Office of Advanced Scientific Computing Research Update

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

U.S. Department of Energy

Office of Science

FY 2007 Current Appropriation Continuing Resolution Impacts

Advanced Scientific Computing Research Program

(dollars in thousands)

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

Largest decreases from President's FY 2007 budget request

- NERSC: -$17.3M
  - Bassi (IBM Power 5) not upgraded
  - Center balanced not maintained
  - New Hires deferred
- Computational Partnerships: -$10.6M
  - Delayed initiation of several SciDAC Centers and Institutes
  - Several University partners placed on no-cost extensions
- Leadership Computing Facilities: -$7.5M
  - Leases extended
  - Site preparation for HPC upgrades deferred

[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.

U.S. Department of Energy

Office of Science

President's FY 2008 Request

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

- **Applied Mathematics ($36.9M)** – Increase of **$7.4M** over FY 2007 President's request to support
  - Critical long-term mathematical research issues relevant to petascale science, multiscale mathematics and optimization control and risk analysis in complex systems
  - $1M increase in Computational Science Graduate Fellowship to $5M.
- **Computer Science ($29M)** – Increase of **$5.1M** over FY 2007 President's request to
  - Develop software and tools to enable both experienced and new researchers to make effective use of petascale systems at the Leadership Computing Facilities and supercomputing facilities.
  - Focus on accelerated visualization, fault tolerance and user interface environments
- **Research and Evaluation Prototypes ($17M)** – Increase of **$4M** over FY 2007 President's request to support joint SC-NNSA (ANL-LLNL) partnership with IBM to explore low power density approaches to petascale computing

[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.

U.S. Department of Energy

Office of Science

House Energy and Water Development Appropriations Report (H.R. 2641)

Advanced Scientific Computing Research Program

ADVANCED SCIENTIFIC COMPUTING RESEARCH

The Committee recommendation is $340,198,000, the same as the budget request and an increase of $56,783,000 over the current fiscal year. The Committee commends the Office of Science and the Office of Advanced Scientific Computing Research for their efforts to provide cutting-edge capabilities to meet current scientific computational needs, and at the same time to extend the boundaries of that cutting edge into the next generation of high-performance scientific computers and supporting software. Perhaps no other area of research at the Department is so critical to sustaining U.S. leadership in science and technology, revolutionizing the way science is done, and improving research productivity.

U.S. Department of Energy

Office of Science

Senate Appropriations Energy and Water Development Subcommittee Report (110-127)

Advanced Scientific Computing Research Program

ADVANCED SCIENTIFIC COMPUTING RESEARCH

The Committee provides $334,898 for Advanced Scientific Computing Research. The increase of $7,700,000 is for the Oak Ridge leadership Computing Facility to maintain budget and cost schedule. The Committee has also included language in the NNSA Advanced Simulation and Computing program to encourage the Office of Science and the NNSA to work together to establish a high performance computing capability within the Department by joining the capabilities of both program support advanced computing architecture, improvements in cyber security and to support the development of advanced software and algorithms to increase the speed and efficiency of existing and future systems. The Committee does not support the Department transferring $19,000,000 to the Department of Defense to lay a minor role in that effort. Instead, the Committee has 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.

U.S. Department of Energy

Office of Science

Protecting America's Competitive Edge Through Energy (PACE-Energy) Act

Advanced Scientific Computing Research Program

- Contained in America Creating Opportunities to Meaningfully Promote Excellence in Technology, Education and Science (COMPETES) Act (Conference committee report from HR 2272 and S 761)

- Establishes Director of Science, Engineering and Mathematics Education
  - Reports to Undersecretary for Science
  - Principle responsibility for administering science, engineering, and mathematics education at DOE

- Establishes Advanced Research Projects Agency – Energy (ARPA-E)
  - To overcome long-term and high-risk technological barriers in the development of energy technologies
    - Identify and promote revolutionary advances in fundamental sciences
    - Translate scientific discoveries into technological innovations
    - Accelerate transformational technological advances in areas that industry is unlikely to take because of technical and financial uncertainty
  - Director is appointed by President and reports to Secretary
  - Program Managers –
    - 3 year renewable terms
    - Appointments not subject to civil service laws
  - Budget separate from DOE's budget
  - No funds may be appropriated in FY 2008 unless the amount appropriated for the Office of Science for FY 2008 exceeds the amount appropriated for the Office in FY 2007 ($3.8B)

U.S. Department of Energy

Office of Science

Facilities Division Draft HPC Strategic Plan

Advanced Scientific Computing Research Program

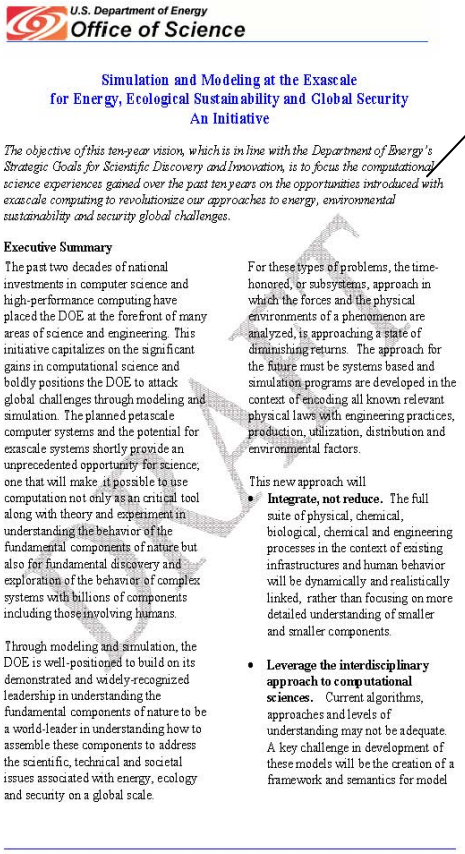
- ASCR's ten-year "terascale to exascale" strategic plan will focus primarily on HPC computing resources and research and evaluation testbeds and the investment needed to stand-up prototypes at the extreme scale for scientific discovery in the 2014-2017 timeframe.
- The key strategic principles that guide ASCR facility investments include:
  - The primary objective of facility investments is to provide support for a broad range of scientific disciplines.
  - An integral part of the development of the next generation HPC resources must include a tight coupling with pioneering scientific applications and a portion of ASCR's computer science and applied mathematics portfolio with the development of the next generation of HPC resources.
  - A strategic focus will be to identify and conquer barriers to success while continually evaluating both risk and reward.
  - The balance between high performance production and leadership class facilities will be determined with input from the Advanced Scientific Computing Advisory Committee (ASCAC) and the mission needs of the other SC program offices.

U.S. Department of Energy

Office of Science

Modeling and Simulation at the Exascale for Energy, Ecological Sustainability and Global Security

Advanced Scientific Computing Research Program



U.S. Department of Energy
Office of Science

Simulation and Modeling at the Exascale
for Energy, Ecological Sustainability and Global Security
An Initiative

The objective of this ten-year vision, which is in line with the Department of Energy's Strategic Goals for Scientific Discovery and Innovation, is to focus the computational science experiences gained over the past ten years on the opportunities introduced with exascale computing to revolutionize our approaches to energy, environmental sustainability and security global challenges.

Executive Summary

The past two decades of national investments in computer science and high-performance computing have placed the DOE at the forefront of many areas of science and engineering. This initiative capitalizes on the significant gains in computational science and boldly positions the DOE to attack global challenges through modeling and simulation. The planned petascale computer systems and the potential for exascale systems shortly provide an unprecedented opportunity for science, one that will make it possible to use computation not only as an critical tool along with theory and experiment in understanding the behavior of the fundamental components of nature but also for fundamental discovery and exploration of the behavior of complex systems with billions of components including those involving humans.

Through modeling and simulation, the DOE is well-positioned to build on its demonstrated and widely-recognized leadership in understanding the fundamental components of nature to be a world-leader in understanding how to assemble these components to address the scientific, technical and societal issues associated with energy, ecology and security on a global scale.

For these types of problems, the time-honored, or subsystems, approach in which the forces and the physical environments of a phenomenon are analyzed, is approaching a state of diminishing returns. The approach for the future must be systems based and simulation programs are developed in the context of encoding all known relevant physical laws with engineering practices, production, utilization, distribution and environmental factors.

This new approach will

- **Integrate, not reduce.** The full suite of physical, chemical, biological, chemical and engineering processes in the context of existing infrastructures and human behavior will be dynamically and realistically linked, rather than focusing on more detailed understanding of smaller and smaller components.
- **Leverage the interdisciplinary approach to computational sciences.** Current algorithms, approaches and levels of understanding may not be adequate. A key challenge in development of these models will be the creation of a framework and semantics for model

DRAFT

The objective of this ten-year vision, which is in line with the Department of Energy's Strategic Goals for Scientific Discovery and Innovation, is to focus the computational science experiences gained over the past ten years on the opportunities introduced with exascale computing to revolutionize our approaches to energy, environmental sustainability and security global challenges.

Town Meetings Held

- **April 17-18 at LBNL**
- **May 17-18 at ORNL**
- **May 31-June 1 at ANL**

U.S. Department of Energy

Office of Science

Other Recent Workshops and Conferences

Advanced Scientific Computing Research Program

- Software Development Tools for PetaScale Computing Workshop
  August 1-2, 2007, Washington DC
- Cyber Security Research Needs for Open Science
  July 23-24, 2007, Bethesda, MD
- SciDAC Annual Conference
  June 24-28, 2007, Boston MA
- DOE CSGF Annual Fellows' Conference
  June 19-21, 2007, Washington DC
- FAST-OS PI Meeting and Workshop
  June 18-19, 2007, Santa Clara, CA
- DOE Visualization and Analytics Workshop
  June 7-8, 2007, Salt Lake City, Utah
- Applied Mathematics Research Program Annual PI Meeting
  May 22-24, 2007, Livermore, CA
- Petascale System Integration into Large Scale Facilities Workshop
  May 15-16, 2007, San Francisco, CA

U.S. Department of Energy

Office of Science

Applied Mathematics Research – PI Meeting

Advanced Scientific Computing Research Program

- Held May 22-24, 2007 at LLNL
- 57 University, 76 Lab participants, 33 talks, 44 posters.
- Main themes: Solvers, Multiscale Math, Numerical Methods, and Optimization.
- Energy and enthusiasm were very high.
- First AMR meeting in 7 years: FY08 meeting planned.

Agenda, abstracts, talks, and posters are posted on the ASCR website at http://www.sc.doe.gov/ascr/WorkshopsConferences/AppMathPIMeet.html

U.S. Department of Energy

Office of Science

Facilities Update

Advanced Scientific Computing Research Program

- NERSC
  - 100+ Cray XT4 (Franklin)
    - delivered in February and underwent integration and acceptance testing.
    - Since June 2007, Franklin has used Compute Node Linux (CNL) - this is the first sustained, large scale testing of CNL which is Cray's future OS of choice. This has accelerated Cray's release of CNL by close to 6 months.
    - Availability testing is underway using CNL and is expected to be completed in Sept/Oct 2007 with full production will be before mid January 2008.
  - NERSC's scalability program has been a great success
    - > 70% of compute time used on Seaborg is for jobs => 768 CPUs (cores) for 2007
    - Many of the "graduates" of NERSC's scalability program now running at scale on leadership systems
  - Mass Storage system holding close to 4 Petabytes of active data and 65 Million files. Most is actually read as well as written.
  - NERSC parallel systems now are a part of the Open Science Grid enabling new application areas such as Nano-Hub
  - 2006 User Satisfaction Survey show excellent overall user satisfaction - 6.3/7.0
  - RFP for NERSC 6 expected in FY2008

- Argonne LCF
  - Acquiring three IBM Blue Gene/P systems: a 111TF, 32K processor system and a 14TF, 4K processor test & development system this Fall, followed by a larger 250-500TF production system.
  - Blue Gene/P is the product of a multi-year R&D partnership between the Office of Science/ANL, NNSA/LLNL, and IBM.
  - ALCF's 111TF Blue Gene/P will be available for 2008 INCITE projects in the Spring, and the larger system for INCITE in 2009.
  - ALCF continues to add staff and infrastructure, wrapping up preparations for the new systems.

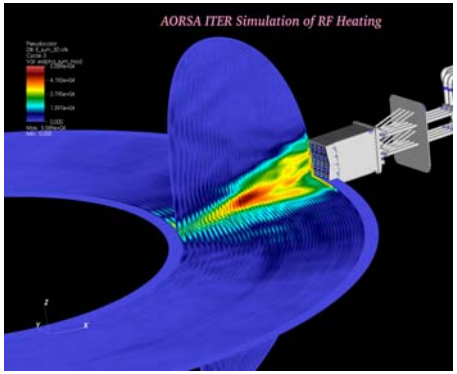
U.S. Department of Energy

Office of Science

Facility Update (Continued)

Advanced Scientific Computing Research Program

- LCF at ORNL
  - Jaguar upgraded to 119 TF in April 2007
  - Jaguar #2 on Top500 list and fastest computer in the world for open science
  - Planned upgrade of Jaguar to 250 TF is on schedule for December 2007
  - AORSA ITER simulation of RF Heating work is pushing the boundaries of the Jaguar using 22,500 processor cores, 87.5 TF
- ESnet
  - ESnet4 in production from coast to coast; below cost and ahead of schedule
  - Partnership with Internet2
  - BER and BES Requirements Workshops held this summer to determine their future networking needs



U.S. Department of Energy

Office of Science

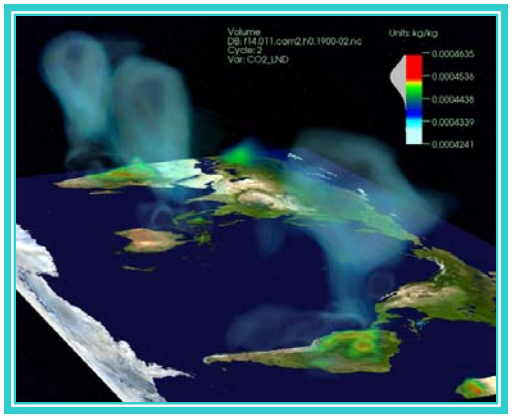
Advanced Scientific Computing Research Program

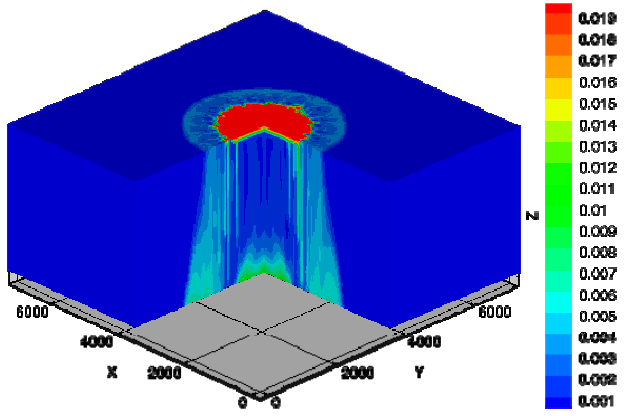
2008 INCITE

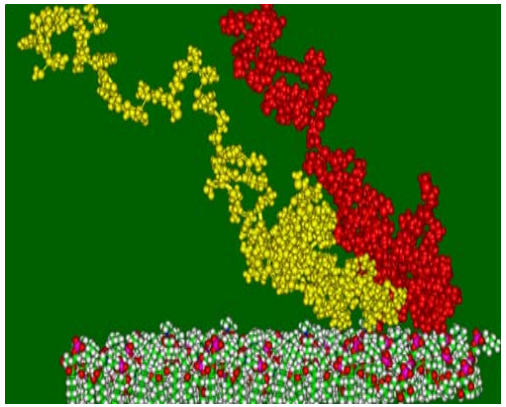
New 2008 Call for Proposals for up to a quarter of a billion processor hours of INCITE allocations announced May 16, 2007

Proposal deadline August 10, 2007

Over 80 proposals received







STAFF ASSIGNMENTS

U.S. Department of Energy

Office of Science

Director's Office

Advanced Scientific Computing Research Program

Staff	Assignment
Michael Strayer	Director
Melea Baker	Administrative Specialist
Nancy White	Program Analyst
Julie Scott	Financial Management Specialist
Norman Kreisman	Senior Advisor

U.S. Department of Energy

Office of Science

Research Division

Advanced Scientific Computing Research Program

Staff	Assignment
Walter Polansky	Acting Division Director, SciDAC
Christine Chalk	Computational Biology partnerships, SciDAC Outreach
Lali Chatterjee	SciDAC SAPS, Nanoscience and Fusion Simulation Project Partnerships
Anil Deane	Base Research—Applied Mathematics (except U. of Maryland and laboratories managed by Battelle)
Barbara Helland	SciDAC Review
Fred Johnson	Base Research—Computer Science, SciDAC--Computer Science Centers for Enabling Technologies (CET) and Institutes
Gary Johnson	Partnerships with Applied Programs, Cybersecurity Research
Robert Lindsay	Distributed Network Environment Research—Collaboratories, Grids and Middleware
Thomas Ndousse-Fetter (currently on assignment to SBIR/STTR office)	Distributed Network Environment Research—Network Research
Mark Sears	Base Research—Applied Mathematics (U. of Maryland and laboratories managed by Battelle), SciDAC--Applied Math CETs and Institutes
Yukiko Sekine	Base Research—Visualization and Data Management, SciDAC--Visualization and Data Management CETs and Institutes
George Seweryniak	Educational programs, ASCR SBIR/STTR

U.S. Department of Energy

Office of Science

Facilities Division

Advanced Scientific Computing Research Program

Staff	Assignment
Michael Strayer	Acting Division Director
Vince Dattoria	OMB Compliance and Project Management
David Goodwin	NERSC User Programs, ESnet User Requirements, Physical Facilities Construction Oversight
Barbara Helland	Leadership Computing Facilities, NERSC Facility Management, INCITE
Dan Hitchcock	ESnet
Fred Johnson	DARPA High Productivity Computer System (HPCS) partnership, IBM-NNSA-SC partnership

Agenda Highlights

- Role of HPC in BER, Jerry Elwood, Biological and Environmental Research
  - Largest SciDAC partner in terms of dollars and number of projects
  - Common PART goal
  - Two joint charges with BERAC

- Improving R&D Integration in DOE, Bill Valdez, Office of Science
  - The Energy Policy Act of 2005 requires the Department of Energy (DOE) to:
    - periodically review all of the science and technology activities of the Department in a strategic framework that takes into account both the frontiers of science to which the Department can contribute and the national needs relevant to the Department's statutory missions; and
    - develop a plan to improve coordination and collaboration in research, development, demonstration, and commercial application activities across Department organizational boundaries