Update on the Applied Mathematics Research Program

ASCAC Meeting
October 28-29, 2008

Sandy Landsberg, Program Manager
Office of Advanced Scientific Computing Research
Office of Science
Department of Energy
Two new program managers:
  - Sandy Landsberg (Permanent fed)
  - Steve Lee (Detailer from LLNL)

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

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

Outreach to external organizations
  - NSF Division of Mathematical Sciences

Large-scale Fundamental Studies of MHD Instabilities, Shadid, SNL
3D fully implicit extended MHD simulations. The upper figure depicts densities and velocities in the nonlinear stage of a 3D Kelvin-Helmholtz unstable configuration with differential rotation. The lower figure depicts temperature during the evolution of a helical perturbation in a 3D toroidal fusion device.
• Research on mathematical models, methods and algorithms to enable scientists to accurately understand complex physical, chemical, biological and engineered systems.

• Currently supported research activities (~ 100 projects):
  • Advanced linear algebra
  • Discretization and meshing
  • Multiscale, multiphysics systems
  • Uncertainty quantification and error analysis
  • Optimization
  • Other research
  • Fellowships & workshops
• FY 2008 Budget: Approximately 75 % Labs, 25% Universities

• Chart: Allocations by area
  • Based on $23.6M (FY08)
  • Does not include
    • Computational Science Graduate Fellowship Program ($5M)
    • New Multiscale Mathematics and Optimization awards
    • Potential new FY09 initiatives:
      • Mathematics for Analysis of Petascale Data
      • Joint Applied Mathematics-Computer Science Institutes
      • High Risk / High Payoff Technologies

FY 2008
Applied Mathematics Research Program

• Today’s program
  • Over ~100 projects
  • Pending awards for Multiscale Mathematics & Optimization for Complex Systems

• Potential new research thrusts
  • Mathematics for Analysis of Petascale Data
  • Joint Mathematics / Computer Science Institute(s)
  • High-Risk / High-Payoff Technologies

• FY10 and beyond
New competition; not a renewal

• Multiscale Mathematics for Complex systems
  • Diverse temporal/spatial scales, multiple physical models
  • Possibly many components (possibly dissimilar), complex connectivity (usually nonlinear), hard-to-predict behavior (often highly sensitive)
  • Complex systems analysis: uncertainty quantification and error analysis
  • Examples: combustion, materials, fluids, plasmas / MHD, porous media, …

• Optimization of Complex Systems
  • Analysis and algorithms for stochastic optimization
  • Theory and algorithms for very large, structured optimization problems
  • Analysis and algorithms for optimization problems with mixed variable types, including continuous, discrete and categorical variables

• Three panel reviews convened in June 2008

• Workshop reports at
  http://www.sc.doe.gov/ascr/Research/AM/ConferencesWorkshops.html

Two awards made in 2008

Large-Scale Optimization for Bayesian Inference in Complex Systems

• Karen Willcox, Massachusetts Institute of Technology
• Youssef Marzouk, Sandia National Laboratories, soon to transfer to MIT
• George Biros, now at Georgia Institute of Technology
• Omar Ghattas, Clint Dawson, University of Texas at Austin

Next-Generation Solvers for Mixed-Integer Nonlinear Programs: Structure, Search, and Implementation

• Sven Leyffer, Todd Munson, Argonne National Laboratory
• Jeffery Linderoth, James Luedtke, Andrew Miller, University of Wisconsin at Madison

• Additional proposals still “Under Consideration”
  • 19 proposals
  • *Multiscale Mathematics*: $5M
  • *Optimization*: $3M

• **Decision Factors**
  • Peer-review comments on technical merit, appropriateness of proposed approach, competency of personnel, and appropriateness of budget
  • Clearly identified new mathematical methods or algorithms beyond advances in a particular application
  • Relevance and potential impact to DOE mission
  • Balance breadth and depth

FY 2009 Budget Request: 
What’s (hopefully) coming

<table>
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<tr>
<th>FY 2007 Spent</th>
<th>FY 2008 Appropriated</th>
<th>FY2009 Requested</th>
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<td>28.8</td>
<td>36.9</td>
<td>43.2</td>
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- FY 2009 request of $43.2M is a $6.3M over the FY 2008 appropriation
- “Applied Mathematics: This increase will support …
  - a new joint Applied Mathematics-Computer Science Institute to focus on the challenges of computing at extreme scales that blur the boundaries between these disciplines,
  - a new effort in the mathematics of large datasets to address the most fundamental issues in finding the key features, understanding the relationships between those features, and extracting scientific insights in extremely large datasets, and
  - increases in key areas of long-term research most relevant to meeting the challenges of computing at extreme scale and risk assessment in complex systems”
Mathematics for Analysis of Petascale Data

Workshop held June 3-5, 2008, Rockville MD

http://www.science.doe.gov/ascr/ProgramDocuments/Docs/PetascaleDataWorkshopReport.pdf


- Need innovative mathematical approaches and techniques for finding the scientific knowledge in massive, complex datasets

- Workshop goals: understand the needs of various scientific domains, translate these into mathematical approaches and techniques, assess the current state-of-the-art, and target gaps and shortfalls that must be addressed.

- Resonates with activities at NSF and DARPA.

Images from the application of Sapphire scientific data-mining software developed at LLNL to characterizing and tracking bubbles and spikes in an 80-terabyte dataset from 3D high-fidelity simulation of the Rayleigh-Taylor instability. Left: a 2D data slice of the data showing the bubble-spike region in pink. Center: the bubble height image. Right: bubble counts using the x-y velocity at the bubble boundary.
New joint Applied Mathematics-Computer Science Institute(s) to focus on the challenges of computing at extreme scales that blur the boundaries between these disciplines

- Workshop held October 7-9, 2008 in Chicago, IL
- Organized by: Mike Heroux (SNL), Al Geist (ORNL) and Phil Colella (LBNL)
- Presentations by: Jack Dongarra (Univ of Tennessee), Trey White (ORNL), Barry Smith (ANL), Brian Van Straalen (LBNL)
- Total number of participants: 32
1. Effective use of many core and hybrid architecture.


3. Addressing complexities of node architectures.

4. Fault detection and tolerant algorithms, resilience.

5. Communication-avoiding and communication-computation concurrent algs.

6. Sensitivity analysis (broad definition)

7. Multiscale/multiphysics modeling


9. Performance degradation at scale due to load imbalance exposed by synchronization

10. Algorithm advances: Magneto-compressive wave reformulation. Time parallel algorithms

11. Efficient multigrid, efficient multi-grid-like time algorithms

12. Effective use of new and emerging memory systems


15. New capabilities to promote efficient development of optimized code.

1. Inability to efficiently develop straight-forward, high-performance portable code.

2. Using machines efficiently:
   - Using computational units (multicore, GPUs).
   - Using memory system efficiently.
   - Using switch-level system efficiently (e.g. ICN).
   - Using system power efficiently.
   - Using synchronizations efficiently.

3. Fault detection, tolerance and management

4. Sensitivities, UQ, etc.

5. Multiscale/Multiphysics.

6. Fast implicit solves.
   - esp: Small coarse problem on big dedicated machine.


8. Debugging of correctness and performance is untenable.

9. Suboptimal algorithms for computer system resource management.
Joint Math/CS Institutes
Cross-cutting tools

3. Portable programming model, execution model.
   • Implicit methods.
   • Reformulations for larger time steps.
   • Discrete optimization for page mapping, router management, etc.
5. Mixed precision, reduced data representations.
6. Libraries can be a test-bed, proof-of-concept for new programming/execution models.
What does a joint Math/CS Institute look like?

- Institute is:
  - Staffing of Math and CS, Labs and Universities, continuum of skills.
  - Approximately 10-20 members, single PI.
  - Single theme with multiple projects.
  - Integrated Math and CS effort.

- Size:
  - $1M too small. $3M OK.

- How do we obtain an integrated effort?
  - Focus on problems that require synergistic Math & CS effort.

- How do we introduce joint accountability?
  - Proposed work must clearly demonstrate need for combined Math & CS research to succeed.
  - Milestones must depend on joint effort.
Need to develop new scientific capabilities that are too high-risk to be carried out as business as usual

- **Case study approach:**
  - Fusion & Accelerator Physics (John Carey, CU Boulder/Tech-X)
  - Climate (John Drake, ORNL)
  - Combustion (John Bell, LBNL)
  - Nuclear Energy (Andrew Siegel, Argonne)

- **Define high-risk / high-payoff projects:**
  - Success could provide large increment in scientific capability
  - Too high-risk for applications community to undertake
Types of Risk

• Type 1: Well-characterized application of a new technology
  • Risk comes from need for hardened implementations of the technology & need for a bridge between application and technology experts.
  • Example: Implementing an existing model in a new programming language or programming framework

• Type 2: Well-established techniques applied to a new problem area
  • Risk comes from attempting to adapt new methodology to meet problem-specific needs
  • Example: AMR for climate

• Type 3: Fundamentally new approaches, particularly in domains where there is little prior art in modeling
  • Example: Uncertainty quantification for multiphysics applications
High-Risk/High Payoff Time Horizon for Case Studies

• For the four applications (fusion, climate, combustion, nuclear energy), consider the following questions:
  • Timeline for progress, over 3-5 years
  • Optimal end state in 10 years
  • Level of effort required to meet these goals
  • Organizational structure of collaboration team
  • External dependencies (e.g., SciDAC support)
High-Risk/High Payoff Cross-cutting topics

- Need for petascale data infrastructure
  - Institutes issue?
- Robust and fast parallel I/O
- Program language support and kernel library support for multicore/NUMA nodes
- Rapid prototyping tools (HPC-MATLAB?)
- Load balancing for new, large machines
- Above items depend on continuing SciDAC in some form
- Workshop report(s) coming soon …
Held Oct 15-17, 2008 at Argonne National Laboratory

http://www.mcs.anl.gov/events/workshops/amr08/index.php

Over 140 researchers

Plenary talks:
- Climate Change, Inez Fung, UC-Berkeley
- Multiscale Modeling, Weinan E, Princeton U
- Large-Scale Data Analysis, Alex Gray, Georgia Tech
- Towards Exascale Computing, Rick Stevens, ANL
- Uncertainty Quantification and Optimization, Karen Willcox, MIT
- Advancing Energy through Algorithms, David Keyes, Columbia U

Theme Areas:
- Linear and Nonlinear Systems
- Multiscale Phenomena
- Uncertainty quantification/sensitivity analysis
- Optimization of complex systems
FY10 and Beyond

- Informed by numerous workshops and panel reports:
  http://www.science.doe.gov/ascr/ProgramDocuments/ProgDocs.html
- **Applied Mathematics at the U.S. Department of Energy: Past, Present and a view to the Future**
  - Predictive modeling and simulation of complex systems
  - Mathematical analysis of the behavior of complex systems
  - Using models of complex systems to inform policy makers
- **Modeling and Simulation at the Exascale for Energy and the Environment Town Hall Meetings Report**
- **Mathematics for Analysis of Petascale Data Workshop Report**
- **Multiscale Mathematics Initiative: A Roadmap**

- **Program Managers are actively working to define new research opportunities that build on and advance traditional ASCR Applied Mathematics strengths**
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Questions?