Report on the Department of Energy Workshop on "Mathematical Research Challenges in Optimization of Complex Systems"

December 7–8, 2006, Bethesda, Maryland

Organizers:

Bruce A. Hendrickson
Sandia National Laboratories
Albuquerque, New Mexico

Margaret H. Wright
Courant Institute of Mathematical Sciences
New York University

Sponsored by:

DOE Office of Advanced Scientific Computing,
Applied Mathematics Research Program

Goal of the workshop

To articulate opportunities for mathematical research relevant to DOE applied science and technology programs

Of particular interest: mathematical areas that do not currently constitute a major fraction of DOE's applied mathematics research portfolio.

Six mathematical areas identified:

- Effective modeling of heterogeneous, coupled human-made systems with nonlinear interactions.
- Analysis and algorithms for a variety of optimization problems involving large systems with a mixture of continuous and discrete variables.
- Methods for analyzing and responding to sensitivity in highly nonlinear systems.
- Statistical approaches for validating and improving mathematical models of non-physical systems with a limited number of observed data.
- Techniques for integrating computational models with real-time data to support decision-making and adaptive control.
- Careful analysis of how risk should be incorporated into complex systems models.

Executive summary:

- There are strong intersections between these six mathematical areas and research needs identified in other recent Office of Science studies.
- These are challenging research areas that will require a sustained long-term effort.
- There is a need to make the research investment now.

Mathematical focus of the workshop:

- Complex systems
- Optimization
- Risk
- Control

Complex systems

Collections of multiple processes, entities, or nested subsystems, where the overall system is difficult to understand because of the following properties:

- The system components need not have mathematically similar structures;
- The number of components can be large, sometimes enormous;
- Components can be connected in a variety of different ways, most often nonlinearly and/or via a network. Furthermore, local and system-wide phenomena depend on each other in complicated ways;
- Taken together, the components form a whole whose behavior can evolve along qualitatively different pathways that may display great sensitivity to small perturbations.

Connections with November 2006 ASCAC review

Performance Assessment and Rating Tool (PART) measures:

- *By 2015, demonstrate progress toward developing mathematics, algorithms, and software that enable effective scientifically critical models of complex systems, including highly nonlinear or uncertain phenomena, or processes that interact on vastly different scales or contain both discrete and continuous elements.*

- *By 2015, demonstrated progress toward developing through the Genomes to Life partnership with the Biological and Environmental Research program, the computational science capability to model a complete microbe and simple microbial community.*

Optimization

The complex systems are meant to accomplish specific aims and ideally should do so in an optimal fashion.

However, the domain application problems of interest tend to differ in both context and character from those physical systems that have been studied under prior DOE funding.

In particular:

- The components of several of the systems of interest are aggregate or non-physical (e.g., power generation plants, prices, target dates for introducing a new technology).

- The purpose of the optimization may be to inform real-time operation, planning, or strategic/policy decision-making.

Risk

Specific goal of including risk in decision-making about complex systems.

Two major factors in formal risk analysis:

- the likelihood that an event will occur and
- the magnitude of the consequences of that event.

The DOE applied mathematics research program has supported work on *uncertainty quantification* and *predictability*, which develop techniques for understanding the potential errors in numerical simulation attributable to uncertainties in data, physics, and modeling.

Risk and uncertainty have different meanings, but measures of uncertainty are essential to assess both elements in risk.

Control

The modeling, design, and study of a system so that it will accomplish a specified set of objectives or display a certain desired behavior.

Predictive control allows prediction of the behavior of system outputs in terms of system inputs.

Adaptive control allows the alteration of system controls in response to changes over time of various parameters.

Organization of workshop

- Four plenary overview talks by application experts associated with DOE applied science and technology programs.

- Parallel cross-cutting breakout sessions to define mathematical research challenges and opportunities relevant to these applications.

Domain application talks:

- **Optimization of fossil fuel power generation**

  Stephen Zitney, National Energy Technology Laboratory

- **The nuclear fuel lifecycle**

  Phillip Finck and Dana Knoll, The Idaho National Laboratory

- **Power grid control and optimization**

  Robert Thomas, School of Electrical and Computer Engineering, Cornell University

- **Risk assessment for cybersecurity**

  Dwayne Ramsey, Lawrence Berkeley National Laboratory

Cross-cutting breakout sessions:

- Networks and Stochastics
- Complex Systems and Statistics
- Control and Optimization
- Model Construction and Validation
- Risk

Mathematicians:

Mihai Anitescu
Argonne National Laboratory

David Applegate
AT&T Research

John Bell
Lawrence Berkeley National Laboratory

John Birge
University of Chicago

Michael Branicky
Case Western University

Joe Chow
Rensselaer Polytechnic Institute

Brenda Dietrich
IBM

Paul Frank
Boeing

John Gilbert
University of California, Santa Barbara

Martin Groetschel
Technical University, Berlin

Seth Guikema
Texas A&M University

Bruce Hendrickson
Sandia National Laboratories

Mathematicians:

Michael Holst
University of California, San Diego

Tim Kelley
North Carolina State University

Tamara Kolda
Sandia National Laboratories

John Lewis
Cray Research

William Massey
Princeton University

Juan Meza
Lawrence Berkeley National Laboratory

Jorge Moré
Argonne National Laboratory

Richard Murray
California Institute of Technology

Cynthia Phillips
Sandia National Laboratories

Vladimir Protopopescu
Oak Ridge National Laboratories

Mathematicians:

William Pulleyblank
IBM

Roman Samulyak
Brookhaven National Laboratory

Radu Serban
Lawrence Livermore National Laboratories

Ellen Stechel
Sandia National Laboratories

Virginia Torczon
College of William & Mary

Stephen Vavasis
University of Waterloo

Bruce West
Army Research Office

Paul Whitney
Pacific Northwest National Laboratory

Alyson Wilson
Los Alamos National Laboratory

Margaret Wright
New York University

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Connections with the DOE Applied Mathematics Research Program

A 2003 internal assessment identified three important gaps in the program portfolio:

- discrete mathematics,
- statistics, and
- methods for coupling different component models (multiphysics).

Connections with BESAC

Basic Energy Sciences Advisory Committee (BESAC) 2004 subcommittee report:

> **Charge to the subcommittee:** *identify current and emerging challenges and opportunities for theoretical research within the scientific mission of Basic Energy Sciences.*

Among the scientific opportunities described in the report:

- Integrated mathematical models of physical systems containing components with differing function or morphologies.
- Control of various processes such as biomolecule-surface interactions or synthesis.

- Optimization of desired physical characteristics.

Opportunities for Discovery: Theory and Computation in Basic Energy Sciences (2005), Report of the Subcommittee on Theory and Computation, Basic Energy Science Advisory Committee, `www.sc.doe.gov/bes/reports/files/OD_rpt.pdf`.

Connections to DOE activities in nuclear energy

The 2004 Workshop on Advanced Computational Material Science: Application to Fusion and Generation IV Fission Reactors:

- Co-sponsored by the Office of Science and the Office of Nuclear Energy, Science, and Technology.
- Produced a detailed account of specific modeling needs, many of which feature the coupling of models with significantly different mathematical characteristics.

Report on the Workshop on Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors, June 30, 2004, `www.sc.doe.gov/bes/reports/files/ACMS_rpt.pdf`.

Connections with BERAC review

Advisory Committee for the Office of Biological and Environmental Research (BERAC) 2006 report.

From the review of the FACE and OTC Elevated CO_2 Projects:

A need is cited for "*a synthesis of results to date combined with modeling...to come up with explicit and testable hypotheses for the next generation of experiments*" in order to "*address the factors associated with the largest uncertainties in model predictions of response*".

Report of the Biological and Environmental Research Advisory Committee Subcommittee Reviewing the FACE and OTC Elevated CO_2 Projects in DOE, October 16, 2006, `www.sc.doe.gov/ober/berac/FACE_2006_report.pdf`.

Connections with BERAC review (cont.)

From the subcommittee reviewing the Climate Change PART Measure:

The report emphasizes "*concerns about the straightforward coupling of carbon cycle, ecological, and ice sheet components to present-day climate models*" because these components are very sensitive to biases in present models.

In considering how DOE can assess the global change research program, the report suggests "*the most crucial elements...are the connections between the components that include human dimensions and economic theory and the components that include models of natural processes.*"

Report of the Biological and Environmental Research Advisory Committee Subcommittee: Review of the Climate Change PART Measure, October 16, 2006, `www.sc.doe.gov/ober/berac/CCRD_PART.pdf`.

Connections with BERAC review (cont.)

From the subcommittee reviewing the Environmental Remediation Sciences PART Measure:

> *By 2015, provide sufficient scientific understanding to allow a significant fraction of DOE sites to incorporate coupled biological, chemical and physical processes into decision making for environmental remediation and long-term stewardship.*

A central point of the report is that BER-sponsored research should produce models that advance understanding of multiple components of contaminant fate and transport.

Report of the Biological and Environmental Research Advisory Committee Subcommittee: Review of the Environmental Remediation Sciences PART Measure, October 16, 2006, `www.sc.doe.gov/ober/berac/ERSD_PART.pdf`.

Executive summary:

- There are strong intersections between the six mathematical areas identified by the DOE Workshop on "Mathematical Research Challenges in Optimization of Complex Systems" and research needs identified in other recent Office of Science studies (e.g., ASCR, BERAC, BESAC, etc.).

- These are challenging research areas that will require a sustained long-term effort.

- There is a need to make the research investment now.

Web page for further information:

DOE Workshop on Mathematical Research Challenges in Optimization of Complex Systems

http://www.courant.nyu.edu/ComplexSystems/

Includes:

- Introduction
- Agenda
- Presentation materials from the application domain experts
- Notes from the focus sessions
- Background and links to related documents