U.S. DEPARTMENT OF ENERGY | Office of Science

Applied Mathematics Program Update

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Advanced Scientific Computing Research
Office of Science
October 19, 2011

Office of Science

Science to Meet the Nation's Challenges Today and into the 21st Century

The frontiers of science

- Supporting research that led to over 100 Nobel Prizes during the past 6 decades—22 in the past decade alone
- Providing 45% of Federal support in the physical sciences
- Supporting over 27,000 Ph.D.s, graduate students, undergraduates, engineers, and support staff at more than 300 institutions

Energy and environmental science and technology

- Fostering research integration and supporting specialized facilities for collaborative studies

21st century tools of science

- Providing the world's largest collection of scientific user facilities to over 26,000 users each year

Simulation & analysis are a critical component to DOE mission

The mission of the Department of Energy is to ensure America's security and prosperity by addressing its energy, environmental, and nuclear challenges through transformative science and technology solutions.

Energy: Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production

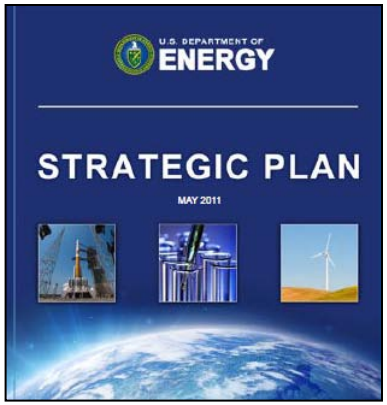
- Reducing time and cost of reactor design & deployment
- Improving the efficiency of combustion energy sources

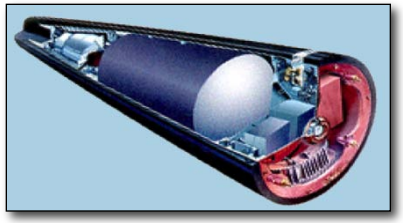
Environment: Understanding, mitigating and adapting to the effects of global warming

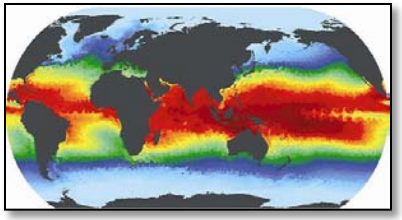
- Sea level rise
- Severe weather
- Regional climate change
- Geologic carbon sequestration

National Security: Maintaining a safe, secure and reliable nuclear stockpile

- Stockpile certification
- Predictive scientific challenges







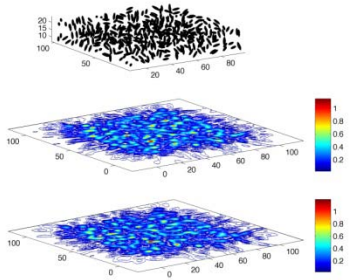
Advanced Scientific Computing Research

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.

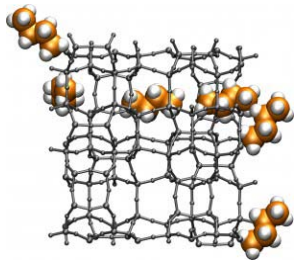
A particular challenge of this program is fulfilling the science potential of emerging multi-core computing systems and other novel “extreme-scale” computing architectures, which will require significant modifications to today’s tools and techniques.

DOE's applied mathematics program has provided significant science impact over ~60 years

- **Sustained support of world-class math researchers has resulted in *models, analysis and algorithms* for PDE-based science**
  - Numerical methods for partial differential equations
  - Numerical linear algebra
  - Optimization
  - Nonlinear systems and solvers
  - Stochastic systems (Predictability program)
- ***Significant applied math developments* have built on this legacy:**
  - Adaptive Mesh Refinement (AMR), Fast multi-pole, Level set methods, Higher-order discretization methods
- **New thrusts addressing DOE challenges with increased complexity and for emerging architectures**
  - Multiscale Mathematics and Optimization for Complex systems
  - Uncertainty Quantification
  - Mathematics for Complex Distributed Interconnected Systems
  - Mathematics for Analysis of Petascale Data
  - Joint Math / Computer Science Institutes
- ***High-performance mathematical software* delivers capability to broad user community**
  - LINPACK – EISPACK – FUNPACK - ODEPACK – MINPACK
  - DASSL – LAPACK - SCALAPACK
  - PETSc - CHOMBO – OVERTURE – MADNESS

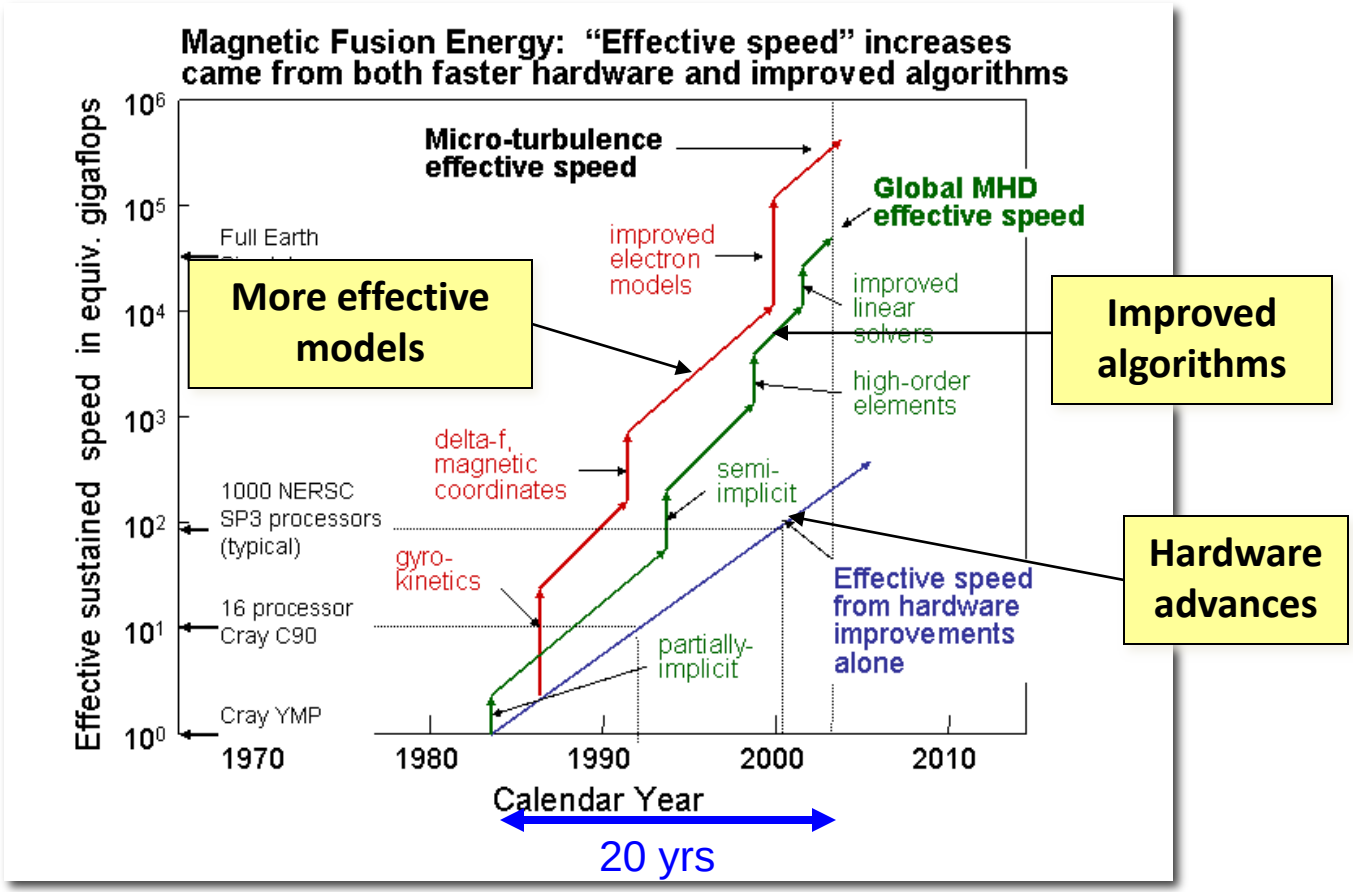


Electromagnetics of microstructured materials
(Gimbutas, Greengard)



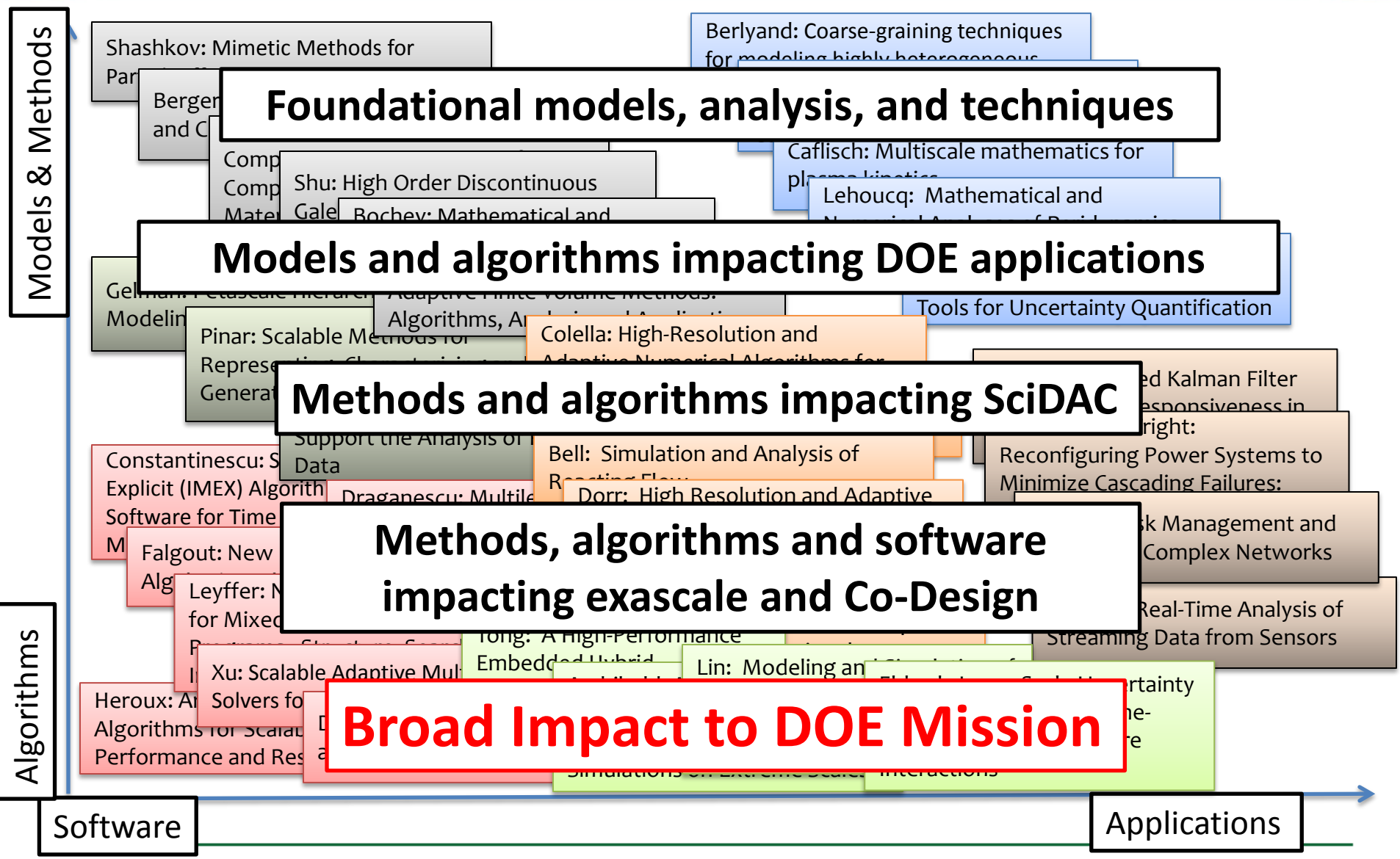
Molecular Pathways in Chemical Systems
(Sethian, Haranczyk & Rycroft)

It's not all about hardware… models and algorithms can dramatically improve effective HPC performance.



http://www.pnl.gov/scales/

Applied Mathematics research has broad impact



Applied Mathematics Committee of Visitors (COV)
May 12-13, 2010

1. PROCESSES - Efficacy and quality of the processes used to:

a) Solicit, review, recommend and document application and proposal actions – 4 Recommendations

1) Improve the level of outreach as regards to new funding opportunities
2) Proposal project descriptions should be limited to 15 pages
3) Large multi-investigator proposals should be appropriately integrated, coordinated and synergistic
4) Actions should be taken to accelerate the processing of approved grants.

b) Monitor active awards, projects and programs – 1 Recommendation

1) Explicit guidelines should be instituted for progress reports

2. PORTFOLIO - Within the boundaries defined by the DOE mission and available funding, comment on how the award process has affected:

a) The breadth and depth of portfolio elements – 1 Recommendation

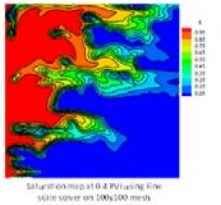
1) The committee finds the portfolio to be *exceptionally strong with regards to both depth and breadth.* The balance of awards with respect to innovation, risk and interdisciplinary research appears to be appropriate. The committee was very *impressed with the long-term perspective* of the DOE applied mathematics program *and its simultaneous agility at funding new program areas.*

b) The national and international standing of the program with regard to other applied mathematics research programs that are also focused on the demands of high performance scientific computing and analysis of petascale datasets – 1 Recommendation

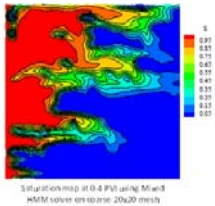
1) The DOE Applied Mathematics program has been, and continues to be, of extremely high quality and standing, both nationally and internationally. A *great strength of the program* is the willingness it has demonstrated to *invest in* projects with a *longer-term perspective* than is possible at most U.S. agencies, enabling the support of breakthrough research and ensuring its success and eventual adoption.

New Awards (FY10): Advancing Uncertainty Quantification (UQ) in Modeling, Simulation, and Analysis of Complex Systems

1. **Modeling and Simulation of High-Dimensional Stochastic Multiscale PDE Systems at the Exascale**
   - Guang Lin (PNNL), Nicholas Zabaras (Cornell), and Ioannis Kevrekidis, (Princeton)
2. **Advanced Dynamically Adaptive Algorithms for Stochastic Simulations on Extreme Scales**
   - Richard Archibald, Ralf Deiterding, and Cory Hauck (ORNL), Dongbin Xiu (Purdue)
3. **A High-Performance Embedded Hybrid Methodology for Uncertainty Quantification with Applications**
   - Charles Tong (LLNL), Barry Lee (PNNL), Gianluca Iaccarino (Stanford)
4. **Enabling Predictive Simulation and UQ of Complex Multiphysics PDE Systems by the Development of Goal-Oriented Variational Sensitivity Analysis and a-Posteriori Error Estimation Methods**
   - John Shadid (SNL), Don Estep (CSU), Victor Ginting (UWyoming)
5. **Bayesian Uncertainty Quantification in Predictions of Flows in Highly Heterogeneous Media and its Application to CO2 Sequestration**
   - Yalchin Efendiev (Texas A&M), Panayot Vassilevski (LLNL)
6. **Large-Scale Uncertainty and Error Analysis for Time-Dependent Fluid/Structure interactions in Wind Turbine Applications**
   - Michael Eldred, et al (SNL) and Juan Alonso (Stanford)

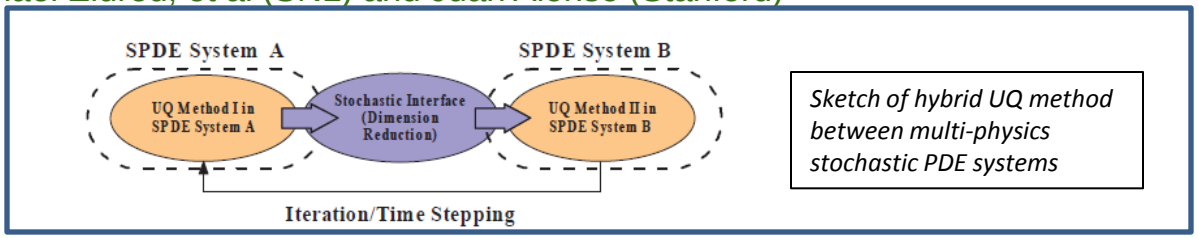


Fine mesh



Coarse-graining

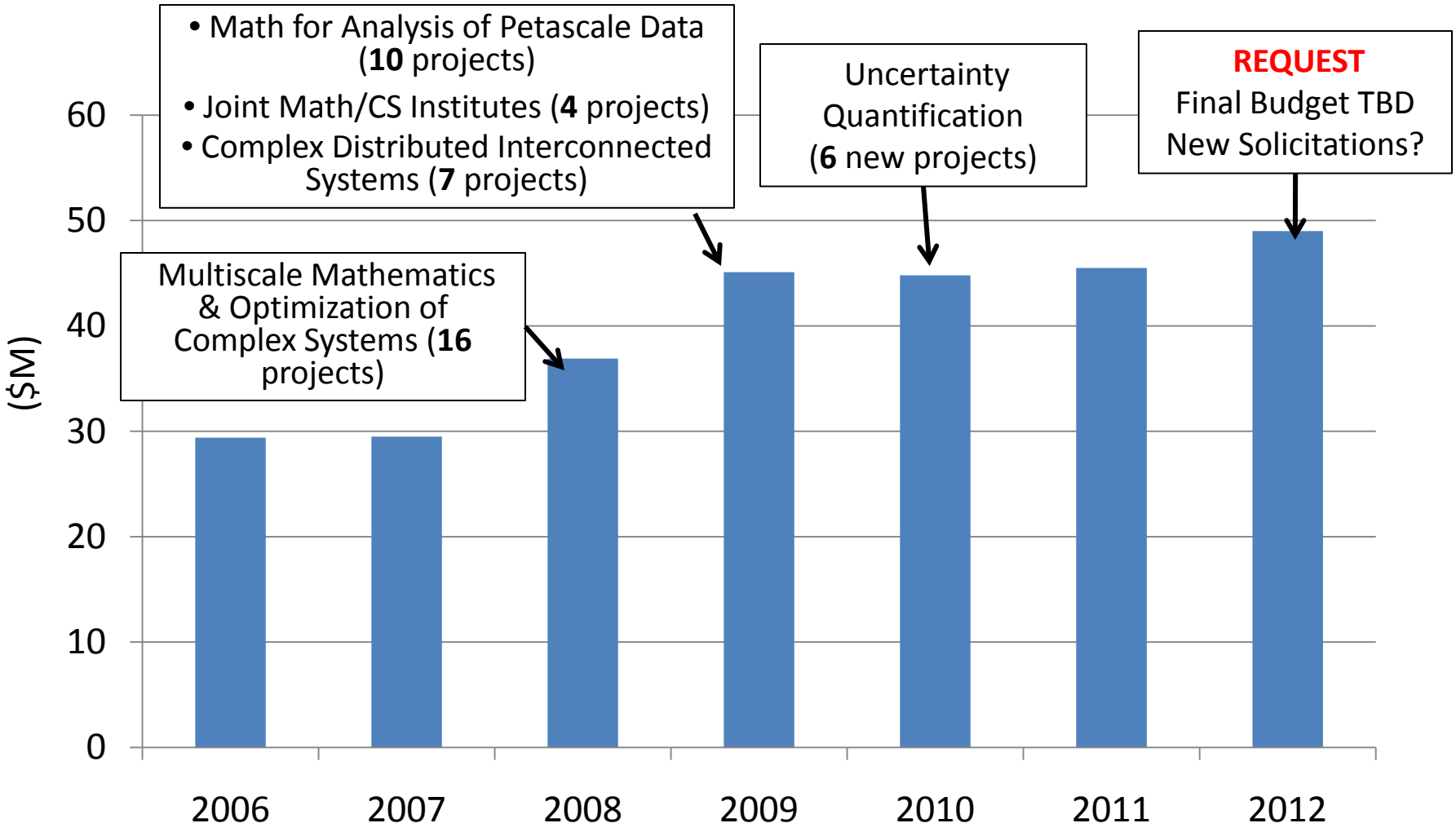
Saturation profile of oil-water porous media flow using fine and multiscale coarse-graining solver



Sketch of hybrid UQ method between multi-physics stochastic PDE systems

http://science.energy.gov/~/media/ascr/pdf/funding/notices/De_foa_0000315.pdf
http://science.energy.gov/~/media/ascr/pdf/funding/notices/Lab_10_315.pdf

ASCR Applied Mathematics Program Budget



Up to Four New Solicitations in FY12

We do not plan on renewing any awards under these solicitations. In order to incorporate new research directions based on community input and aligned with ASCR and DOE priorities, we plan on issuing **up to four new solicitations** updating research projects related to:

- Multiscale Mathematics and Optimization of Complex Systems
- Mathematics for Complex Distributed Interconnected Systems
- Mathematics for Analysis of Petascale Data
- Joint Math / Computer Science Institutes

For existing awards (available to all):

- A "No Funds Extension (NFE)" will be granted to awardees who provide a justification for more time to complete their research.

Depending on when we received our budget and based on availability funds:

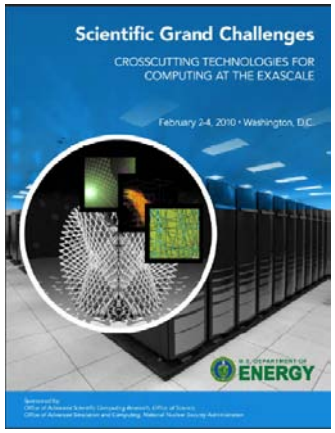
- We may issue a new solicitation in FY12 and issue new awards in FY12.
- We may issue a new solicitation in FY12, but issue new awards in FY13. An NFE may be issued to provide continuity.
- We may issue a new solicitation in FY13 with new awards late in FY13. In this case, we may allow projects to submit a proposal for a one-year extension with supplemental funds, or a NFE may be issued.

Relevant Workshops and Reports

- Workshop on Mathematics for the Analysis, Simulation and Optimization of Complex Systems, September 13-15, 2011
  - http://www.orau.gov/mathworkshop2011/
- 2011 ASCR / BES Data Workshop, October 24-25, 2011
  - http://www.orau.gov/dataworkshop2011/default1.htm
- Office of Electricity Delivery and Energy Reliability (OE) Workshop: Computational Needs for the Next Generation Electric Grid, April 18-20, 2011, Cornell University
- Workshop on Cross-cutting Technologies for Computing at the Exascale, February 2-4, 2010
  - http://extremecomputing.labworks.org/crosscut/index.stm
  - http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Crosscutting_grand_challenges.pdf

Highlights from Cross-cut Technologies report

- Recast critical applied mathematics algorithms
  - New PDE discretizations to reflect shift from FLOP - to memory- constrained hardware
  - Take advantage of data-movement constraints to redesign UQ and data analysis algorithms and techniques
  - Need for reduced global communication in linear and nonlinear solvers and optimization methods
  - Understanding the mathematical structure of complex systems enabled by exascale
  - Alternative formulations for emerging architectures



- Address numerical analysis issues associated with moving away from bulk synchronous programming
  - Accuracy and stability of multi-physics and multi-scale coupling
  - High-order coupling methods

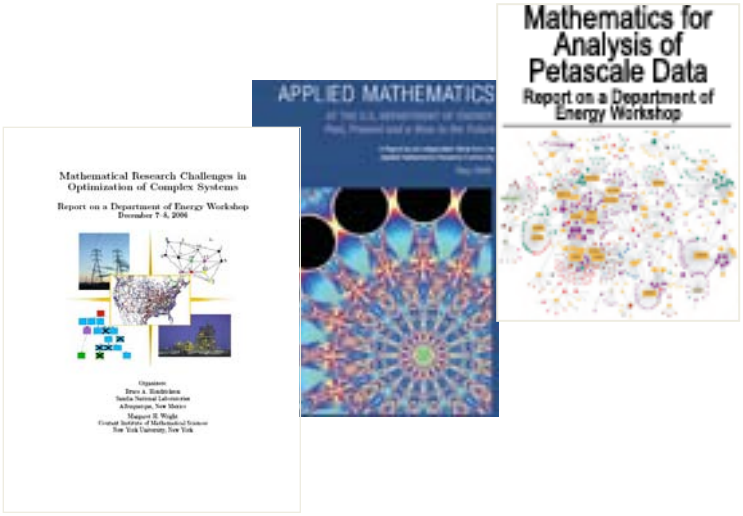
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Crosscutting_grand_challenges.pdf

Relevant Workshops and Reports

- Exascale Research PI Meetings
  - http://exascaleresearch.labworks.org/ascrOct2011/ascr
  - http://exascaleresearch.labworks.org/ascrMar2011/ascr2011
- Scientific Grand Challenges Workshop Series
  - Climate change, quantum universe, nuclear science, fusion energy science, nuclear energy systems, basic energy sciences, biology and national security
  - http://science.energy.gov/ascr/news-and-resources/workshops-and-conferences/grand-challenges/
- ASCAC Subcommittee Report: The Opportunities and Challenges of Exascale Computing
  - http://science.energy.gov/~/media/ascr/ascac/pdf/reports/Exascale_subcommittee_report.pdf

Community Involvement: How can I help ASCR?

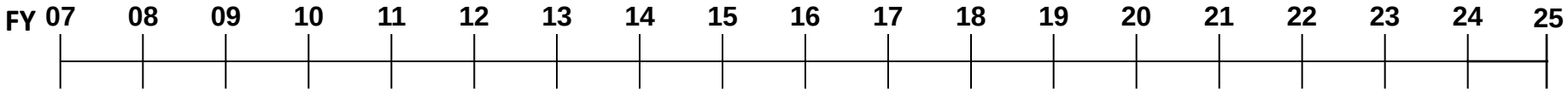
- **Learn more about DOE & ASCR programs**
- **Be a reviewer**
  - Panel reviews
  - Mail reviews
- **Identify future research needs**
  - Encourage "strong" community interest



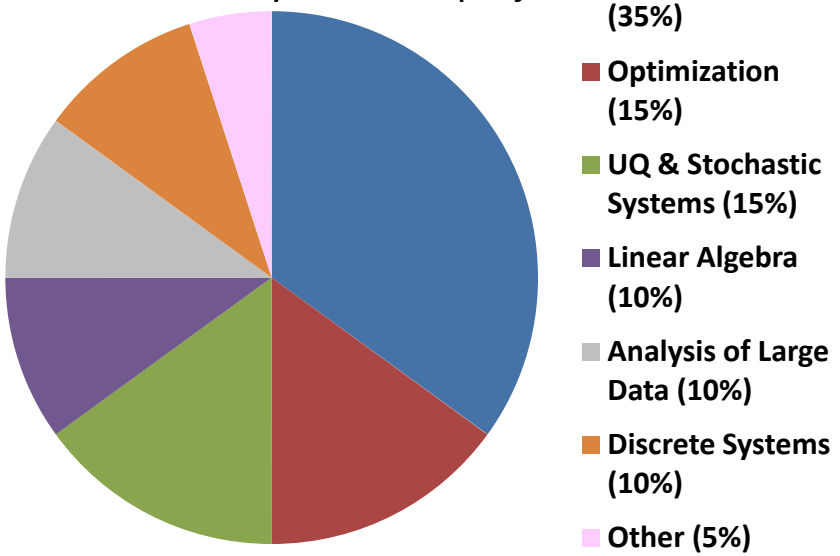
- **Participate in DOE workshops**
  - ASCR-sponsored workshops
  - Basic Energy Sciences (BES), Biological and Environmental Research (BER), Fusion Energy Sciences (FES), Electricity Delivery and Energy Reliability (OE), Nuclear Energy (NE), Environmental Management (EM)
- **ACCOMPLISHMENTS!**
  - Quad chart with notes
  - Progress reports: Technical & DOE relevance
  - E-mail updates on awards or other noteworthy accomplishments

Applied Mathematics program future directions

The DOE Applied Mathematics program supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions; analysis and development of robust mathematical models, algorithms and software for enabling predictive scientific simulations of DOE-relevant complex systems.



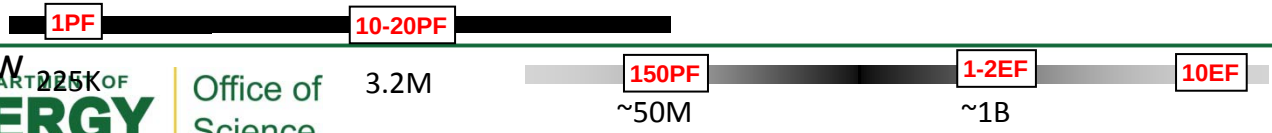
FY11: $45M/year, ~110 projects



Future directions: Modeling, analysis, and algorithms for simulation of DOE complex systems:

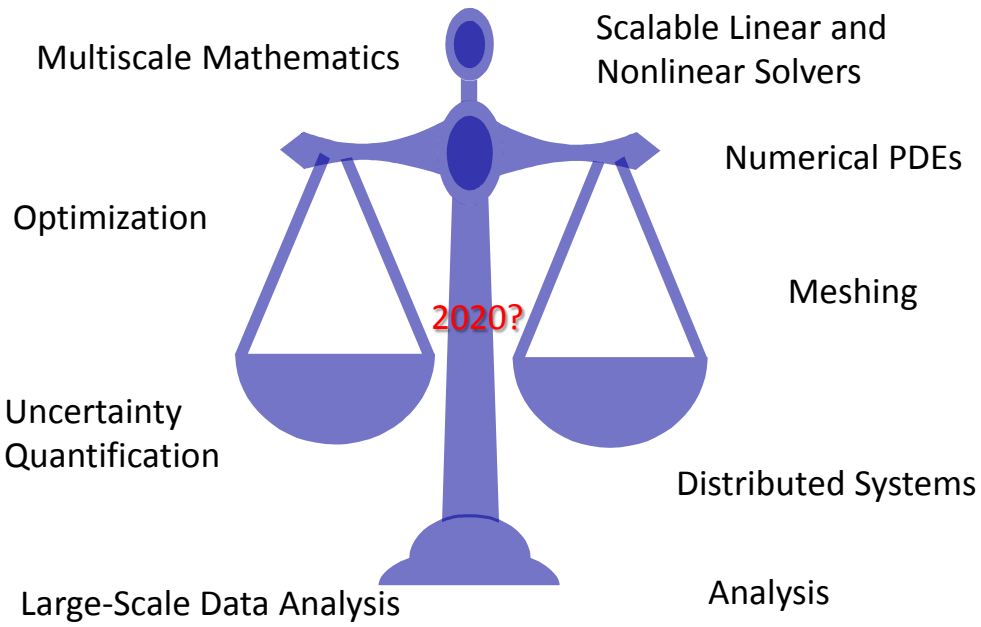
- Increase fidelity: develop new multi-scale, multi-physics models, analysis of coupled systems
- Uncertainty Quantification and V&V
- Approaches for systems that are inherently stochastic
- Methods that integrate data and simulation
- Novel analysis of algorithms for large data / streaming data
- Solvers and optimization methods with reduced global communication
- Higher-order methods; accuracy, stability of methods that move away from bulk synchronous programming models
- Algorithms resilient to machine errors
- Analysis of algorithms for emerging architectures

Multicore: Here and now



Manycore / Hybrid Architectures

The goal & challenge is maintaining a balanced Applied Mathematics program in a dramatically changing computing environment.



Applied Mathematics Committee of Visitor Report (2010):
The committee finds the portfolio to be ***exceptionally strong with regards to both depth and breadth.*** The balance of awards with respect to innovation, risk and interdisciplinary research appears to be appropriate. The committee was very ***impressed with the long-term perspective*** of the DOE applied mathematics program ***and its simultaneous agility at funding new program areas.***

Plan and change gracefully:

- Internal coordination within ASCR, synergies with Computer Science, SciDAC, Co-Design
- Awareness and coordination with DOE: SC, Applied Offices, NNSA
- Awareness of other agencies activities: NSF, AFOSR, ONR, etc.
- Engage the scientific community, e.g. SIAM Committee on Science Policy, SIAM Computational Science and Engineering, exascale research community and international community

Closing Remarks

- **Comments and questions on panel on "Impacting Science through Applied Mathematics and Emerging Architecture"**
  - Mike Heroux, maherou@sandia.gov
  - John Bell, jbbell@lbl.gov

- **The $90M Question ???**

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Questions, comments, feedback, solutions all graciously accepted.

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