leverage to foster transformational changes to cyber security;
- Innovative research program models developed and implemented by the Office of Science, such as Scientific Discovery through Advanced Computing (SciDAC), are available to apply to cyber security challenges.
- Ceding leadership to others will compromise our ability to do mission critical science;

ASCR News
"Celebrate our Partners"

David Keyes named recipient of 2007 Sidney Fernbach Award

"Outstanding contributions to the development of scalable numerical algorithms for the solution of nonlinear partial differential equations (PDEs) and for his exceptional leadership in high-performance computation."

ASCR in the News



http://www.science.doe.gov/ascr/News/NewsRoundup.html

DOE and IPCC

2007 Nobel Peace Prize: Former Vice President Al Gore and United Nations Intergovernmental Panel on Climate Change (IPCC)

Supercomputers at the NCCS at ORNL and NERSC at LBNL provided more than half of the simulation data for the joint DOE/NSF) data contribution to the IPCC Fourth Assessment Report.

SC07 ASCR PIs Meeting

Monday, November 12, from 4 - 6 pm (Reno time) in Meeting Rooms **A8 & A9** of the Reno Convention Center.

DOE at SC


SC 2007
NOVEMBER 2007
RENO SPARKS CONVENTION CENTER
RENO, NEVADA
Latest Revision: 9-7-07
Closed Off
DoD
HPCMP
NASA
IBM
HP
Microsoft
SCinet
ENTRANCE
ENTRANCE
ENTRANCE
Loading Docks
Warehouse
Loading Docks
Warehouse