



U.S. DEPARTMENT OF
ENERGY

OFFICE OF
SCIENCE

Opportunities in Biology at the Extreme Scale of Computing

August 17-19, 2009

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Office of Science, U.S. Department of Energy



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ENERGY

Vision

-- Advanced Scientific Computing Research --

▪ Deliver Petascale Science Today

- Continue to make the Leadership Computing Facilities available to the very best science through Innovative and Novel Computational Impact on Theory and Experiment (INCITE).
- Continue to work with Pioneer Applications to deliver scientific results from day one.

▪ Build the Intellectual Foundation for the Future

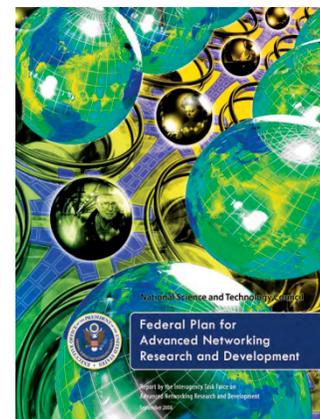
- Continue to nurture –
 - World class mathematics and computer science research efforts
 - Applications critical to DOE missions through Scientific Discovery through Advanced Computing (SciDAC).
- Provide direct support for “bleeding-edge” research groups willing to take on the risk of working with emerging languages and operating systems.
- Foster innovative research at the ever blurring boundary between Applied Mathematics and Computer Science.

▪ Realize the Promise of Extreme Scale

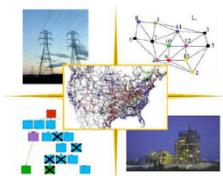
- Work with key science applications to identify opportunities for new research areas only possible through extreme scale computing.
- Support innovative research on advanced architectures and algorithms that accelerates the development of hardware and software that is well suited to extreme scale computational science.



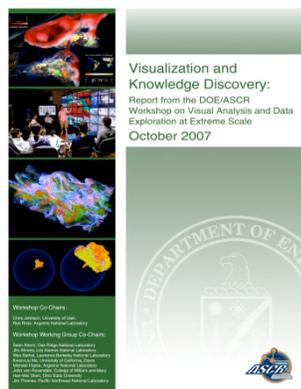
- Provide forefront research knowledge and foundational tools:
 - Continuing excellence in applied mathematics, computer science and next generation networking research
 - Advancing scientific discovery through cross-disciplinary partnerships (SciDAC)



Mathematical Research Challenges in Optimization of Complex Systems
Report on a Department of Energy Workshop
December 7-8, 2006



Organizers:
Bruce A. Barlow
Sandia National Laboratories
Albuquerque, New Mexico
Magaret S. Wright
Cornell Institute of Mathematical Sciences
New York University, New York

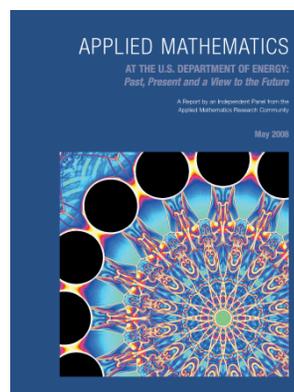
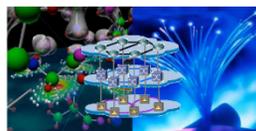


Visualization and Knowledge Discovery:
Report from the DOE/ASCR
Workshop on Visual Analysis and Data
Exploration at Extreme Scale
October 2007

US Department of Energy
Office of Science

Workshop Report on
Advanced Networking for
Distributed Petascale Science:
R&D Challenges and Opportunities

April 8-9, 2008



APPLIED MATHEMATICS

AT THE U.S. DEPARTMENT OF ENERGY:
Past, Present and a View to the Future

A Report to the Independent Panel from the
Applied Mathematics Research Community

May 2008

Mathematics for Analysis of Petascale Data

Report on a Department of Energy Workshop
June 3-5, 2008



Organizers and Authors:

Philip Kegelmeyer, Chair	Sandia National Laboratories
Robert Calderbank	Princeton University
Terence Cochran	Pacific Northwest National Laboratory
Leif Johansson	National Science Foundation
Chandrika Kamath	Lawrence Livermore National Laboratory
Juan Meza	Lawrence Berkeley National Laboratory
Nagiza Samalova	North Carolina State University/Cornell University
Alyson Wilson	Louisiana State University



Applied Mathematics and Computer Science

Software Developed under ASCR Funding

Programming Models

Active Harmony

ARMC1
ATLAS
Berkeley UPC Compiler
Charm++
Fountain

FT -MPI
Global Arrays
Kepler
MVAPICH
OPEN-MPI
OpenUH
PVM

Development/ Performance Tools

BABEL
Berkeley Lab Checkpoint Restart
(BLCR)
Dyninst API
Fast Bit
Goanna
HPCtoolkit

Jumpshot
KOJAK
MPIP
MRNet
Net PIPE
OpenAnalysis
PAPI
ROSE
ScalaTrace
STAT
TAO

TAU
Hpcviewer

Math Libraries

ACTS COLLECTION

ADIC
Hypre
ITAPS Software Suite
LAPACK
Mesquite

MPICH2
OpenAD
OPT++
PETSc
ROMIO
ScaLAPACK
Sparskit -CCA
Trilinos

System Software

Cluster Command & Control
High-Availability OSCAR HA -
OSCAR
LWK-Sandia
PVFS
ZeptoOS

Collaboration

enote

Visualization /Data Analytics

BeSTMan
Parallel netCDF
Virtual Data Tool Kit

Miscellaneous

Libmonitor



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Scientific Discovery through Advanced Computing (SciDAC)

- Advancing Science through large-scale data, modeling and simulation
 - Science Application and Science Applications Partnerships: *Astrophysics, Accelerator Science, Climate, Biology, Fusion, Petabyte data, Materials & Chemistry, Nuclear physics, High Energy physics, QCD, Turbulence, Groundwater*
 - Centers for Enabling Technology: Address mathematical and computing systems software issues
 - Institutes: Assist Scientific Applications teams and foster next generation computational scientists



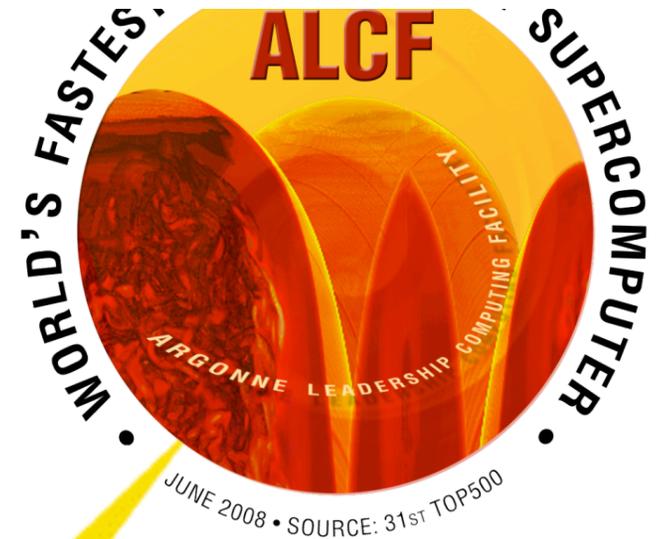
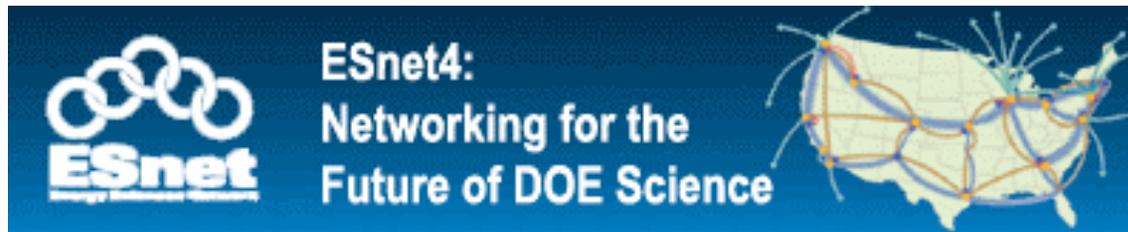
<http://www.scidac.gov>



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ASCR Facilities

- Providing the Facility – High-End and Leadership Computing
- Investing in the Future - Research and Evaluation Prototypes
- Linking it all together – Energy Sciences Network (ESnet)

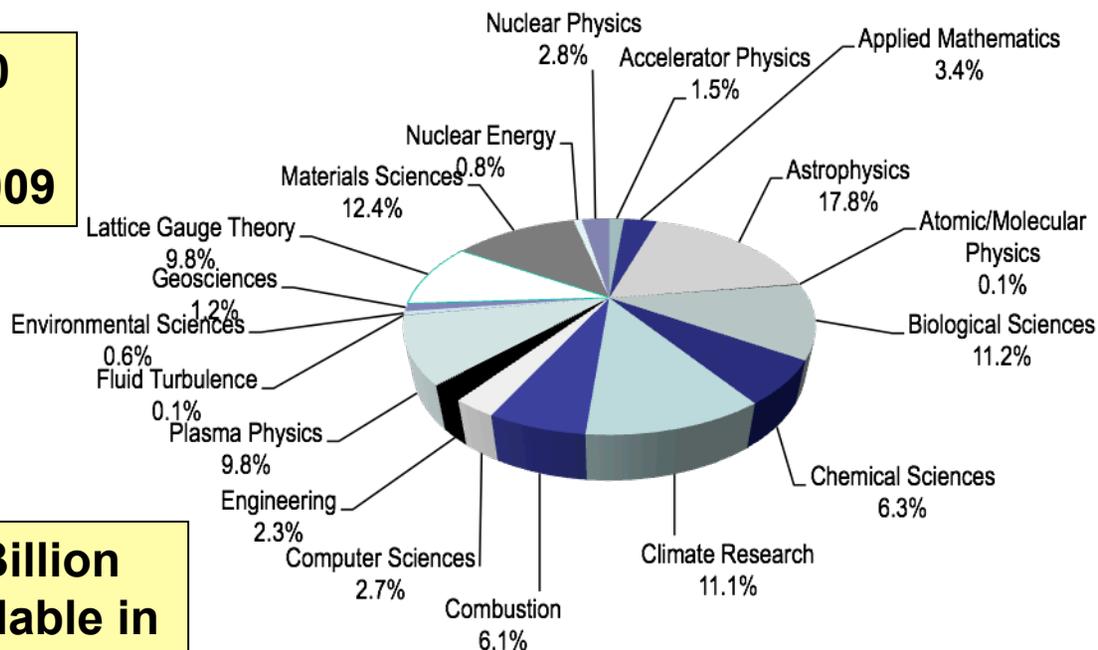




- **Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program started in 2004.**
 - Small number of computationally intense, high impact projects
 - Open to all national and international researchers, including industry
 - No requirement of DOE or Office of Science funding or topic area
 - Peer and computational reviews

2009 INCITE projects

**Approximately 890
million processor
hours awarded in 2009**



**Approximately 1.3 Billion
processor hours available in
2010**



Realizing the promise of Extreme Scale

Listening to the Community

Three Town Hall Meetings held April-June, 2007

**Climate, Combustion, Fusion, Fission
Solar, Biology, Socioeconomic Modeling
and Astrophysics**

**Mathematics, Computer Science
Algorithms, Software infrastructure and
Cyberinfrastructure**

**Integrated program- investments in
hardware, algorithms and scientific
software research and development**

**Tightly coupled to a selected set of
scientific communities and the
associated applied mathematics
research.**

**Modeling and
Simulation at the
Exascale for
Energy and the
Environment**

Co-Chairs:
Horst Simon
*Lawrence Berkeley National Laboratory
April 17-18, 2007*
Thomas Zacharia
*Oak Ridge National Laboratory
May 17-18, 2007*
Rick Stevens
*Argonne National Laboratory
May 21-June 1, 2007*



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Science Needs at the Extreme Scale Workshop calendar

■ Prior

- **BER/Climate Workshop:** Challenges in Climate Change Science and the Role of Computing at the Extreme Scale, November 6-7, 2008
- **HEP/High Energy Physics Workshop:** Scientific Challenges for Understanding the Quantum Universe and the Role of Computing at the Extreme Scale, December 9-11, 2008
- **NP/Nuclear Physics Workshop:** Forefront Questions in Nuclear Science and the Role of High Performance Computing
- **FES/Fusion Workshop:** Extreme Scale Computing Challenges in Fusion Science, March 2009
- **NE/Nuclear Energy Workshop:** Science-based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale, May 11-12, 2009
- **BES/Materials&Chemistry Workshop:** Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, August 13-15, 2009 in Bethesda, MD

■ Now

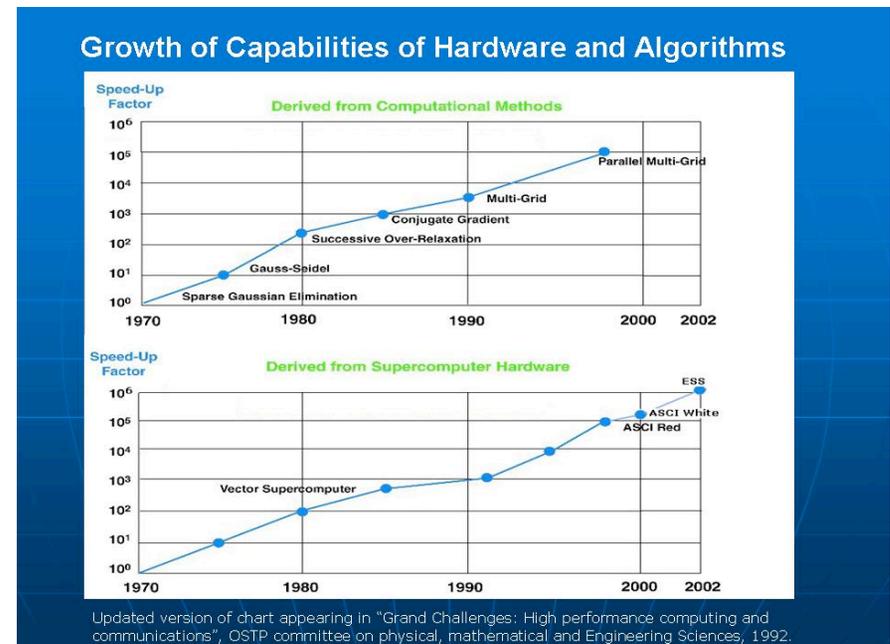
- **BER/Biology Workshop: Opportunities in Biology at the Extreme Scale of Computing, August 17-19, 2009 in Chicago**

■ Planned

- **NNSA/ASCR Workshop:** Science Grand Challenges, October 6-8, 2009, in Washington, DC

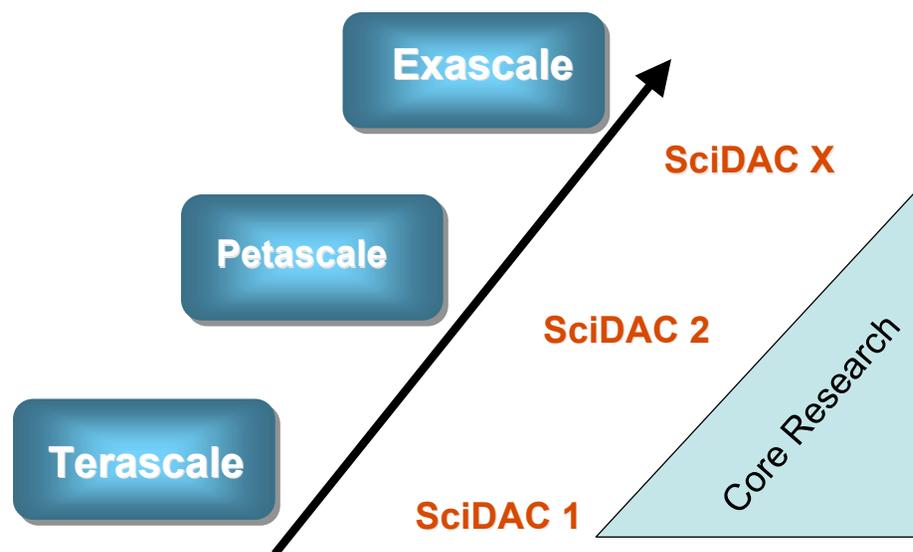
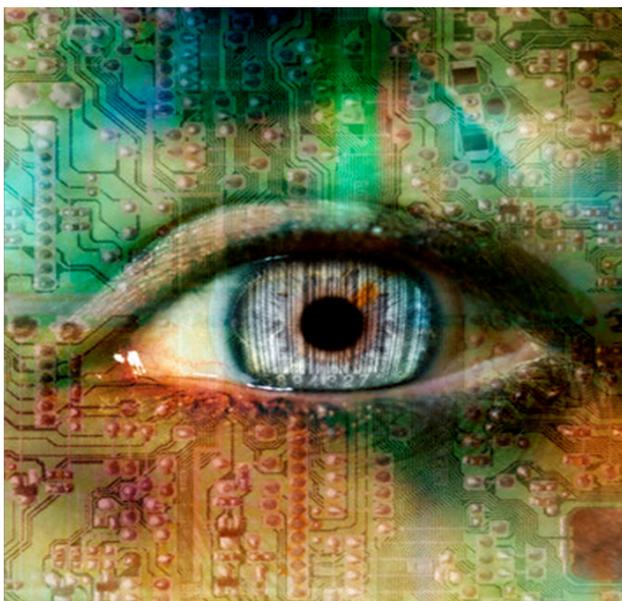
Next Steps

- ASCR will hold several cross-cutting workshops next FY as part of the process.
- ASCR will use the output from these workshops to prioritize funding opportunities all relevant areas:
 - Applied math and numerical algorithms,
 - Computer science including system software and tools, advanced computing architectures
 - Expanded partnerships
 - Pioneer/risk taking applications
 - New mission areas
 - Next generation networks
 - High Performance and Leadership Facilities





What computing is needed to enable the grand challenges in the Biological Sciences ?



Perhaps the most significant applications of scientific computing come not in the solution of old problems, but in the discovery of new phenomena through numerical experimentation, Lax Report on Large Scale Computing in Science and Engineering, 1982