U.S. DEPARTMENT OF ENERGY

Advanced Scientific Computing Research

-- An Introduction --

Texas Research Exchange Fest
September 7-8, 2009
College Station, TX

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DOE Mission Elements

- *Energy*
  - Nuclear power, clean coal, fusion reactors, enhanced oil recovery, bio-fuels, reliability & security of electric power grid, new engine designs
- *Environment*
  - Carbon sequestration, nuclear waste storage, environmental cleanup, climate research
- *National Security*
  - Nuclear stockpile stewardship

MISSION
Discovering the solutions to power and secure America's future
U. S. DEPARTMENT OF ENERGY
STRATEGIC PLAN

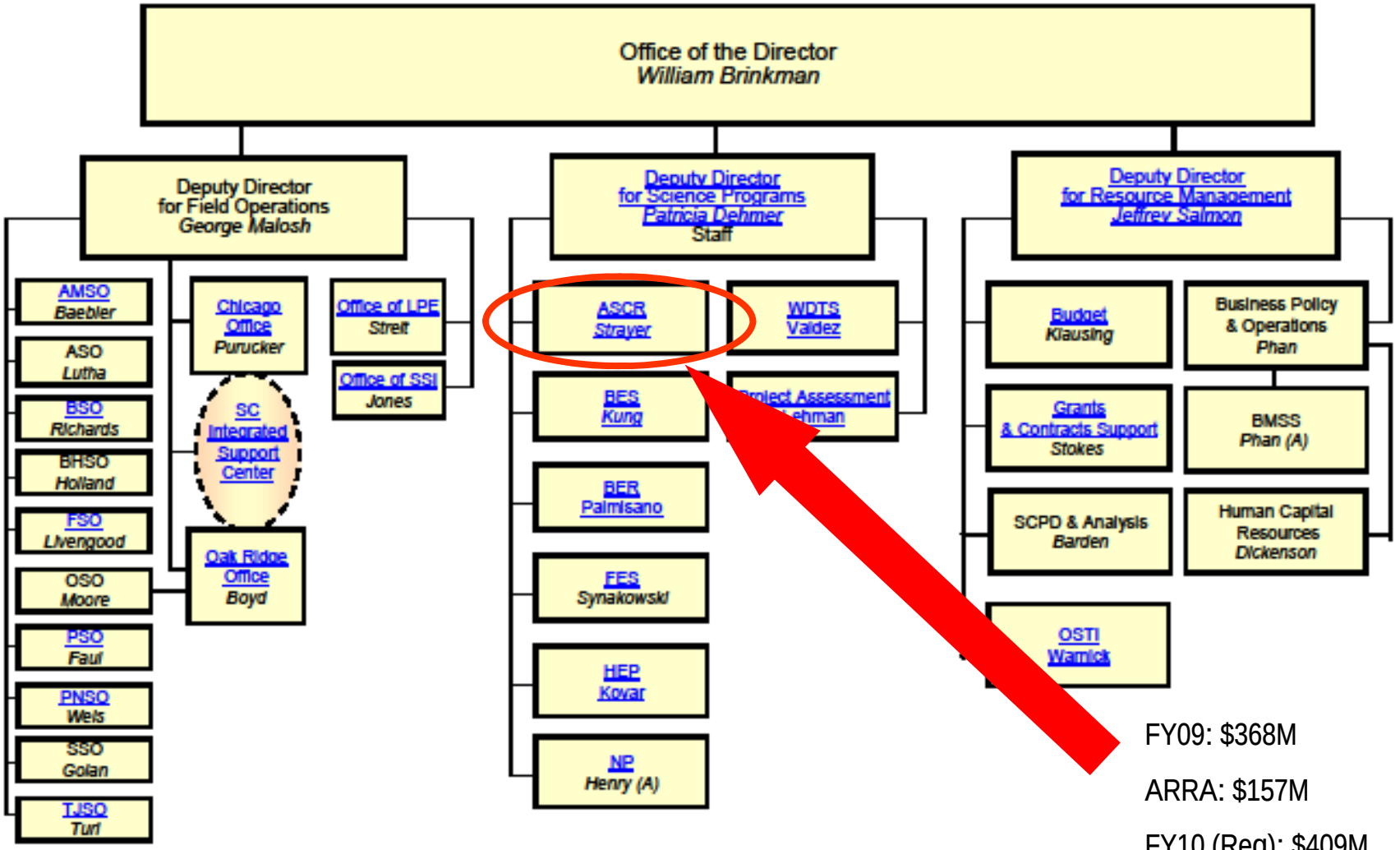
FY09: $4.8B

ARRA: $1.6B

FY10 (Req): $4.9B

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

OFFICE OF SCIENCE



FY09: $368M

ARRA: $157M

FY10 (Req): $409M

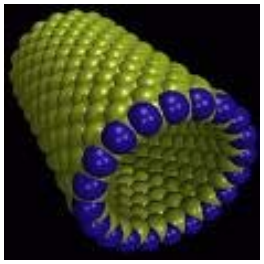
What kinds of questions can ASCR help answer for DOE?

- Can we predict the operating characteristics of a clean coal power plant?

- How stable is the plasma containment in a Tokamak?

- How quickly is climate change occurring and what are the uncertainties in the predicted time scales?

- How quickly can the US recover if part of the power grid became inoperable?



- How can new materials be designed with a specified desirable set of properties?

Answering these and other important questions involves study of increasingly complex physical and engineered systems

ASCR Vision

- **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.

http://www.sc.doe.gov/ascr/index.html

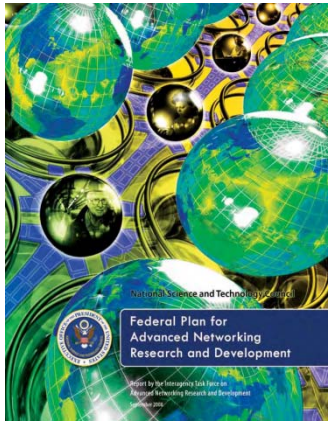
Office of Advanced Scientific Computing Research (ASCR)

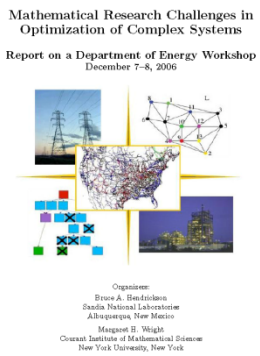
Mission:
Discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the Department of Energy.

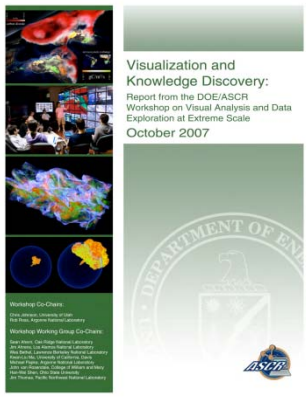
	FY 2009 Budget
Applied Mathematics	40,164
Computer Science	33,618
Computational Partnerships	52,064
Next Gen. Networking	14,321
SBIR/STTR	4,038
Total Research	**144,205**
High Performance Production Computing	54,790
Leadership Computing Facilities	115,000
High Performance Network Facilities & Testbeds	25,000
Research and Evaluation Prototypes	23,900
SBIR/STTR	5,925
HPC and Network Facilities	**224,615**
Total, ASCR	**368,820**

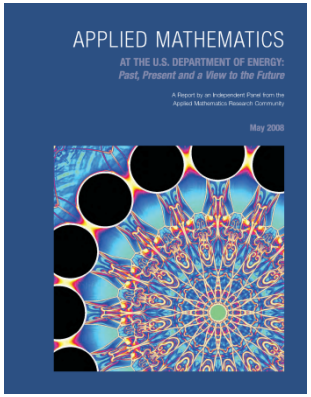
ASCR Research

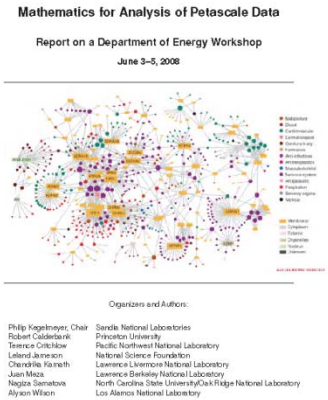
- **Provide forefront research knowledge and foundational tools:**
  - **Continuing excellence in applied mathematics, computer science and next generation networking research**
  - **Advancing scientific discovery through cross-disciplinary partnerships (SciDAC)**











Applied Mathematics and Computer Science

Software Developed under ASCR Funding

Programming Models

Active Harmony

ARMCI
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

ASCR funded R&D 100 Awards

Three ASCR funded projects win R&D 100

PETSc, a suite of data structures and routines for solving PDEs.
Funded by TOPS SciDAC project and ASCR Base Math

ROSE, a compiler infrastructure.
Funded by ASCR Computer Science program.

Catamount N-Way (CNW) lightweight kernel, operating system.
Supported by ASCR built on work funded by NNSA-ASC program.

SIAM Fellows

A Cadre of Game Changers

Of the 191 SIAM Fellows in Class of 2009:

- Over 40 have been or are currently funded by ASCR

Currently Funded SIAM Fellows

John B. Bell	LBNL
Marsha J. Berger	Courant
Russel E. Caflisch	UCLA
Alexandre J. Chorin	UC Berkeley
Phillip Colella	LBNL
Howard C. Elman	U. MD College Park
James W. Demmel	UC Berkeley
Jack J. Dongarra	UT Knoxville
C. William Gear	NEC Research
James G. Glimm	SUNY Stony Brook
Leslie F. Greengard	Courant
John Guckenheimer	Cornell
James M. Hyman	LANL
Thomas Yizhao Hou	Caltech
Christopher R. Johnson	U Utah
Sven Leyffer	ANL
Thomas A. Manteuffel	CU Boulder
Jorge J. More	ANL
J. Tinsley Oden	UT Austin
Dianne P. O'Leary	U MD College Park
Michael L. Overton	Courant
Linda R Petzold	UCSB
James A. Sethian	UC Berkeley
Michael J. Shelley	Courant
Chi-Wang Shu	Brown
Margaret H. Wright	Courant
Mary F. Wheeler	UT Austin

ASCR PECASE Winners

Cecilia Aragon, staff scientist at LBNL, received the PECASE for her groundbreaking research in data-intensive scientific workflow management, and pioneering development of innovative methods for visualization, analysis, and organization of massive scientific data sets. She is funded by ASCR.

Alexandre Tartakovsky, computational mathematician at PNNL, received the PECASE for his research on subsurface flow that addresses past and future energy needs: cleaning up buried nuclear or toxic contaminants and storing carbon dioxide from fossil fuels underground. He is also supported by the BER program.

Oliver Fringer, assistant professor of civil and environmental engineering at Stanford University, received a PECASE. Dr. Fringer was a fellow in the ASCR Computational Science Graduate Fellowship (CSGF) program from 1997-2001.

Solicitations Just Closed:
Applied Mathematics Program

- Mathematics for Analysis of Petascale Data: $4M/year
  - 81 proposals from universities & national labs, closed May 29
  - Mathematical challenges in extracting insights from “petascale” datasets
  - Topic areas include anomaly detection, machine learning, streaming data, dimensionality reduction, visualization
  - Proposals described wide variety of university, lab projects and collaborations
  - 11 awards made: 50% funds to labs, 50% funds to universities
- Mathematics for Complex, Distributed, Interconnected Systems: $3.5M/year
  - 38 proposals, all DOE national lab-led projects, closed June 12
  - Emphasis on interconnected systems operating within purview of DOE: computer networks, electric power grid, critical infrastructures
  - Lab-based projects: foundation for engaging university researchers in 2010
  - 6 awards made: 100% funds to labs (w/ some university subcontracts)

Solicitations Just Closed:

Joint Math/CS Institute

- Solicitation
  - Sought "*applications for research under a unified management structure to address key challenges where collaborative research in applied mathematics and computer science efforts are required to bridge the gap between large complex scientific applications software and next-generation hardware*"
  - Closed June 5, 2009
- $4M/year available
- 29 applications received
  - 25 were reviewed in a combination of panel and mail reviews;
  - 4 were deemed out of scope.
- Three awards have been made so far
  - Two laboratory-led
  - One university-led

Solicitations Just Closed:

Ice Sheet Modeling

- Joint ASCAC-BERAC Report in March 2008 identified the need to
  - include fully dynamic ice sheet models and ocean/ice shelf interactions
  - assess the rate and magnitude of sea level rise due to rapid ice sheet melting as a high priority for climate models.
- Solicitation
  - Sought "*computational science/applied mathematics/computer science research to accelerate scientific and computational breakthroughs to improve Ice Sheet Modeling*
  - Complements DOE SC SciDAC, ASCR and BER funded research
  - Closed May 26, 2009
- $3M/year available for three years
- Eight proposals received & reviewed
- Six Projects awarded late June, 2009
  - Two University -led
  - Four Laboratory-led

Office of Science
Early Career Research Program

- Eligibility: less than 10 years post PhD
- Full Proposals due: Sept 1, 2009 8:00PM Eastern Time
- Universities:
  - Announcement: http://www.sc.doe.gov/grants/FAPN09-26.html
  - Expected number of awards in ASCR: 4 awards
  - Budget: $150K/year over five years
- National Laboratories:
  - Announcement: http://www.sc.doe.gov/grants/LAB09_26.html
  - Expected number of awards: 2 awards
  - Budget: $500K/year over five years
- Review Criteria
  - Scientific and/or Technical Merit of the Project
  - Appropriateness of the Proposed Method or Approach
  - Competency of the Research Team and Adequacy of Available Resources
  - Reasonableness and Appropriateness of the Proposed Budget
  - Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the application/proposal is submitted
  - Leadership within the scientific community.

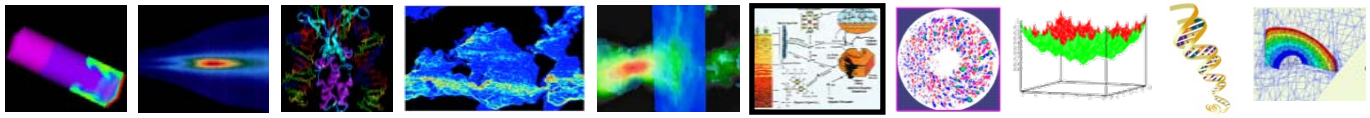
Scientific Discovery through Advanced Computing (SciDAC)

- 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

SciDAC 2: Path to Petascale

Scientific Discovery



Applications

SciDAC 2

- Accelerator science and simulation
- Climate modeling and simulation
- Fusion science
- Petabyte high-energy/nuclear physics
- Nuclear physics
- Radiation transport
- Astrophysics
- Computational Biology
- High-energy physics
- Materials science and chemistry
- QCD
- Turbulence
- Groundwater reactive transport modeling and simulation

- Centers for Enabling Technology

- Scientific Applications Partnerships
- Institutes (University-lead)

Computing/ Networking

INCITE NERSC Allocation

Leadership Computing- ANL	556 TF IBM BG/P
Leadership Computing- ORNL	263 TF Cray XT4 → 1 PF Cray XT5
Production Computing- NERSC	104 TF Cray XT4 → 360 TF Cray XT4
ESnet	On path toward Dual rings 40Gbps/ 10 Gbps fault tolerant

Top 10 Computational Science Accomplishments

Rank	Title
1	Scientists Model the Molecular Basis of Parkinson's Disease (Tsigelny)
2	Astrophysicists Discover Supernova Shock-Wave Instability and a Better Way to Spin up Pulsars (Blondin)
3	Designing Proteins at Atomic Scale and Creating Enzymes (Baker)
4	First-Principles Flame Simulation Provides Crucial Information to Guide Design of Fuel-Efficient Clean Engines (Yoo)
5	Breakthrough Fusion Simulation Sheds Light on Plasma Confinement (Tang)
6	Closing in on an Explanation for High-Temperature Superconductivity (Scalapino)
7	Powerful Mathematical Tools Resolve Complex Simulations (Smith)
8	A Billion Particle Simulation of the Dark Matter Halo of the Milky Way (Madau)
9	Exploring the Mysteries of Water (Galli)
10	Novel Solver Enables Scalable Electromagnetic Simulations (Kolev)

ASCR Budget

	FY 2009 Appropriation	FY 2010 Request	Change from FY09 to FY 10
Advanced Scientific Computing Research			
Applied Mathematics	40,164	44,850	4,686
Computer Science	33,618	46,800	13,182
Computational Partnerships (includes SciDAC)	52,064	53,235	1,171
Next Generation Networking for Science	14,321	14,321	0
SBIR/STTR	4,038	4,586	548
Total, Mathematical, Computational, and Computer Sciences Research	***144,205***	***163,792***	***+19,587***
High Performance Production Computing (NERSC)	54,790	55,000	210
Leadership Computing Facilities	115,000	130,000	15,000
Research and Evaluation Prototypes	23,900	23,900	0
High Performance Network Facilities and Testbeds (ESnet)	25,000	29,862	4,862
SBIR/STTR	5,925	6,446	521
High Performance Computing and Network Facilities	***224,615***	***245,208***	***+20,593***
Total, Advanced Scientific Computing Research	**368,820**	**409,000**	**+40,180**

FY2010 Budget Request
Highlights

- Applied Mathematics
  - Cyber Security research moved from Next Generation Networking
  - Proposed new fellowship program in Applied Math and High performance computer science
- Computer Science
  - New effort in Advanced Computer Architecture design for science
  - Bridges efforts in advanced computer architecture design with ongoing efforts in computer science and applied mathematics to address needs of DOE science applications
- Computational Partnerships
  - Support for interdisciplinary teams focused on transforming critical DOE applications for extreme scale computing
- Facilities
  - Increases support lease payments and site preparation at ANL for proposed upgrade
  - ESnet will begin to deliver 100-400 Gbps to SC laboratories

Realizing the promise of Extreme Scale

Listening to the Community

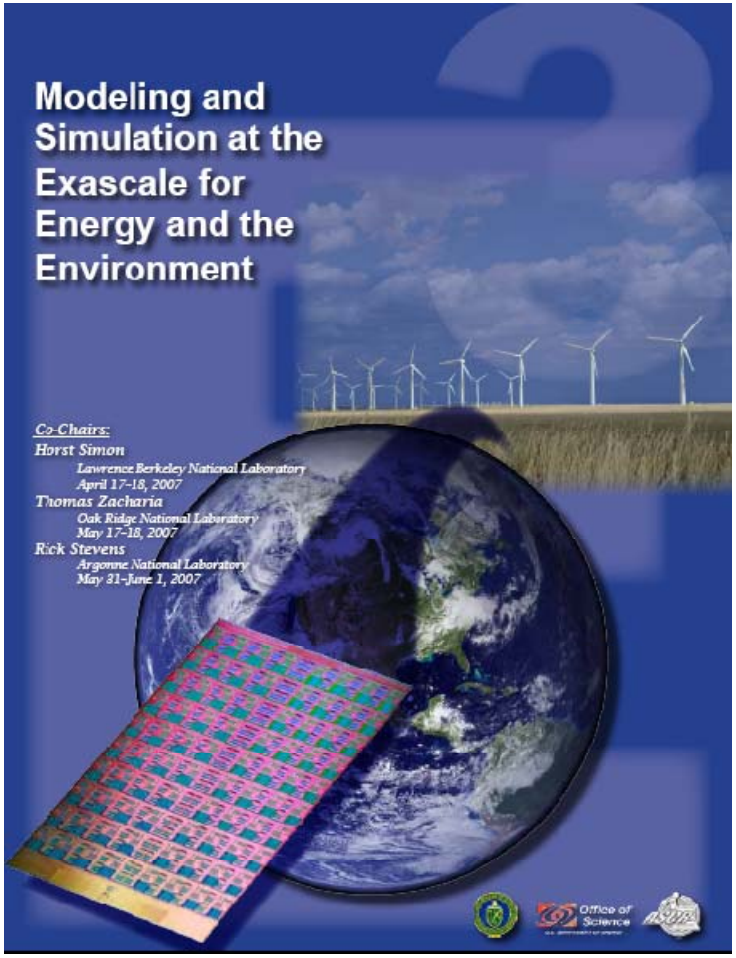
Three Town Hall Meetings held April-June, 2007

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.

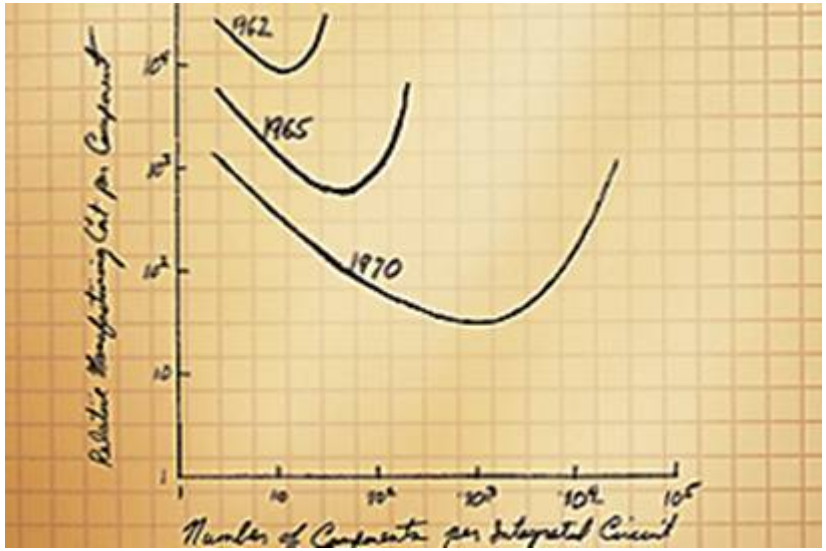


Workshop calendar

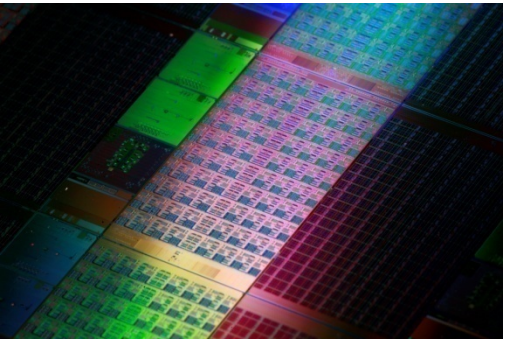
Exascale

- Previous
  - BER/Climate Workshop: Challenges in Climate Change Science and the Role of Computing at the Extreme Scale, 11/08
  - HEP/High Energy Physics Workshop: Scientific Challenges for Understanding the Quantum Universe and the Role of Computing at the Extreme Scale, 12/08
  - NP/Nuclear Physics Workshop: Forefront Questions in Nuclear Science and the Role of High Performance Computing, 2/09
  - FES/Fusion Workshop: Extreme Scale Computing Challenges in Fusion Science, 3/09
  - NE/Nuclear Energy Workshop: Extreme Scale Computing Challenges in Nuclear Energy, 5/09
  - BES/Materials Workshop: Extreme Scale Computing Challenges in Materials Science, August 12-14, 2009 in Washington DC
  - BER/Biology Workshop: Extreme Scale Computing Challenges in Biology, August 17-19, 2009 in Chicago
- Planned
  - NNSA/ASCR Workshop: Science Grand Challenges, October, 6-7, 2009, in Washington DC

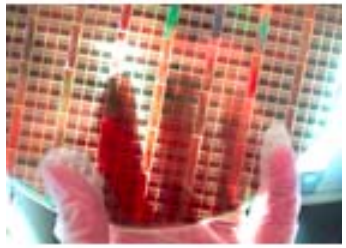
An Era of Challenge



Moore's original graph predicting Moore's Law in 1965. Chip capacity will double every 2 yrs.



Intel Teraflops Research Chip



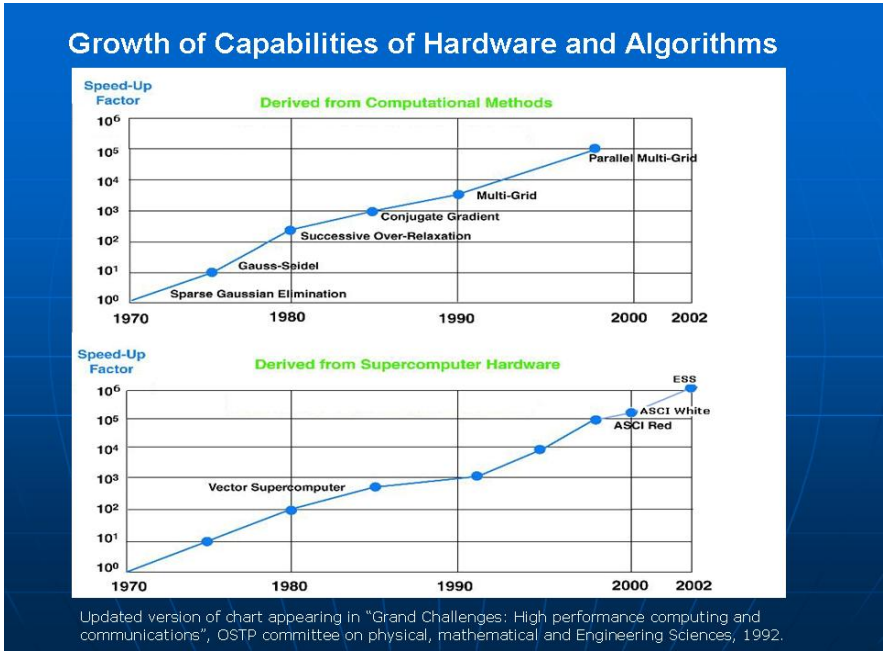
IBM Stacked Chip

- **Unpredictable evolution of hardware**
- **Multilevel and heterogeneous parallelism; memory hierarchies**
- **Programming models must work at scale (numbers of core, lines of code, numbers of components)**
- **Managing data, simulation, experimental and observed**
- **Communications: synchronous → asynchronous**
- **Reliability**

It's not just extreme scale, it's also extreme complexity

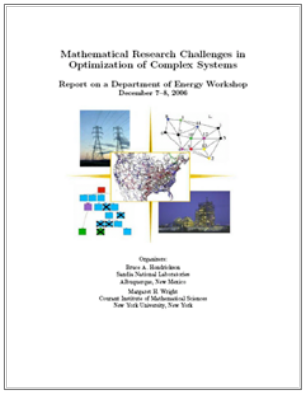
Next Steps

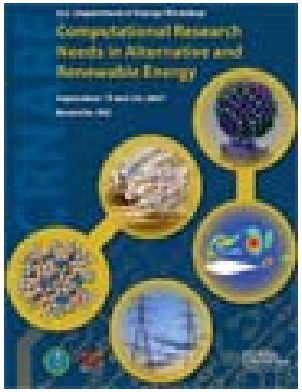
- ASCR will hold several cross-cutting workshops next FY as part of the process.
- ASCR will use the output from these workshops to prioritize funding opportunities in all relevant areas:
  - Applied math and numerical algorithms,
  - Computer science including system software and tools, advanced computing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

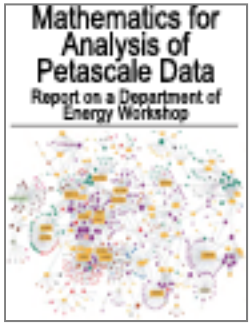


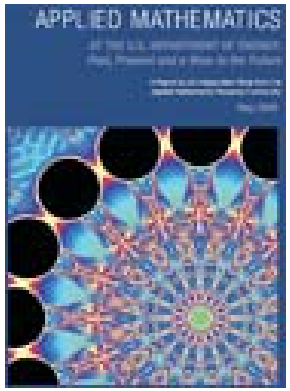
Community Involvement

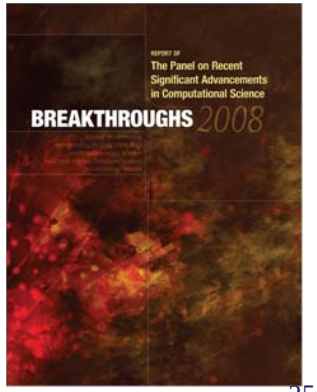
- Learn more about ASCR programs
- Be a reviewer
  - Panel reviews
  - "Postal" reviews
- Participate in DOE workshops
  - ASCR-sponsored
  - Basic Energy Sciences (BES), Biological and Environmental Research (BER), Electricity Delivery and Energy Reliability (OE), Energy Efficiency and Renewable Energy (EERE), Nuclear Energy (NE)
- Identify future research needs
  - Generate "strong" community interest





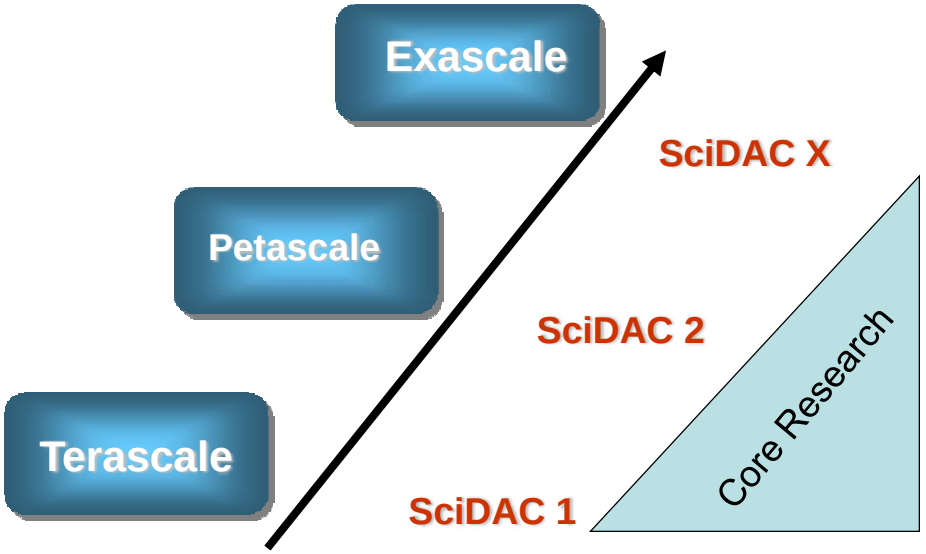






The Challenge Ahead

What computing is needed to enable scientific grand challenges?



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