Preliminary Report on the "Workshop for the Analysis, Simulation, and Optimization of Complex Systems"

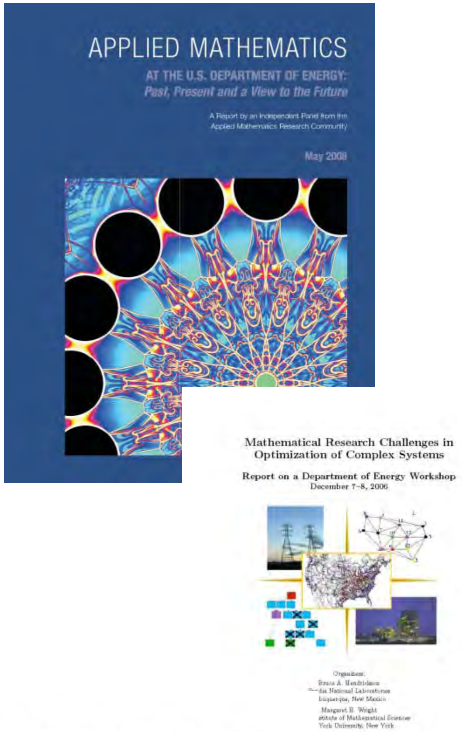
John Bell
Advanced Scientific Computing Advisory Committee
Washington, DC
November 1-2, 2011

Overview

- Workshop on Mathematics for the Analysis, Simulation and Optimization of Complex Systems
  - Organized at the request of the program managers for the ASCR Applied Mathematics Program
  - Organizing committee
    - Mihai Anitescu
    - John Bell
    - David Brown
    - Michael Ferris
    - Bob Moser
  - September 13-14, 2011
  - http://www.orau.gov/mathworkshop2011/

Background

- Understanding and predicting the behavior of complex systems is central to the Department of Energy meeting it mission requirements
  - Energy
  - Environment
  - National security
- Workshop motivated by need to identify the research in Applied Mathematics required to address DOE mission requirements
  - Scientific discovery
  - Engineering design
  - Risk Analysis



APPLIED MATHEMATICS

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

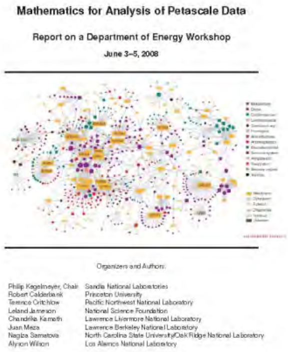
A Report by an Independent Panel from the
Applied Mathematics Research Community

May 2008

Mathematical Research Challenges in
Optimization of Complex Systems

Report on a Department of Energy Workshop
December 7–8, 2006

Organizers:
Bruce A. Hendrickson
dia National Laboratories
buquerque, New Mexico
Margaret H. Wright
stitute of Mathematical Sciences
York University, New York



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 Critchlow	Pacific Northwest National Laboratory
Leland Jameson	National Science Foundation
Chandrika Kamath	Lawrence Livermore National Laboratory
Juan Meza	Lawrence Berkeley National Laboratory
Nagiza Samatova	North Carolina State University/Oak Ridge National Laboratory
Alyson Wilson	Los Alamos National Laboratory

DOE Applied Mathematics Program

- Background
  - DOE has a long history of support for research in applied mathematics
  - Founded in 1950's at request of von Neumann
  - Currently a $40M program
- Core strengths
  - Numerical methods for partial differential equations
  - Numerical linear algebra
  - Optimization
  - Nonlinear systems and solvers
  - Stochastic systems and UQ (more recent)
- Core areas remain critical and active areas of research addressing
  - Increasingly complex systems
  - Novel emerging architectures
  - Components of broader efforts

Recent thrust areas / solicitations (FY09)

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

Workshop goal

- Identify important new areas of applied mathematics research needed to complement and enhance existing ASCR Applied Mathematics program to address challenges in understanding complex systems relevant to DOE
- Key elements of complex systems
  - Hierarchy of models with differing length and time scales as well as physical fidelity
  - Potential increased role for data, possibly from multiple sources, and its coupling to simulation
  - Need to address a broad set of questions: how good is my prediction, how do I control the systems, what are the inherent risks in the system
- Participants were asked to identify several types of research needs
  - Key gaps – new areas that need to be investigated
  - Areas from recent thrusts that require additional effort – what role do these areas need to play
  - Linkages with core research areas – specialized work within a core area needed to address a class of problems
  - Combinations of technologies need to address a set of problems

Workshop Organization

- Plenary session to survey complex systems arising from various DOE mission areas to serve as prototypes for the types of problems that Applied Math Program needs to address
- Organized as a panel with representatives from various DOE offices
  - Energy Efficiency and Renewable Energy
    - Offshore Wind Program -- Chris Hart
    - Integration of renewable systems -- Charlton Clark
  - Electricity Delivery and Energy Reliability
    - Modeling of the electric grid -- Gil Bindewald
  - Nuclear Energy
    - Nuclear Energy Advanced Simulation and Modeling – Alex Larzelere
  - Environmental Management
    - Advanced Simulation Capability for Environmental Modeling – Juan Meza
  - Basic Energy Sciences
    - Challenges for Computational Discovery in Basic Energy Sciences – Mark Pederson

Process

- Over a series of breakout sessions participants were asked to:

- Identify broad mathematical themes
  - Survey problem areas
  - Identify state of the art – what is known? what isn't known?
  - Look at potential solution strategies and underlying mathematical elements
  - How do different mathematical elements fit together

- For each theme
  - What is the state of the art for a given theme
  - What are the research needs in this area
  - What problems will this area address
  - Are there other problems where this area is applicable
  - How does this area interplay with other topics

Participants identified needs for research in four mathematical themes

- Themes were ubiquitous across all of the application areas that were surveyed
  1. Building and using hierarchies or collections of models
  2. Modeling systems characterized by diverse phenomena
  3. Systems that are inherently chaotic, stochastic, and/or uncertain
  4. Integration of data and observations with modeling and simulation

- Greatest potential impact from synergistic use of combinations of methodologies

Examine the computational challenges in these areas associated with emerging multicore architectures

Building and using hierarchies and collections of models

- Model selection, competition, and integration
  - Information-theoretic approaches (quantifying information content)
  - Analysis of coupled models (stability, asymptotic properties)
- Scale bridging
  - Bi-directional coupling
  - Non-equilibrium, microinstantiation, kinetic acceleration
  - Renormalization techniques
- Hierarchical decision-making
  - Analysis and algorithms for multi-level decisions
  - Inclusion of stochastic elements
  - Dealing with continuous and discrete, nonconvex elements

Modeling systems characterized by diverse phenomena

- Interfacing models from different domains
    - Limited visibility into highly distinct models
    - Techniques to deal with lack of derivatives and/or noisy responses
- Rigorous mathematical analysis of coupling
    - Key to developing effective numerical methods
    - Need for higher-order approaches
- Numerical methods
    - Architecture aware
    - Communication among models vs. data locality
    - Possible asynchronous computations

Systems that are inherently chaotic, stochastic, and/or uncertain

- Propagation of uncertainty through hierarchical models, models that represent a diverse set of processes or chaotic systems
  - Multiscale, multiphysics models
  - Uncertainty in chaotic systems
- Efficient techniques for capturing rare events
  - Risk mitigation
  - System robustness
- Optimization of stochastic systems
- Numerical algorithms for large systems of stochastic differential equations

Integration of data and observations with modeling and simulation

- Using data to constrain system dynamics
    - Inverse problems
    - Reducing uncertainty
- Techniques for solving inverse problems with sparse and noisy data
- Particle algorithms for data assimilation
    - Predictions based on direct combination of simulation and data
- Optimization and control based on combined use of model and data (possibly real-time)

Synergy example 1: ASCEM

- Risk mitigation for environmental remediation
  - How do we bridge the gap from pore scale to field scale in defining geochemical rates
  - How do we bound predictions of flow in heterogeneous subsurface that is not well characterized
  - How do we use available data to constrain overall system behavior
  - How do we assess potential risks associated with alternative remediation strategies

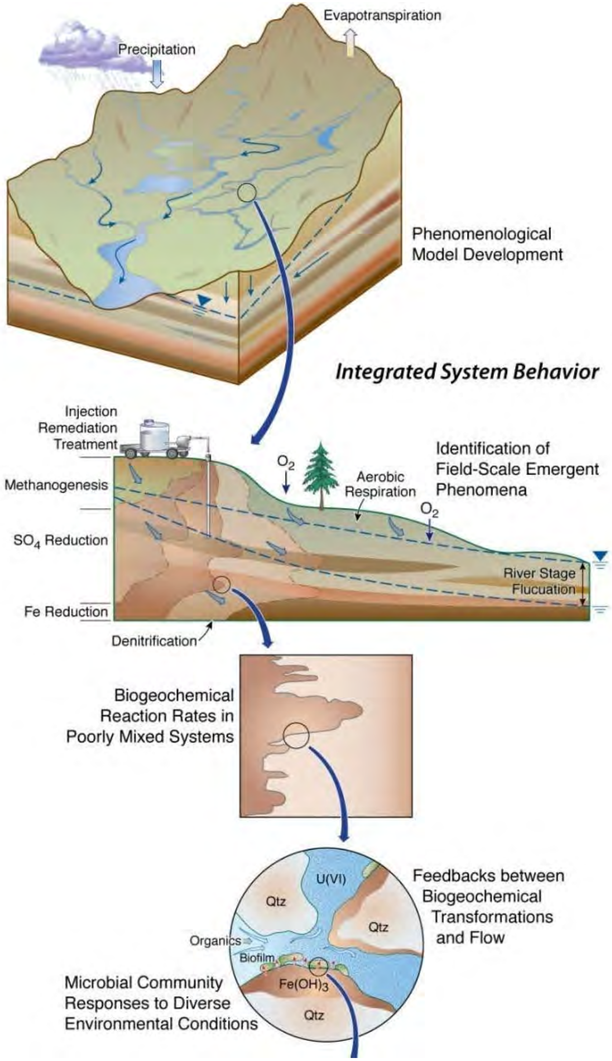
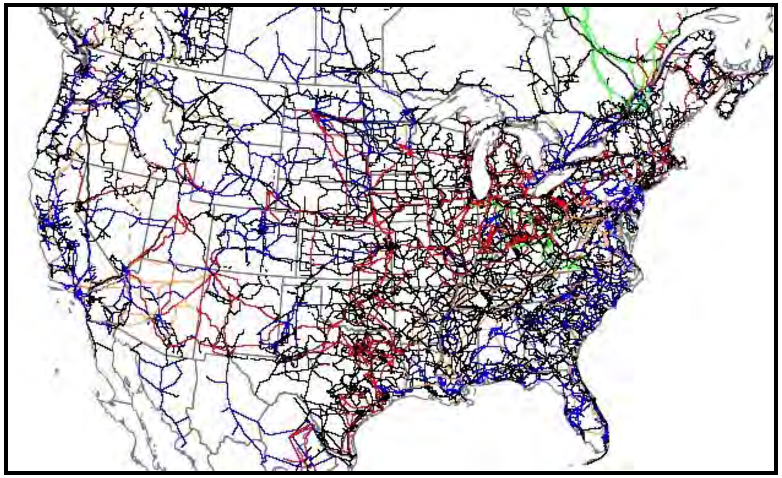


Image courtesy of J. Meza

Synergy example 2: Electric power grid

- Increase reliability of the power grid and prevent cascading failures
    - Can we develop a predictive multiscale model of the electric power grid
    - How do we use real-time noisy data from SmartGrid sensors to improve predictive capability of model
    - Can one develop distributed control algorithms to prevent cascading failures
    - Can we develop strategies to operate the grid in the presence of variable generation characteristics of wind and solar power

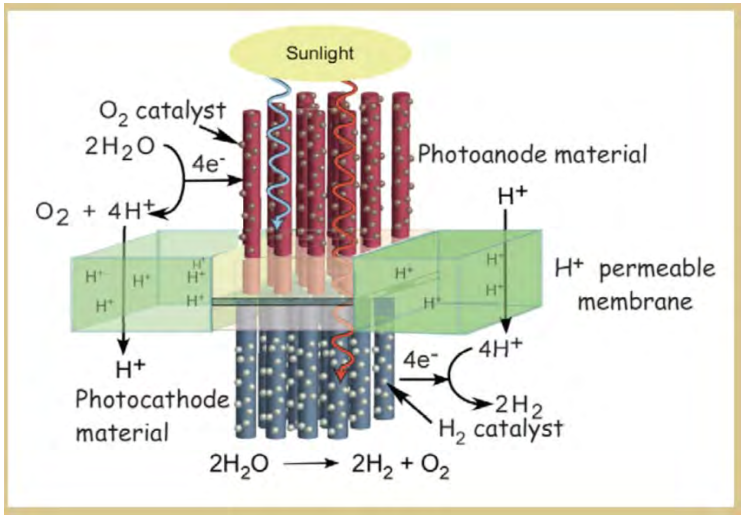


Electric Power Grid

Courtesy of G. Bindewald

Synergy example 3: Catalysts for fuel generation

- Develop the tools needed for the discovery of new catalysts for fuel generation
  - Integrate of quantum chemistry, molecular dynamics and mesoscale modeling
    - Coupling disparate types of physical models
    - Bridging significant spatial and temporal scales
  - Optimization techniques for energy minimization
  - Stochastic inverse problems to link models with high-resolution experimental data



Joint Center for Artificial Photosynthesis

Synergy example 4: Nuclear energy

- Maximize nuclear fuel utilization when reloading reactor core
  - High fidelity modeling of nuclear core behavior
    - Thermal fluids
    - Neutronics
    - Chemistry
    - Accurate coupling of processes
  - Quantified uncertainty in prediction of behavior
  - Complex combinatorial optimization problem for placement of new rods and distribution of old rods
    - Cluster versus distributed placement

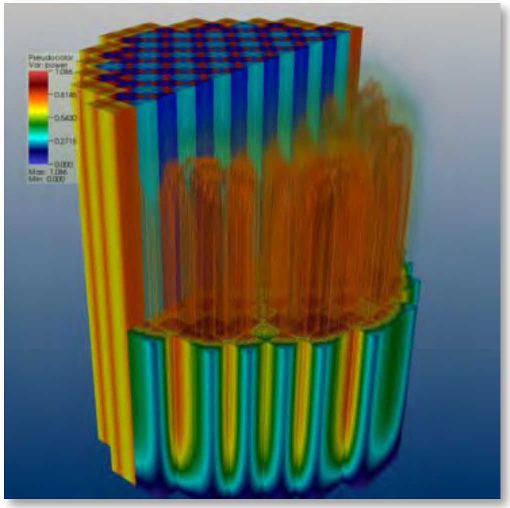


Image courtesy of
A. Larzelere

Summary

- There is a huge range of important DOE problems whose solution require significant efforts in Applied Mathematics
    - Building and using hierarchies or collections of models
    - Modeling systems characterized by diverse phenomena
    - Inherently chaotic, stochastic and/or uncertain
    - Integration of data and observations with modeling and simulation

- Greatest impact from synthesis of elements from multiple themes
    - Relies on advances in component methodologies

- The synthesis of these mathematical topics will lead to fundamental mathematical questions that span a range of activities from basic analysis to the design of new numerical algorithms to software that exploits next generation parallel architectures