

U.S. Department of Energy



Office of Science

U.S. Department of Energy's Office of Science

Advanced Scientific Computing Research Program

Office of Advanced Scientific Computing Research

View From Washington

Michael R. Strayer
Associate Director



2006 DOE Strategic Plan

Advanced Scientific Computing Research Program

Strategic Theme 3: Scientific Discovery and Innovation



•**Goal 3.1: Scientific Breakthroughs** – Achieve the major scientific discoveries that will drive U. S. competitiveness, inspire America, and revolutionize approaches to the Nation’s energy, national security, and environmental quality challenges.

- Strategy: Advance the computational sciences and the leadership-class computational capabilities required for today’s frontiers of scientific discovery.

•**Goal 3.2: Foundations of Science** – Deliver the scientific facilities, train the next generation of scientists and engineers, and provide the laboratory capabilities and infrastructure required for U.S scientific primacy.

- Strategy:
 - Complete construction and begin operation of major scientific user facilities
 - Better communicate the importance of science and technology to inspire participation in the innovation economy

•**Goal 3.3: Research Integration** – Integrate basic and applied research to accelerate innovation and to create transformational solutions for energy and other U. S. needs.

- Strategy: Strengthen ties between the basic research and applied mission programs in Departmental planning.

(<http://www.energy.gov/about/strategicplan.htm>)



President's Budget Request FY 2008 ASCR Highlights

Advanced Scientific Computing Research Program

(dollars in thousands)

FY 2006 Current Appropriation	FY 2007 Request	FY 2007 House Mark	FY 2007 Senate Mark	FY 2007 Appropriation	FY 2008 Request
228,382 [a]	318,654	318,654	318,654	***	347,698

- **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 CSGF 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, uncertainty and user interface environments
- **Research and Evaluation Prototypes (\$17M)** – Increase of **\$4M** over FY 2007 President's request to support joint SC-NNSA 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.



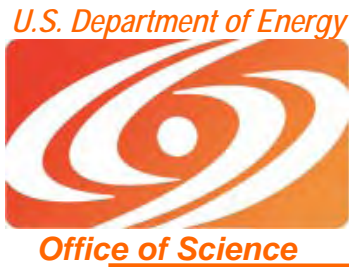
Continuing Appropriation Resolution (CR) 2007

Advanced Scientific Computing Research Program

H.J. Res. 20

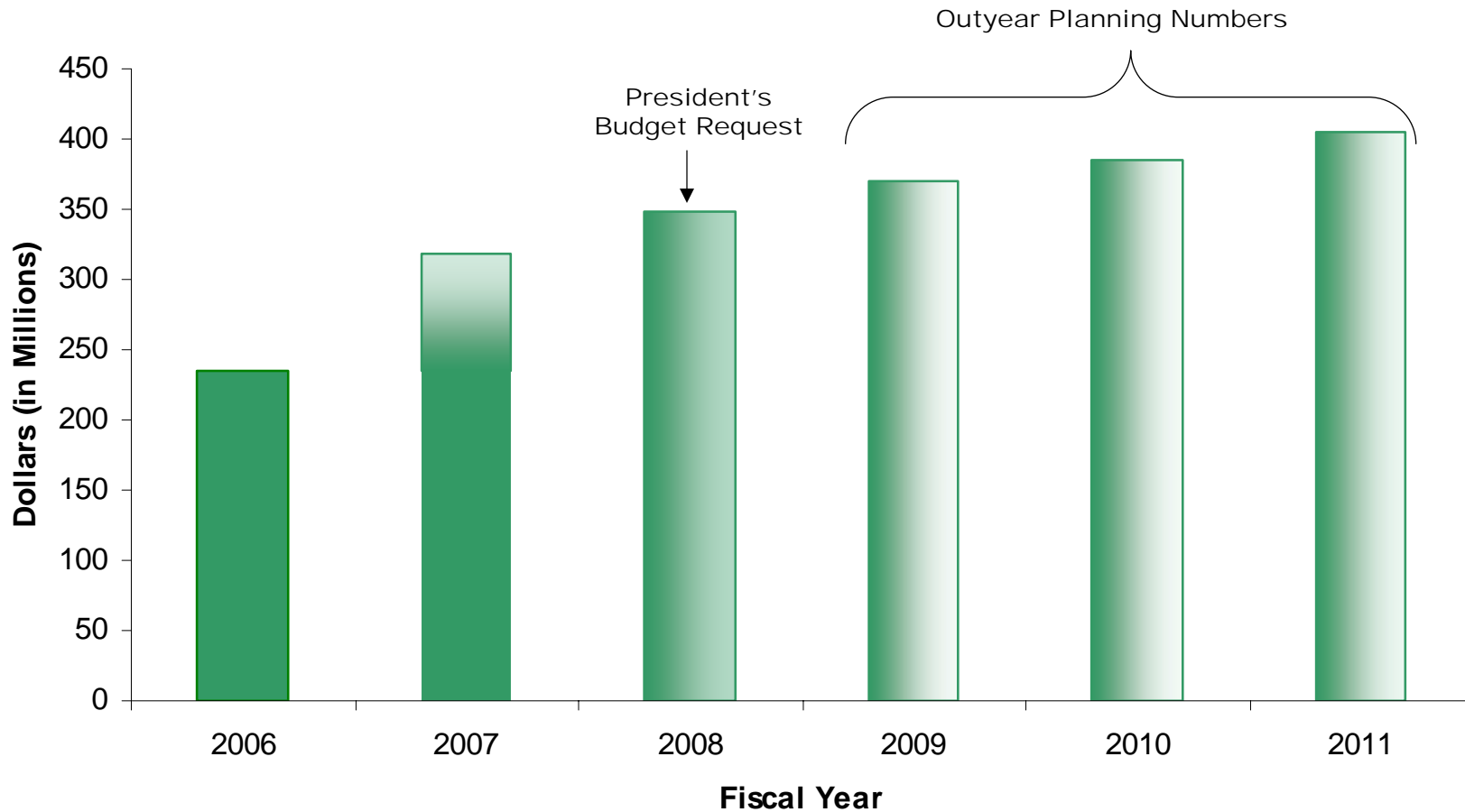
- Signed by President February 15, 2006
- **Sec. 113.** Within 30 days of the enactment of this section, each of the following departments and agencies shall submit to the Committees on Appropriations of the House of Representatives and the Senate a spending, expenditure, or operating plan for fiscal year 2007 at a level of detail below the account level. (Department of Energy)

FY 2006 SC Appropriation	\$3,515,231,000	
FY 2007 SC President's Request	\$4,101,710,000	17% increase over FY 2006 SC appropriation
FY 2007 SC H.J. Res. 20	\$3,796,393,000	8% increase over FY 2006 SC appropriation



ASCR Budget Comparison FY 2006 – FY 2011

Advanced Scientific Computing Research Program





SC Lab Appraisals

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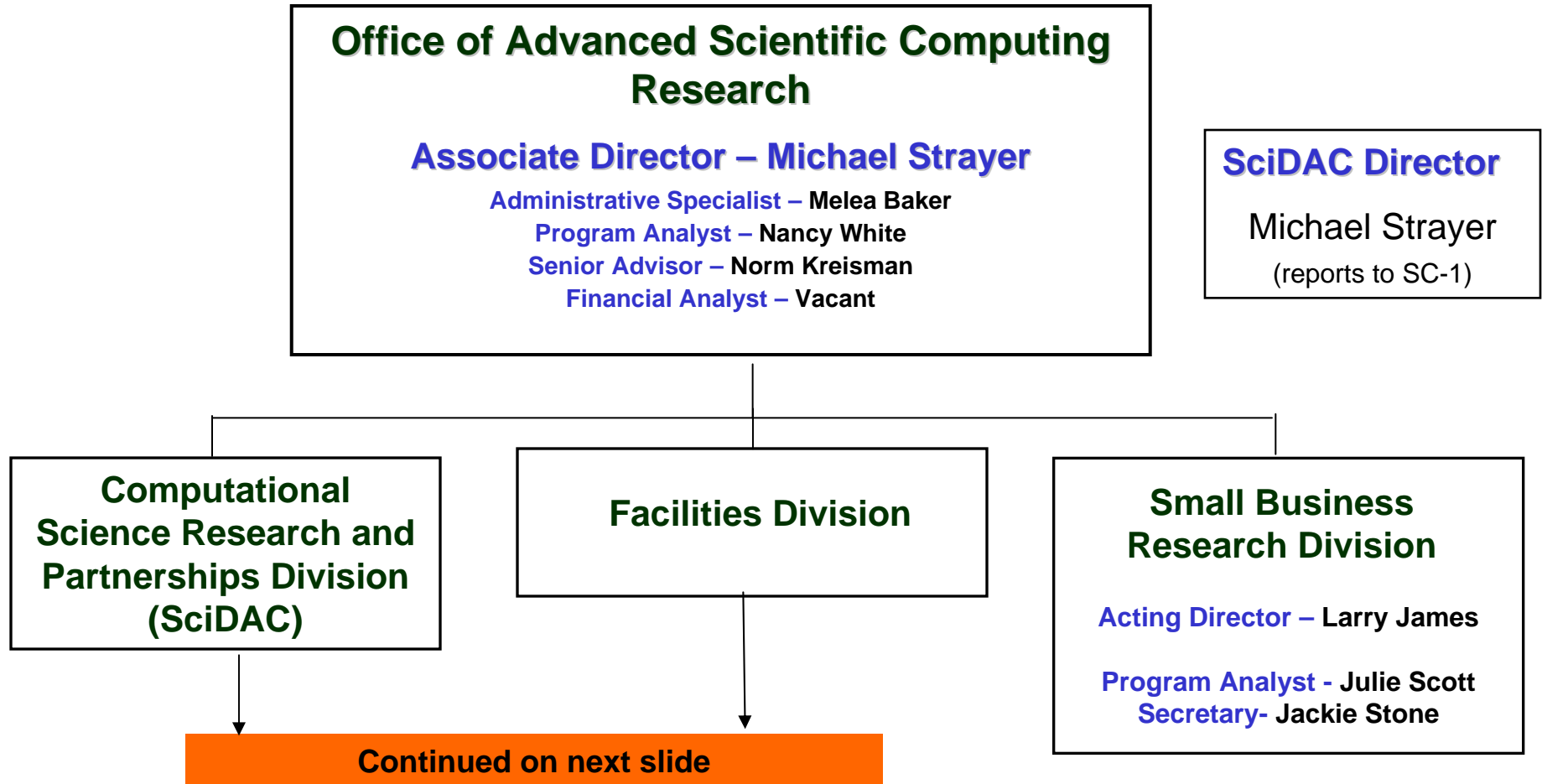
- SC's new laboratory appraisal system offers a common platform to evaluate all laboratories and is a significant improvement over the old evaluation system.
- All laboratories are evaluated against the same goals and objectives.
- Performance measures and metrics under the objectives, however, can vary to address unique aspects at each laboratory. This provides both commonality and flexibility in the performance evaluation process.
- The old SC laboratory appraisal system had less consistency across the laboratories in what was considered in evaluating their overall performance in science and operations.
- This new system will be more fair and consistent in evaluating the performance at our laboratories.
- This new system results in a laboratory report card based on an approach similar to graduate school grading, in which a B+ means the laboratory performance meets our expectation.

http://www.er.doe.gov/News_Information/News_Room/2007/Appraisal_0Process/index.htm



ASCR Staff

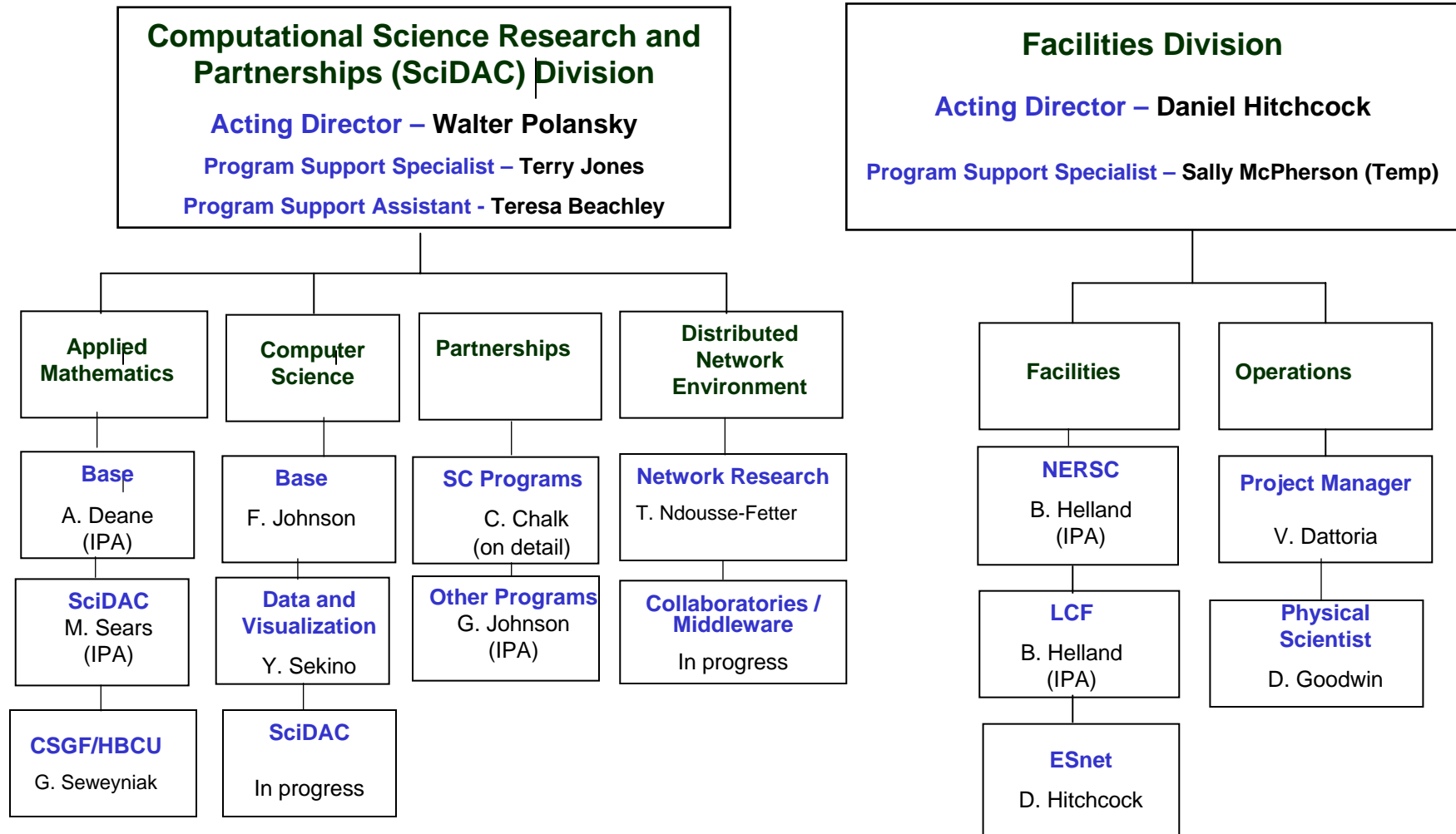
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ASCR Staff (cont)

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Recent Workshops

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- Mathematics Research Challenges in Optimization of Complex Systems, December 7-8, 2006
- Computational Subsurface Sciences, January 9-12, 2007
- DOE Cybersecurity R&D Challenges for Open Science, January, 24-26, 2007

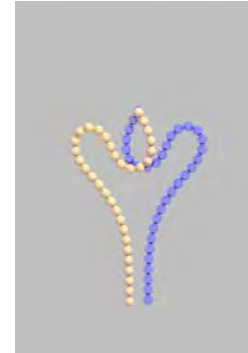
ASCAC presentations on workshops planned for Tuesday afternoon and Wednesday morning



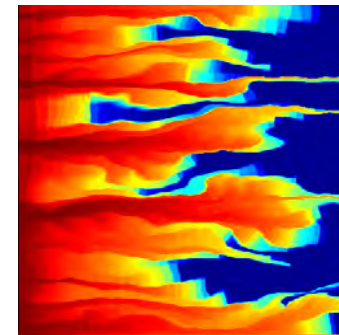
Recent Accomplishments Applied Mathematics

Advanced Scientific Computing Research Program

- Numerical model of two-phase viscoelastic flow, which can be used to simulate a wide collection of nanoscale devices and flow phenomena with applications ranging from ink jet plotters to plasma screens to automated drug design- LBNL
- Novel multiscale approach to enable system-level simulations of nanoscale systems, involving millions of atoms (100-1,000 x improvement over existing methods); places nanoscale system prediction and design within reach- ANL
- Fundamental advances in multiscale methods for flow and transport in highly heterogeneous porous media which lack apparent scale separation; Systematic multiscale analysis and efficient coarse-scale models that can capture global effects- Caltech, Stanford and Texas A&M



Microscopic scale actin filaments can exhibit “coiling” patterns

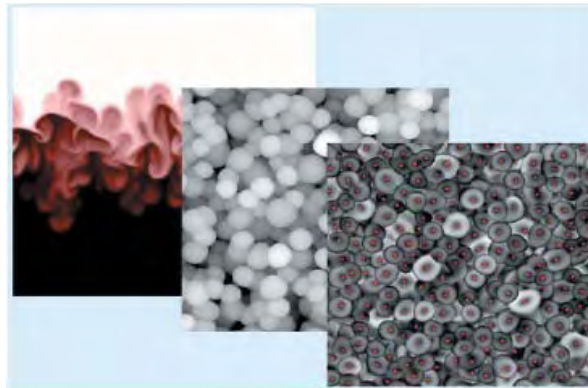


Fine-scale saturation

Recent Accomplishments Computer Science

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- Recent enhancements to MPICH2 includes support for multi-core CPUs and multithreading. Both of these features enable applications using MPI to take advantage of key features in the Cray and IBM architectures. **MPICH2 won a 2005 R&D100 award.**
- Many scientific data sets are now so large and complex that useful information is overlooked and the potential benefits of increased data are only partially realized. **Sapphire**, developed at LLNL, provides powerful data mining capabilities for end-to-end data analysis that finds useful information in raw datasets and **won a 2006 R&D100 award.**



Sapphire software is being used to characterize and track bubbles and spikes in an 80 terabyte dataset from a three-dimensional, high fidelity simulation of the Rayleigh-Taylor instability.

(a) A 2-D slice of the data, indicating the bubble-spike region in pink. (b) The bubble height image. (c) The bubble counts using the magnitude of the X-Y velocity at the bubble boundary. Only 1/36 of the two dimensional data are displayed.



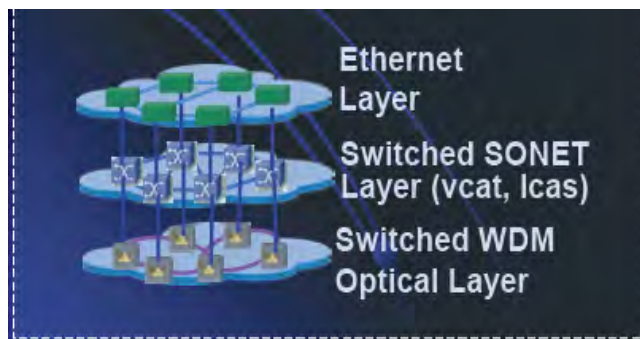
Recent Accomplishments

Distributed Network Environment Research

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Switched Optical Network Technologies for large-scale Science

Researchers working with *UltraScience Net testbed* have successfully developed and tested advanced optical network technologies that enable a single backbone network to provide conventional Internet services as well as dynamic switched optical services to support large-scale science applications



Network with multiple layers designed to be dynamically reconfigurable at the optical layer to support scientific applications with diverse network requirements.

Demonstrates that reliable transfer of scientific data can be increased 100x.

Method ready for transfer to next-generation, high-performance science networks.



ASCR Facilities Update

Advanced Scientific Computing Research Program

- **ALCF**
 - 100 teraflop IBM Blue Gene/P package awaiting approval from Chicago Operations
- **LCF - Oak Ridge**
 - Cray XT3 upgraded from 25 to 54 teraflops in FY 2006
 - 100 teraflop upgrade in final acceptance testing.
- **NERSC**
 - 100+ teraflop Cray XT4 delivered and acceptance testing will begin in March, 2007
- **ESNET**
 - The second and third MAN were completed in the Chicago and New York-Long Island Areas. They provide dual connectivity at 20 gigabits per second.
 - Partnership agreement with Internet2 was signed in August, 2006



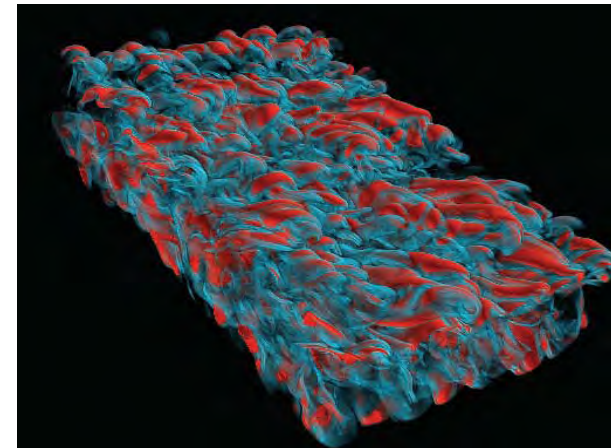
Management Principles for HPC facilities tailored from DOE Order 413.3 and OMB Guidance



INCITE Accomplishments

Advanced Scientific Computing Research Program

- “The INCITE award has enabled us to extend our computations to three dimensions so that we may investigate interactions between turbulence, mixing, and finite-rate detailed chemistry in combustion.”
Direct Numerical Simulation of Turbulent Non-Premixed Combustion (Jacqueline Chen, Sandia National Laboratories, California)
- “Using our 2006 INCITE award, we have simulated fracture of the largest-ever 3-D lattice systems. For the first time, these simulations confirmed and explained the anomalous scaling observed in fracture experiments, a result which could only be achieved by simulating very large systems. These large scale simulations, possible only through INCITE allocation, have been instrumental in advancing the current understanding of physics of how materials fracture.”
Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture, Phani Nukala, Oak Ridge National Laboratory, Tennessee



NERSC – INCITE - Chen
Simulated planar jet flame, colored by the rate of molecular mixing, critical for determining the interaction between reaction and diffusion in a flame.

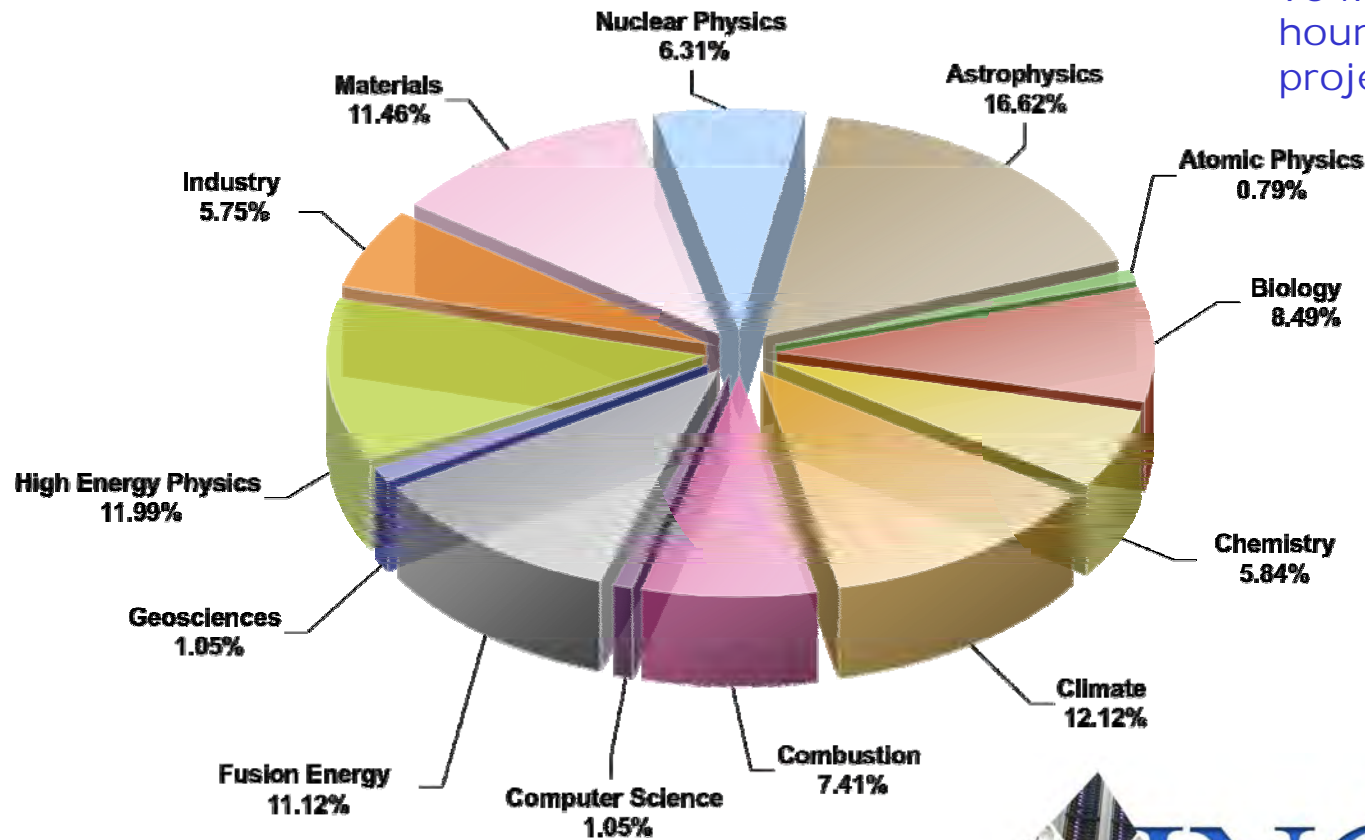
See <http://www.sc.doe.gov/ascr/incite/ResearcherRemarks.pdf>



2007 INCITE Allocations by Disciplines

Advanced Scientific Computing Research Program

95 Million processor hours allocate to 45 projects





Other Activities

Advanced Scientific Computing Research Program

- National Plan for Advanced Networking Research, Dan Hitchcock, ASCR co-chair with Susan Iacono, NSF

“In 2007, participating agencies will undertake the development of a Federal Plan for Advanced Networking R&D, analogous to the recent Plans for High-End Computing and for Cyber Security and Information Assurance R&D. The Federal Plan for Advanced Networking R&D will provide a strategy for addressing current and future networking needs of the Federal government in support of science and national security missions, and provide a process for developing a more detailed roadmap to guide future multi-agency investments in advancing networking R&D.” *(page 48 of the Analytical Perspectives of the 2008 budget, <http://www.whitehouse.gov/omb/budget/fy2008/pdf/apers/crosscutting.pdf>)*



Planned Workshops

Advanced Scientific Computing Research Program

- 2007 Computational Science and Engineering Conference, April 10-12, 2007 at the Omni Shoreham Hotel.
 - The application focus of this meeting will be Nuclear Energy and Reactor Simulations.
- Cybersecurity Research Needs for Open Science, May 2007
- Applied Mathematics Research PI Meeting, May 22-24, 2007
- Development of sub-program in Math for Large Data Sets, June 2007
 - Mathematics for Understanding the Science in Petascale Data: *Finding the Dots, Connecting the Dots, Understanding the Dots*
- Computational Science Research Needs in Alternative & Renewable Energy, August, September 2007



New ASCR Website

Advanced Scientific Computing Research Program



<http://www.sc.doe.gov/ascr/>