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

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Applied Mathematics Research Program Update

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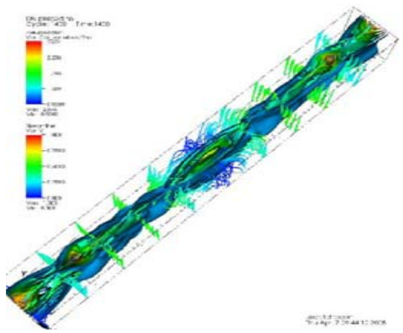
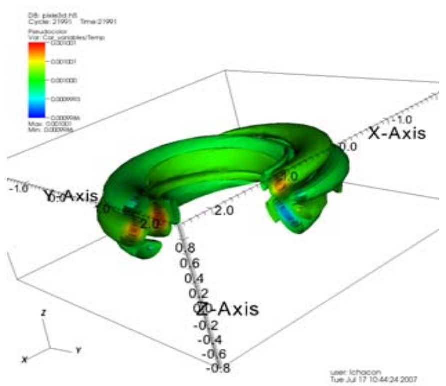
- Two new program managers:
  - Sandy Landsberg (Permanent fed)
  - Steve Lee (Detailee from LLNL)
- Multiscale Mathematics and Optimization for Complex Systems call
  - 2 proposals in Optimization funded in FY2008
  - 19 proposals “under consideration” pending continuing resolution
  - 77 proposals 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.

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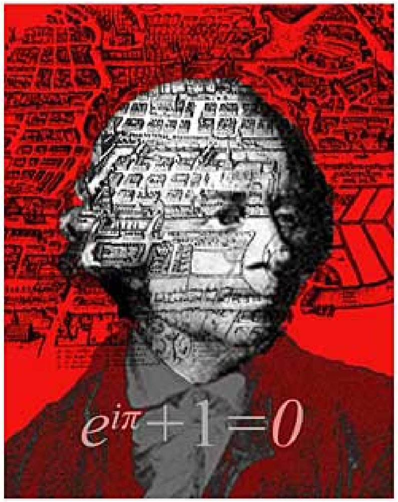
Applied Mathematics Research Program

- **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***



Leonhard Euler 1707 - 1783

Applied Mathematics Research Allocations

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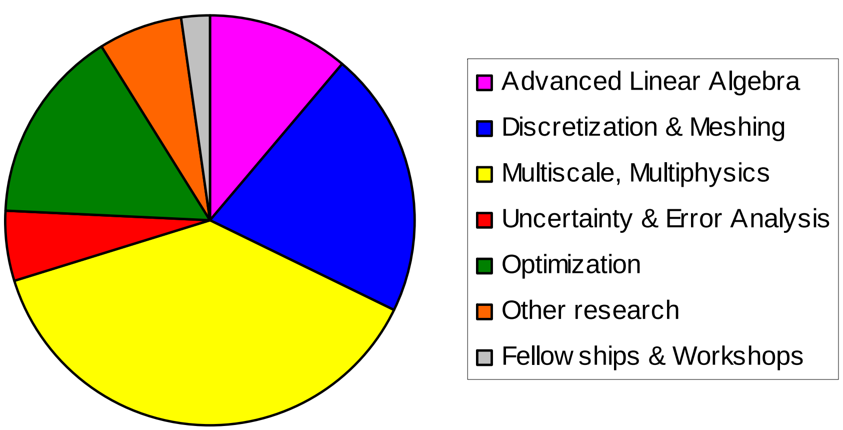
- **FY 2008 Budget: Approximately 75 % Labs, 25% Universities**
- **Chart: Allocations by area**
  - **Based on $23.6M (FY08)**
  - **Does not include**
    - **Computational Science Graduate Fellowship Program ($5M)**
    - **New Multiscale Mathematics and Optimization awards**
    - **Potential new 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

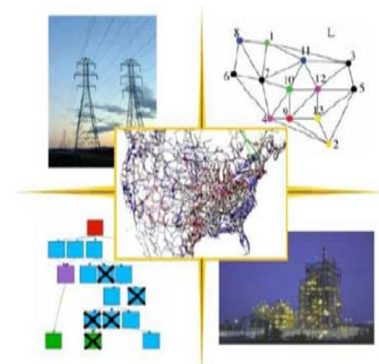
- Today's program
  - Over ~100 projects
  - Pending awards for Multiscale Mathematics & Optimization for Complex Systems
- Potential new research thrusts
  - Mathematics for Analysis of Petascale Data
  - Joint Mathematics / Computer Science Institute(s)
  - High-Risk / High-Payoff Technologies
- FY10 and beyond

Multiscale Mathematics and Optimization for Complex Systems

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



From "Mathematical Research Challenges in Optimization of Complex Systems," report on a DOE Workshop, December 7-8, 2006, organizers Bruce A. Hendrickson and Margaret H. Wright.

Multiscale Mathematics and Optimization for Complex Systems

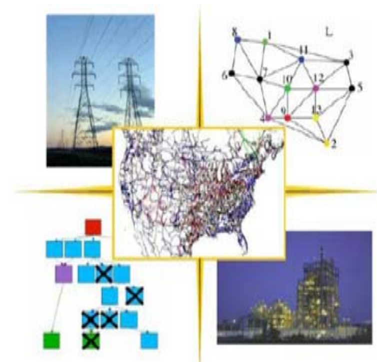
Two awards made in 2008

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



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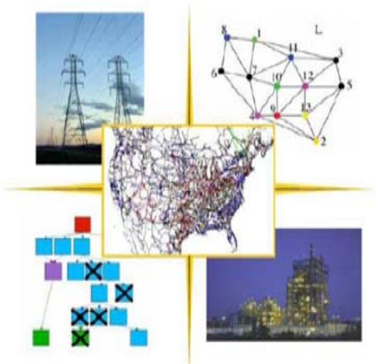
Multiscale Mathematics and Optimization for Complex Systems

- **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**



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

FY 2007 Spent	FY 2008 Appropriated	FY2009 Requested
28.8	36.9	43.2

- **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"***

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Mathematics for Analysis of Petascale Data

Workshop held June 3-5, 2008, Rockville MD

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

- ***R. L. Orbach AAAS talk, Feb. 2006, "New Opportunities for Data and Information Management: Finding the Dots, Connecting the Dots, Understanding the Dots"***
- ***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.

Joint Mathematics / Computer Science Institute(s)

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
- Workshop briefings available at: http://www.csm.ornl.gov/workshops/institutes/index.html

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Joint Math/CS Institutes Key Topics Discussed

1. Effective use of many core and hybrid architecture.
2. Exploiting mixed precision. Single/double and double/quad..
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
8. Fast implicit solves.
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
13. Debugging of correctness and performance.
14. Motifs, interoperable motifs.
15. New capabilities to promote efficient development of optimized code.
16. New discrete optimization methods for computer system resource management.

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Joint Math/CS Institutes Key Problems

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.
7. Numerical stability of transient problems at scale.
8. Debugging of correctness and performance is untenable.
9. Suboptimal algorithms for computer system resource management.

Joint Math/CS Institutes Cross-cutting tools

1. Code, algorithm and model transformations.
2. Motifs and their interoperability.
3. Portable programming model, execution model.
4. Algorithms.
   - 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.

High-Risk / High-Payoff Technologies

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 …

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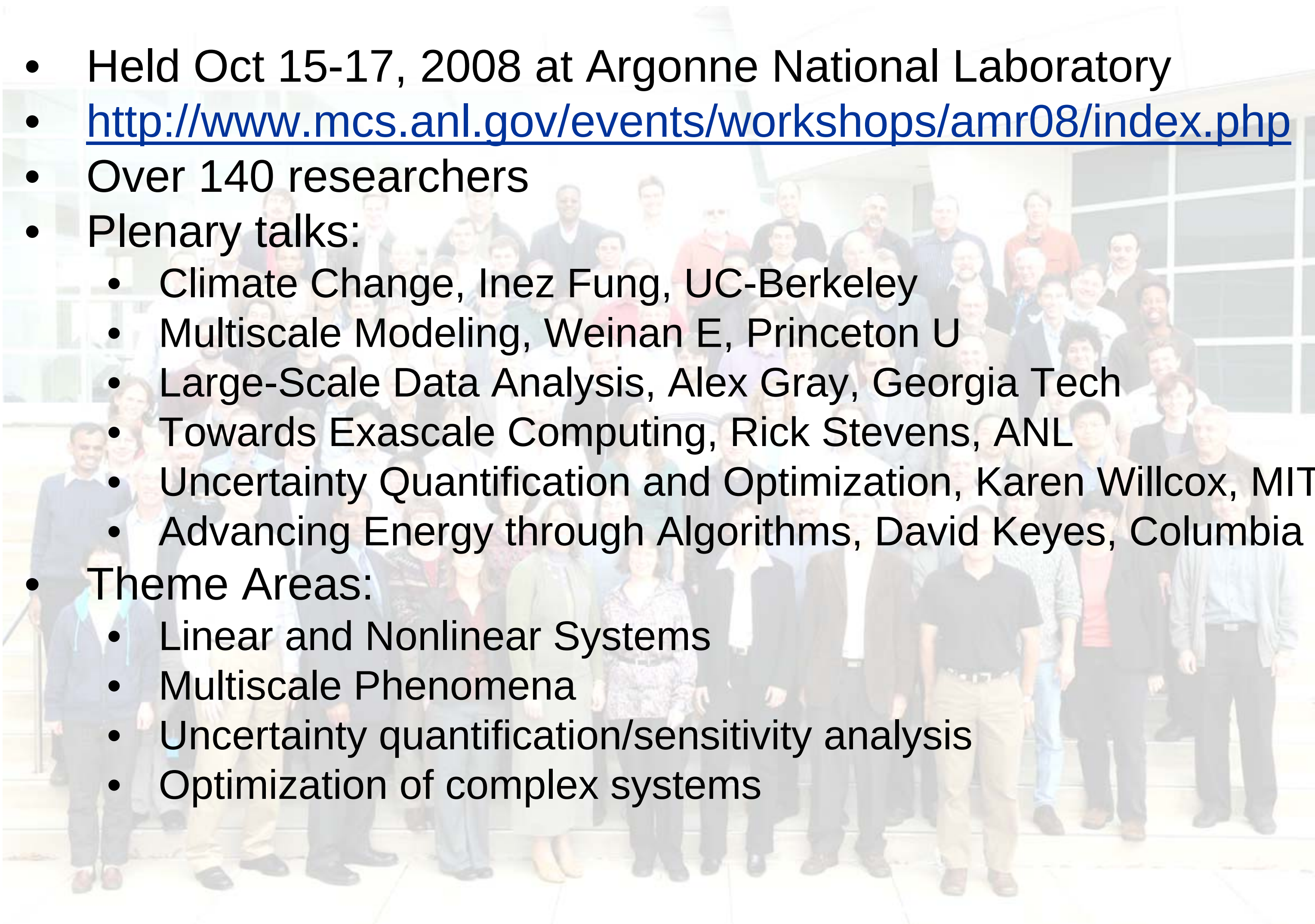
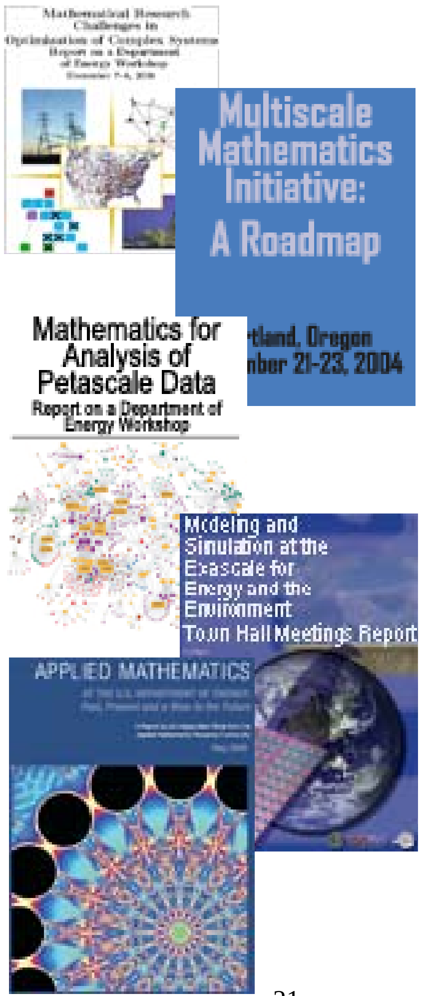
Applied Mathematics PI Meeting



- 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***](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***
  - ***Report on the Mathematical Research Challenges in Optimization of Complex Systems***
  - ***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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Applied Mathematics Research

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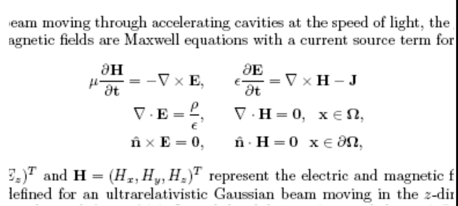


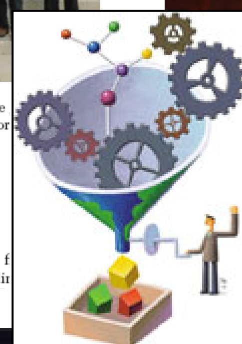
eam moving through accelerating cavities at the speed of light, the agnetic fields are Maxwell equations with a current source term for

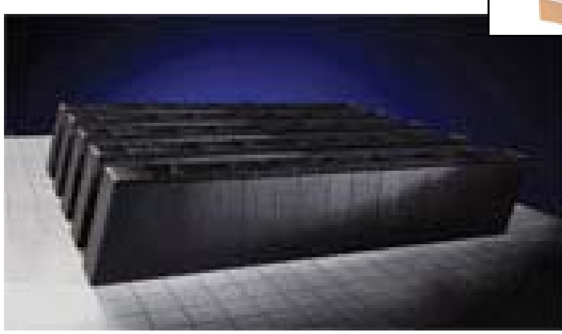
$$\mu\frac{\partial \mathbf{H}}{\partial t} = -\nabla\times\mathbf{E}, \qquad \epsilon\frac{\partial \mathbf{E}}{\partial t} = \nabla\times\mathbf{H} - \mathbf{J}$$

$$\nabla\cdot\mathbf{E} = \frac{\rho}{\epsilon}, \qquad \nabla\cdot\mathbf{H} = 0, \quad \mathbf{x}\in\Omega,$$

$$\hat{\mathbf{n}}\times\mathbf{E} = 0, \qquad \hat{\mathbf{n}}\cdot\mathbf{H} = 0 \quad \mathbf{x}\in\partial\Omega,$$

$E_z)^T$ and $\mathbf{H} = (H_x, H_y, H_z)^T$ represent the electric and magnetic f lefined for an ultrarelativistic Gaussian beam moving in the z-dir





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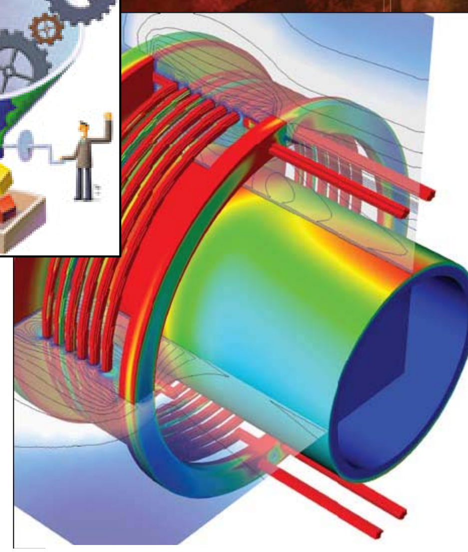

Novel Solver Enables Scalable Electromagnetic Simulations

ABSTRACT: A team based at Lawrence Livermore National Laboratory has developed the first provably scalable solver code for Maxwell's equations, a set of partial differential equations that are fundamental to numerous areas of physics and engineering. This new software technology enables researchers to solve larger computational problems with greater accuracy.

Contributors/Authors

Tzanio Kolev and Panayot Vassilevski, LLNL; Jinchao Xu, Penn State University; Ralph Hiptmair, ETH, Zurich; Joseph Pasciak, Texas A&M University

Questions?