

U.S. Department of Energy



Office of Science

Advanced Scientific Computing Research Program

View from Washington and Germantown

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August 5, 2008



Talk Outline

Advanced Scientific Computing Research Program

Advanced Scientific Computing Research (ASCR) Update

- Budget
- Staffing
- Research Program Highlights
- International Collaborations
- Innovative and Novel Computational Impact on Theory and Experiment (INCITE) update
- Small Business Innovative Research (SBIR)



Advanced Scientific Computing Research Budget Status

Advanced Scientific Computing Research Program

- Under a Continuing Resolution (CR) until 03/09.
 - Third year of prolonged CRs – makes budget and planning hard.
- Both Senate and House have Energy and Water Bills that have passed the Committee.
- After the Bills are passed by the full Senate and House the two committees go to Conference and then the conference Bill goes back to both houses for votes and if passed without amendment the Bill goes to the President and, if signed, becomes law. All of this needs to happen before Jan. 1 or we start all over again.
- New FY 2010 Budget request delivered in Jan.
- Probability CR will be extended to year long.



ASCR 2009 Budget Action House Report

Advanced Scientific Computing Research Program

“The Committee recommendation is **\$378,820,000, an increase of \$10,000,000 over the budget request and \$27,647,000 over the current fiscal year.** The increase includes **\$5,000,000 above the budget request to expand its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) activities,** which leverage the Department’s leadership computational facilities and expertise by pairing them with scientists and engineers in other fields from universities, national laboratories, and industry to address critical scientific and technological questions. **A further \$5,000,000 is provided to enhance advanced scientific computing research activities relevant to two of the six integrated research and development research and development areas identified in the request.** Including these additional funds, \$5,000,000 is provided for Advanced Mathematics for Optimization of Complex Systems, Control Theory, and Risk Assessment, and \$2,969,000 is provided for Carbon Dioxide Capture and Storage. These increases reflect the Committee’s view of the importance of scientific computation not only in revolutionizing the way science is done, but also for applying these techniques to a wide range of modeling efforts relevant to the broader missions of the department.”



ASCR 2009 Budget Action Senate Report 110-416

Advanced Scientific Computing Research Program

“The Committee provides **\$368,820,000 for Advanced Scientific Computing Research, the same as the budget request.** The Committee is concerned that the Department has limited cooperation between the NNSA and DOE laboratories in supporting the advanced computing architecture and algorithm development. The Committee expects the Office of Science to continue to support joint research through the Institute for Advanced Architecture and Advanced Algorithms.”



ASCR Budget Details

Advanced Scientific Computing Research Program

	FY 2008 Approp.	FY 2009 Request	FY 2009 HEWD	FY 2009 SEWD	FY 2009 CR
Applied Mathematics	36,885	43,164	46,164	43,164	36,885
Computer Science	27,226	34,618	34,618	34,618	27,226
Computational Partnerships	53,767	52,064	54,064	52,064	53,767
Next Gen. Networking for Science	12,017	17,221	17,221	17,221	12,017
High Performance Production Computing	54,200	54,790	54,790	54,790	54,200
Leadership Computing Facilities	110,158	115,000	120,000	115,000	110,158
High Performance Network Facilities & Testbeds	23,936	25,000	25,000	25,000	23,936
Research and Evaluation Prototypes	23,585	17,000	17,000	17,000	23,585
<i>Subtotal, ASCR</i>	<i>341,774</i>	<i>358,857</i>	<i>368,857</i>	<i>358,857</i>	<i>341,774</i>
All other (GPP, GPE, SBIR/STTR)	9,399	9,963	9,963	9,963	9,399
Total, ASCR	351,173	368,820	378,820	368,820	351,173



Impacts of a Year long CR

Advanced Scientific Computing Research Program

- Joint Applied Mathematics-Computer Science Institute
- Mathematics of large datasets
- Direct support for science application “leading edge developers”
- Partnership with BER in climate models to improve the representation of ice sheets in global circulation
- Basic research effort in Cyber Security for Open Science
- *However, the CR fully funds the Department’s commitment to the DARPA High Productivity Computing Systems (HPCS)*

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Advanced Scientific Computing Research Program

ASCR Staffing



ASCR

Organizational Structure

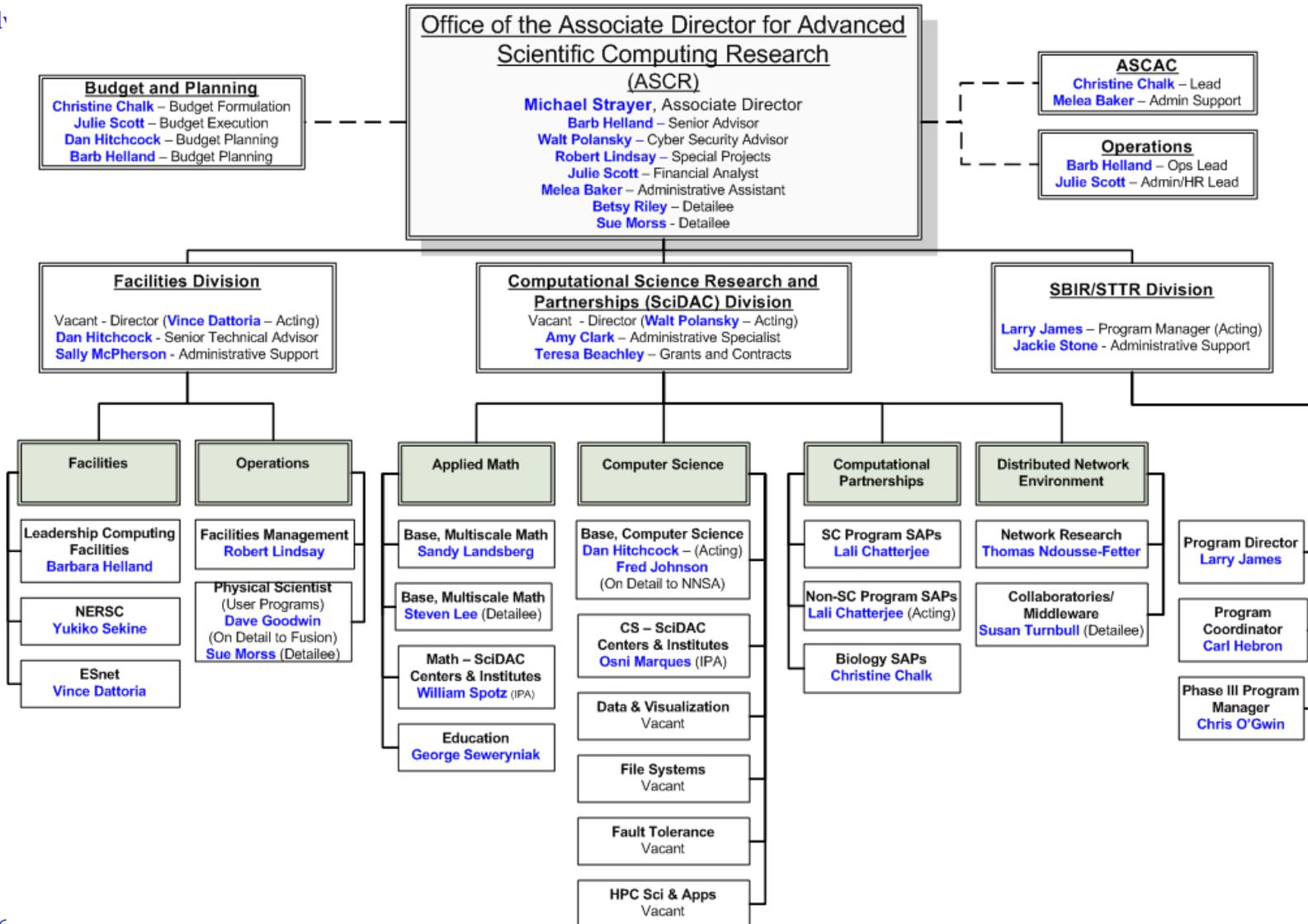
Advanced Scientific Computing Research Program





Staff Assignments October, 2008

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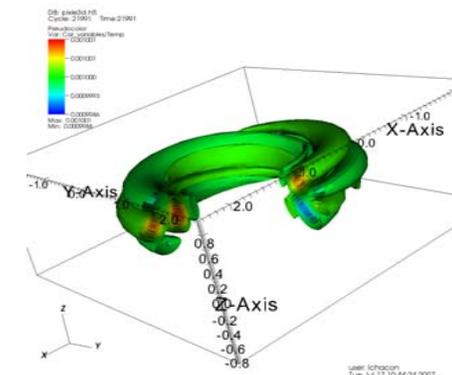
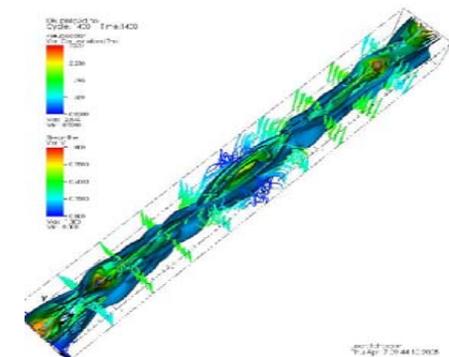
Advanced Scientific Computing Research Program

Research Program Highlights

Applied Math Research Program Update

Advanced Scientific Computing Research Program

- **Staffing Changes:**
 - Sandy Landsberg, Team Lead
 - Steve Lee, Detailee from LLNL, Program Manager
- **Multiscale Mathematics and Optimization for Complex Systems call**
 - 2 proposals in Optimization funded in FY2008
 - 19 proposals “under consideration” pending continuing resolution
 - 77 proposals declined
- **Recent workshops**
 - Meeting held in Chicago, IL Oct 7-9, 2008 with parallel tracks on
 - Joint Mathematics/Computer Science Institutes
 - High-Risk / High Payoff Technologies
- **Outreach to external organizations**
 - NSF Division of Mathematical Sciences





Applied Mathematics 2008 PI Meeting

Advanced Scientific Computing Research Program

- Held at Argonne National Laboratory Oct 15-17, 2008
- Over 140 researchers in attendance





Computer Science Research Program Update

Advanced Scientific Computing Research Program

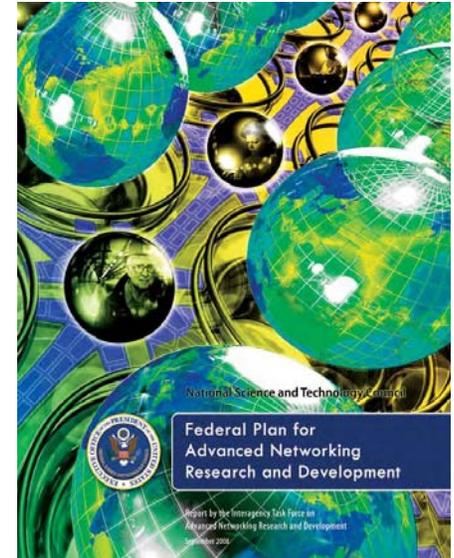
- **Staffing changes:**
 - Dan Hitchcock: Team Lead
 - Osni Marques, IPA from LBNL, Program Manager
- **Software Development Tools for Improved Ease-of-Use of Petascale Systems call**
 - 97 proposals received representing 34 projects
 - Topics included Performance tools, Correctness tools, Development Environment and
 - Scalable Infrastructure
 - Review was for August 26-27
- **CS Strategic plan**
 - Started (informal) discussions/consultations with community
 - Format to be decided (e.g. 10 most difficult problems?)



Next-Generation Networks Program Update

Advanced Scientific Computing Research Program

- **Staffing Changes**
 - Susan Turnbull, detailee from GSA, Team Lead
- **Program elements:**
 - **Network research** – core network research
 - **Middleware research** – Grid technologies
- **The next-generation program**
 - supports R&D activities to develop advanced networks to enable distributed high-end science
 - coordinates with ESnet to develop and deploy networks that enable scientists to push the limits of today's networks
- Next-generation network technologies has enabled the efficient and rapid distribution of massive data generated by the LHC experiment and climate modeling
- Major activities in FY09: Network research program announcement





ASCR Education Programs

Computational Science Graduate Fellowship

Advanced Scientific Computing Research Program

- The Computational Science Graduate Fellowship (DOE-CSGF) is a strategic investment to develop the next generation of computational scientists, providing support and guidance to some of the nation's best scientific graduate students.
- According 2006 DOE-CSGF Program Review:
 - “This relatively small, but incredibly effective program has succeeded in the critical area of advanced scientific computing by operating a program that attracts and selects students through a competitive process that results in an enhanced graduate education in this important field...The success of this program is clearly evident...”
- Recommendations
 - DOE should seek funding to double the size of the current program and should work closely with the contractor to be sure that the current excellent management approach is maintained.
 - The notion of starting follow-on programs, such as named postdoctoral fellowships or Young Investigator award programs in scientific computing is worthwhile and should be considered by DOE...But it is important that the existing graduate student efforts not be diluted.



ASCR Education Programs

DOE-CSGF (cont)

Advanced Scientific Computing Research Program

- Currently 68 fellows; 18 new fellows started in September, 2008
- 222 DOE-CSGF alums:
 - 18% at DOE Laboratories
 - 33% in academia
 - 30% in industry
 - 19% other (other federal or state agencies, non profit, etc)
- Next Annual Conference: July 14 - July 16, 2009 in D.C.



<http://www.krellinst.org/csgf>



ASCR Education Programs

Research Alliance in Math and Science

Advanced Scientific Computing Research Program

- The Research Alliance in Math and Science (RAMS) was designed to provide collaborative research experiences among faculty and students at colleges or universities and DOE national laboratory researchers.
 - Undergraduate and graduate students intern at the Oak Ridge National Laboratory (ORNL) during a summer term of 10 - 12 weeks.
 - Each student is assigned to a research mentor to work on a project of interest to the student, the student's professor(s), and the ORNL researcher.
 - 17 students participated in 2008
 - RAMS intern, Jessica Traviero, won first place in poster competition at the TeraGrid '08 Student Competition.
 - Program Review planned for Dec 3-4, 2008



<http://computing.ornl.gov/internships/rams/>

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INTERNATIONAL COLLABORATIONS



International Collaborations

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- Meetings with French and European Commission in September, 2008
- Potential Areas of Collaboration
 - Applications software and algorithms for petascale computing with a particular emphasis in areas of energy, environment and basic science,
 - Open source systems software, I/O, data management, visualization, and libraries of all forms targeting petascale computing platforms,
 - New programming models and tools addressing extreme scale, multicore, heterogeneity and performance,
 - Large-scale systems deployments for attacking global challenges,
 - Education and training for the next generation of computational scientists.



International Collaborations

First Steps

Advanced Scientific Computing Research Program

Joint workshops - targeting workshops where international cooperation could be of value – HPC or exascale or computing science/domain science.

- Open software workshops; Jack Dongarra, the University of Tennessee, Knoxville will be the U.S. lead for this.
- ASCR HPC Best Practices Workshop series
 - 2007—Integration issues
 - 2008—Risk Management

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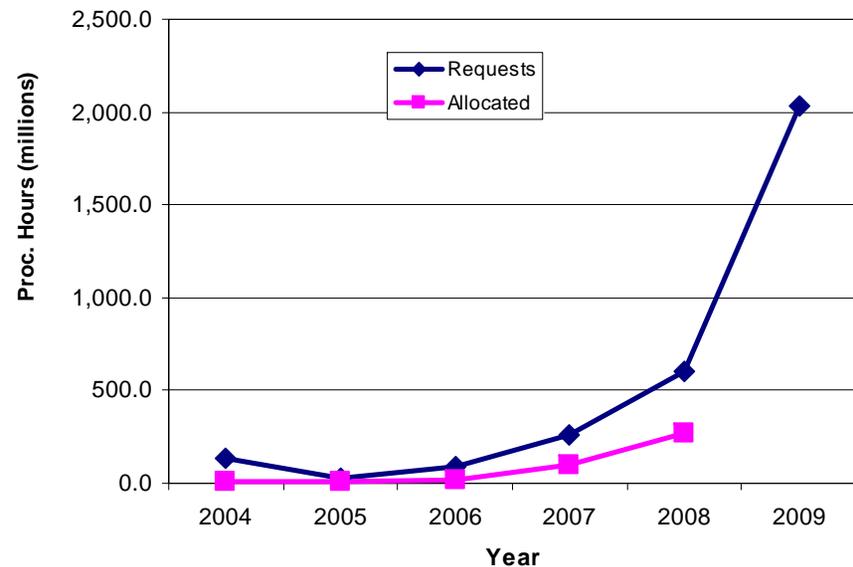
Innovate and Novel Computational Impact on Theory and Experiment (INCITE)



INCITE Background

Advanced Scientific Computing Research Program

- Initiated at National Energy Research Scientific Computing Center (NERSC) at LBNL in 2004
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer and computational reviews





2009 Proposals

Advanced Scientific Computing Research Program

- 79 unique proposals received from scientific disciplines of accelerator physics, astrophysics, chemical sciences, climate research, computer science, engineering physics, environmental science, fusion energy, life sciences, materials science, and nuclear physics
- 21 renewal proposals

Over **2 Billion processor hours** requested for 2009 from new and renewal proposals

Over 600 Million processors hours available for 2009 awards, including renewals

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SBIR/STTR Update



SBIR/STTR

Advanced Scientific Computing Research Program

- Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs in separate division in ASCR
- Current set asides for SBIR and STTR are 2.5% and 0.3%, respectively on all DOE R&D programs except NNSA
- New SBIR/STTR Request for Proposals (RFP) issued September 17th and will close November 20th (<http://www.sicence.doe.gov/sbir>)
- Anticipate selecting 350 SBIR Phase I and 25 STTR Phase I awards (at \$100K each) in April with awards made in June.
- ASCR-related Topic Areas:
 - 50. Software Libraries and Applications Maintenance and Scaling to Petascale
 - 51. Scientific Visualization and Data Understanding
 - 52. High Performance Networks
 - 53. Scalable System Software for Petascale Computer Systems
 - 54. Scalable Middleware and Grid Technologies

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SC08

Advanced Scientific Computing Research Program

ASCR PI Meeting

Salon E

Hilton Hotel -- Austin Downtown

Monday November 17, 2008

4:00 pm – 6:00 pm