



U.S. Department of Energy's
Office of Science
Advanced Scientific Computing Research Program

View from Germantown

ASCAC Meeting
February 26-27, 2008

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Department of Energy

U.S. Department of Energy



Budget Update... ...FY2009 Budget Request

Advanced Scientific Computing Research Program

Office of Science

	FY2007 Current Appropriation	FY2008 Current Appropriation	FY2009 Request
Advanced Scientific Computing Research			
Applied Mathematics	28,804	36,900	43,164
Computer Science	23,020	29,000	34,618
Computational Partnerships	41,695	50,246	52,064
Next Generation Networking for Science	13,598	13,764	17,221
SBIR/STTR	—	3,742	4,237
<i>Total, Mathematical, Computational, and Comp. Sciences Research</i>	<i>107,117</i>	<i>133,652</i>	<i>151,304</i>
High Performance Production Computing	37,554	54,200	54,790
Leadership Computing Facilities	94,910	110,158	115,000
Research and Evaluation Prototypes	14,313	23,100	17,000
High Performance Network Facilities and Testbeds	21,840	24,336	25,000
SBIR/STTR	—	5,727	5,726
<i>Total, High Performance Computing and Network Facilities</i>	<i>168,617</i>	<i>217,521</i>	<i>217,516</i>
Total, Advanced Scientific Computing Research	275,734²	351,173¹	368,820

¹ Reflects a reduction for the 0.91% rescission in P.L. 110-161, the Energy and Water Development and Related Agencies Appropriations Act, 2008.

² Total is reduced by \$7,681,000: \$6,858,000 of which was transferred to the SBIR program and \$823,000 of which was transferred to the STTR program.



Budget Update... ...FY2008 Appropriation Highlights

Advanced Scientific Computing Research Program

“Advanced Scientific Computing Research.

Funding under this heading in the amended bill includes **\$354,398,000^a** for **Advanced Scientific Computing Research**. Within Advanced Scientific Computing Research, **\$19,500,000** is included for the Office of Science to continue the Department's participation in the **Defense Advanced Research Projects Agency High Productivity Computing Systems partnership** and an **increase of \$7,700,000** is included for the **Oak Ridge Leadership Computing Facility** to maintain the planned budget and cost schedule.

The **Office of Science** and the **National Nuclear Security Administration (NNSA)** are directed **to establish the Institute for Advanced Architectures and Algorithms with Centers of Excellence at Sandia National Laboratories and Oak Ridge National Laboratory**. These Centers will execute a national program involving industry, universities and national laboratories that is focused on technologies to sustain the U.S. leadership in high performance computing. The NNSA ASC and Office of Science ASCR programs will jointly fund the program and provide direction needed to support the goal of developing exascale computing for the Nation.” — from **DIVISION C - ENERGY AND WATER DEVELOPMENT AND RELATED AGENCIES APPROPRIATIONS ACT, 2008** – Committee Report, Page 40

^a This amount was reduced by \$3,225,000 to \$351,173,000 due to a 0.91% across-the-board rescission.



FY2009 Budget Request Research Highlights: Applied Math and CS

Advanced Scientific Computing Research Program

- **Broaden world-class research in Applied Math & Computer Science:**
 - New Joint Math-CS Institute **responds to the recognition that emerging complex non-traditional computer node architectures and the simultaneous need for extreme algorithm scalability will likely require cooperative research among mathematicians and computer scientists. The joint institute activity is intended to foster this new approach and will be focused on basic research.**
 - New support for science application “leading edge development teams” willing to take on the risks of working with new and emerging languages and tools
 - New Applied Math effort in the Mathematics of Large Datasets



FY2009 Budget Request Research Highlights: Computational Partnerships and Networking Research

- **Expand SciDAC partnership with BER in climate models to improve the representation of ice sheets in global circulation.**
- **Next Generation Networking for Science will begin to implement key elements of the President's networking plan most relevant for open science networks.**
 - New basic research effort in Cyber Security for Open Science



FY2009 Budget Request Facilities Highlights

- The facilities will develop and implement a unified approach to supporting and maintaining the software, languages and tools that are critical to effective utilization of the resources.
- Operate ORNL LCF (OLCF) at one Petaflop
- Operate ANL LCF (ALCF) at 500 Teraflops
- Operate NERSC at 100+ Teraflops to meet SC program needs
- Continue ESnet upgrades (with Internet2) to meet LHC commitments (40-60Gbps)
- R&E prototypes support IBM-ANL-LLNL Blue Gene Research effort and SC contribution to DARPA HPCS



Path to the Extreme Scale

As we move into the next decade, ASCR must capitalize on the significant gains in computational science realized over the past decade and aggressively deliver Leadership Computing to attack critical challenges that advance scientific discovery and economic competitiveness.



Research for Extreme Scale

In the next decade targeted investments throughout ASCR's research program will focus on

- Harnessing the potential of petascale systems and datasets
- Supporting critical research efforts to prepare for exascale systems that enable entirely new scientific applications and require radically new algorithmic and computational approaches
- Building on lessons learned at the petascale



Research Strategies: Applied Math and CS

- **Expand current investments in**
 - Mathematics of complex/multiscale systems as called for in ASCR/BER reports
 - Math libraries
 - Usable tools for systems with one million cores/cpus
- **New investments in**
 - Uncertainty quantification and other methodology for validating complex models
 - Autonomous system software, fault tolerance, and other approaches for managing large systems
 - Exascale file systems and I/O issues
 - Testbeds for software scaling and evaluation

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Research Strategies: Partnerships & Networking

- **Increase breadth of computational partnerships**
 - Develop high risk/high payoff branches of application code teams to explore and evaluate new applied mathematics/computer science methodology requiring major code changes
- **Distributed Networking**
 - New focus on usability in a hostile network environment
 - Develop inter-domain tools for managing Federated Optical Networks
 - Explore innovative solutions to data sharing and workflow issues in petascale datasets

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Facilities Strategies

- **Robust upgrade strategy for**
 - Two Leadership Computing Facilities
 - NERSC
 - ESnet
- **R&E Prototype investments to**
 - Ensure that development of HPC resources continues to benefit open science applications
 - Understand research challenges that must be overcome for scientific applications to realize the potential of these new systems

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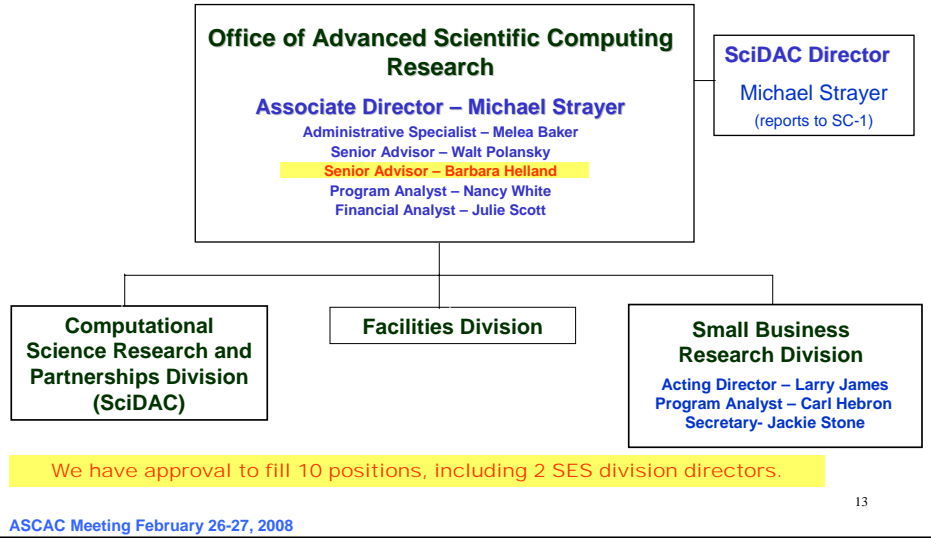
New Facilities

- **New Data Facility Initiative to support exponential growth of scientific data from observations and experiments**
 - Production infrastructure includes hardware platforms and software for scientific data management, analysis/analytics and interfaces.

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Staffing



INCITE: 2008 Awards

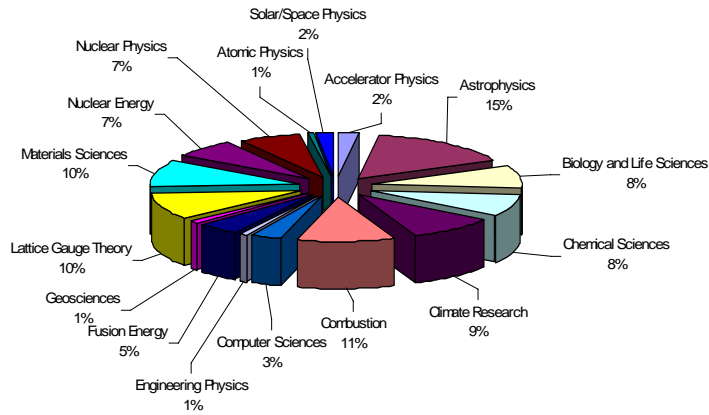
The 2008 INCITE awards provide the largest amount of supercomputing resource awards donated in DOE's history -- three times that of last year's award.

- 265 million processor-hours
- 55 scientific projects

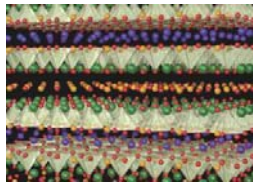
Applications were chosen based on their potential breakthroughs in the science and engineering research and their suitability of the project for using supercomputers.



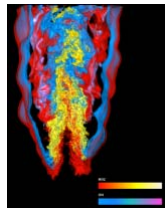
2008 INCITE Awards: Allocations by Discipline



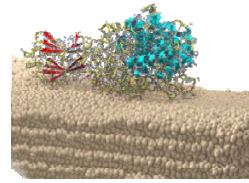
INCITE Accomplishments



Resolved decades-long controversy about modeling physics of high temperature superconducting cuprates



First 3-D simulation of flame that resolves chemical composition, temperature, and flow



New insights into protein structure and function leading to better understanding of cellulose-to-ethanol conversion



Recognitions

Vern Paxson
of Berkeley Lab Honored with ACM's
Grace Murray Hopper Award
for Research Characterizing the Internet



The award is presented annually to the outstanding young computer professional of the year, selected on the basis of a single recent major technical or service contribution. The award recognizes Paxson's work in the mid-1990s, which "[laid] the groundwork for the exciting resurgence in research in Internet measurement during the last ten years".



Recognitions

James Sethian
of Berkeley Lab elected to
**National Academy
of Engineering**
*For his development of efficient
methods of tracking moving interfaces*



Election to the National Academy of Engineering is among the highest professional distinctions accorded to an engineer.