Mathematical Research Challenges in Optimization of Complex Systems

Report on a Department of Energy Workshop
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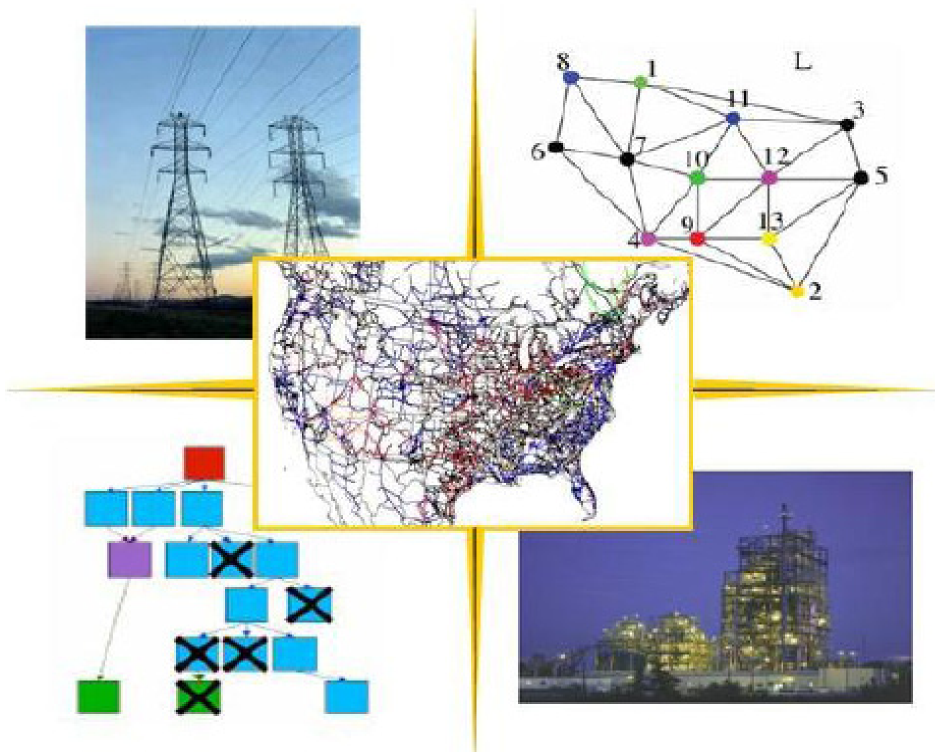

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Executive Summary

In December 2006, an invitation-only workshop sponsored by the Office of Advanced Scientific Computing Research, Office of Science, Department of Energy (DOE), brought together a diverse group of 32 distinguished mathematical scientists to consider "Mathematical Research Challenges in Optimization of Complex Systems". The goal of the workshop was to articulate opportunities for mathematical research relevant to DOE applied science and technology programs, in mathematical areas that are not already a major part of the DOE applied mathematics research portfolio.

Domain experts gave presentations on four applications of great interest to DOE: (*i*) fossil fuel power generation, (*ii*) the nuclear fuel lifecycle, (*iii*) power grid control and optimization, and (*iv*) risk assessment for cybersecurity. Participants then met in cross-cutting breakout sessions to define research challenges and opportunities.

The workshop applications as well as the associated mathematical research areas involve *systems that are not primarily physics-centered.* This description, which is intended to be broadly inclusive, applies to systems whose components range from aggregated engineered objects (e.g., power plants) to non-tangible elements (e.g., prices and decisions).

For the workshop applications as well as innumerable related problems, further illumination of fundamental issues requires new mathematical insights in the following six categories:

1. Modeling of heterogeneous, coupled systems with nonlinear interactions;
2. Optimization of large nonlinear systems with a mixture of variable types (including continuous, discrete, and categorical);
3. Methods for analyzing sensitivity and assessing uncertainty in highly nonlinear systems;
4. Statistical approaches, especially those that use a limited number of observed data, for validating and improving mathematical models;
5. Techniques for integrating models with data to support decision-making and adaptive control;
6. Analysis of how risk should be incorporated into complex systems models.

It is our conviction that sustained investments in these mathematical research areas would make a significant contribution to the solution of many important problems across the Department of Energy. Support for this research is especially timely because recent advances in high-end computing, stimulated by the Office of Science, allow progress far beyond the simplified models and inadequate heuristics previously dictated by computational limitations.

1 Workshop Overview

An invitational workshop on "Mathematical Research Challenges in Optimization of Complex Systems", organized on behalf of the Office of Advanced Scientific Computing Research (ASCR), Office of Science, Department of Energy (DOE), was held on December 7–8, 2006. The scientific focus of the workshop is discussed in Section 2.

The operational goal of the workshop was to identify mathematical research challenges arising in selected problems of great importance to DOE applied science and technology programs. Of particular interest were mathematical areas that do not currently constitute a major fraction of DOE's applied mathematics research portfolio, and a majority of the 32 distinguished mathematical scientists invited to the workshop accordingly represented expertise in such areas. An additional goal for workshop invitees was institutional breadth; eleven were from U.S. universities, two from non-U.S. universities, five from industry, one from a Department of Defense research agency, and thirteen from DOE laboratories. Details about the workshop's context within DOE are given in Section 3.

Four overview talks were given during the first day by application experts associated with DOE applied science and technology programs on

(i) optimization of fossil fuel power generation;

(ii) the nuclear fuel lifecycle;

(iii) power grid control and optimization; and

(iv) risk assessment for cybersecurity.

The applications talks are summarized and discussed in Section 4.

An extended question-and-answer session, designed to enhance delineation of the major open mathematical issues, followed each of these presentations. Participants then met in focus groups—three on the first day, two on the second—organized by cross-cutting mathematical areas to identify topics for mathematical research relevant to these applications. The three topics in the first set of focus groups were "Networks and stochastics", "Complex systems and statistics", and "Control and optimization"; the second set of topics comprised "Model construction and validation" and "Risk". The focus group titles were deliberately made broad and slightly ambiguous to reflect the wide-ranging nature of the workshop.

The workshop closed with presentations from the five focus group leaders, interspersed with questions and commentary from the participants. Presentation materials and notes from the focus sessions can be found at the workshop Web site [25].

2 Mathematical Focus of the Workshop

To clarify the scientific scope of the workshop, we provide brief definitions of four of the mathematical focus areas. Only two of these—"complex systems" and "optimization"—appear in the workshop name; "risk" and "control" were omitted in the interests of brevity. Nonetheless, the importance of the latter two was recognized in advance and reflected in the expertise of the invited mathematical scientists.

Complex systems. The intent of the workshop was to focus on *systems*, meaning collections of multiple processes, entities, or nested subsystems, where the overall system is difficult to understand and analyze 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 at any stage.

Unfortunately, although the term "complex systems" is widely used, it is not precisely defined. The properties listed above, and the systems described at the workshop, fit well with the broad interpretations of several academic institutes devoted to complex systems (for example, the New England Complex Systems Institute [13] and the Northwestern Institute on Complex Systems [14]).

A crucial property of the systems considered at the workshop is that *they are not primarily physics-centered*. This characterization applies to systems whose components range from aggregated engineered objects (e.g., power plants) to non-tangible elements (e.g., prices and decisions).

Optimization. The theme of optimization was highlighted in the workshop title because the complex systems described in Section 4 are meant to accomplish specific aims, and ideally they should do so in the best possible way. However, many of the associated problems tend to differ in both context and character from optimization problems in physics-centered systems such as those mentioned in Section 3.3. For example, the purpose of optimization in the workshop applications may be to inform planning, strategic decision-making, or real-time operation; the parameters to be optimized may include a mixture of continuous, integer, and categorical variables; and there may be a hierarchy of optimization problems that differ substantially in nature.

Risk. An explicit concentration of this workshop was on mathematical challenges arising from inclusion of risk in decision-making about complex systems. Risk analysis has been the subject of research in economics and business since the 1920s, and the journal *Risk Analysis*, published by the Society for Risk Analysis, has been in existence for more than 25 years [21]. Two factors are typically included 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 previously 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. (See, for example, the "big picture" overview in [24].) "Risk" and "uncertainty" have different meanings, but they are often closely related in the sense that measures of uncertainty are essential to assess both elements in risk. (See [9] for a discussion of risk and uncertainty in climate change assessment.)

Control. Happily, the mathematical definition of "control" is very close to its meaning in ordinary parlance. Control involves the modeling, design, and study of a system so that it will accomplish a specified set of objectives or display a certain desired behavior. As its name implies, predictive control allows prediction of the behavior of system outputs in terms of system inputs. In adaptive control, the system controls are altered depending on how various parameters change over time.

3 The DOE Context for the Workshop

Before describing the substance of the workshop, we review its context within the Department of Energy. Motivation for the workshop arose from two common motifs in DOE's Strategic Plan and the requirements of the Energy Policy Act of 2005, Section 994. It is also appropriate to ground the workshop within the history and current state of the Applied Mathematics Research program.

3.1 The DOE Strategic Plan

Strategic Goal 3 of the DOE Strategic Plan [5], labeled as "Scientific Discovery and Innovation", involves "strengthening U.S. scientific discovery and economic competitiveness" and "improving the quality of life through innovations in science and technology".

As part of this enterprise, Goal 3.1 stresses that DOE will "provide the base of new knowledge and the resulting new options and solutions to these ... challenges". In addition, Goal 3.3 states that DOE will "integrate basic and applied research to accelerate innovation and to create transformational solutions for energy and other U.S. needs". Two of the strategies for reaching Goal 3.3 are to "strengthen the ties between the basic research and applied mission programs" and "ensure continuous cooperation and information flow between basic and applied research efforts".

3.2 DOE's response to the 2005 Energy Policy Act

In the same vein as Goals 3.1 and 3.3 of the DOE Strategic Plan, the Energy Policy Act of 2005, Section 994 [6, page 322], requires periodic review by DOE of all of its science and technology activities "in a strategic framework that takes into account both the frontiers of science to which the Department can contribute and the national needs relevant to the Department's statutory missions".

DOE's first mandated report to Congress on satisfying the requirements of Section 994, submitted in the summer of 2006 [4], states that the Secretary of Energy will "ensure that the Department's overall research agenda includes, in addition to fundamental and curiosity-driven research, basic research related to topics of concern to DOE's applied technology programs".

One of the efforts launched by DOE in response to the Energy Policy Act was to identify gaps in its science and technology portfolio, stressing the identification of cross-cutting scientific and technical issues and the associated potential benefits for DOE's major programs. During this process, the general area of "advanced mathematics for optimization of complex systems, control theory, and risk assessment" was identified as "highly cross-cutting". In discussing this topic, the DOE response stresses that the required mathematics is "fundamentally different" from what DOE has historically pursued (see Section 3.3), and that "further development would benefit DOE in many of its other complex systems challenges". Confirmation of these views is evident from the description of research challenges in Section 5.

3.3 The Applied Mathematics Research Program

The DOE Applied Mathematics research program was created in the early 1950s by the Atomic Energy Commission (a predecessor of DOE) at the suggestion of John von Neumann. For more than 50 years, this distinguished program has nurtured leading applied mathematics researchers in the DOE national laboratories and academia, while at the same time fostering close ties between researchers in these two settings.

The DOE applied mathematics program is most famous for a portfolio of remarkable accomplishments in the theory and numerical solution of partial differential equations that describe time-dependent physical processes in complex three-dimensional geometries. Such equations are at the heart of fluid and solid mechanics, electromagnetism, radiation transport, and atomic and molecular systems. DOE-supported research has included the fundamental mathematics of stability and accuracy for finite-difference methods, as well as the theoretical foundations for numerical methods capable of solving problems with shock waves and other discontinuities.

Furthermore, in keeping with DOE's role as a mission agency, interactions have been actively encouraged between mathematical research and the DOE community, with greatest emphasis on physical sciences applications from the Office of Science (formerly the Office of Energy Research). Some of the applications intimately tied to the DOE applied mathematics program are: atmospheric fluid dynamics; chemical-vapor deposition; climate change; combustion; fusion; macromolecular modeling; modeling of materials; particle accelerator design; subsurface flows; and turbulence.

A consistently distinctive feature of DOE's applied mathematics program has been its close connection with computation, particularly at the highest end. For more than 30 years, DOE has been a leader in supporting the development of efficient and mathematically well-crafted algorithms and general-purpose numerical software. For the past few years, as part of DOE's emphasis on ultrascale computing, a major theme in its applied mathematics research has been "mathematical research and software that impact the future of high-performance computing" [15, 1]. In addition, a recent ASCR initiative has specifically targeted research in multiscale mathematics, to develop "new high-fidelity simulations to address important Office of Science research" [15].

4 Workshop Applications

The workshop was organized around four technical presentations that discussed mathematical challenges in the following applications: (*i*) fossil energy power generation, (*ii*) the nuclear fuel lifecycle, (*iii*) power grid control and optimization, and (*iv*) risk assessment for cybersecurity. Although different in detail, the associated mathematical problems share several common features:

- As already observed in Section 2, the high-level systems of interest are *not primarily physics-centered*: they may involve aggregations that are themselves systems of engineered objects (for example, a power plant), and they may involve economic, temporal, or strategic elements (for example, prices, construction start dates, and choices of new technologies);
- There is a need to analyze, design, improve, and/or control the overall system and/or its subsystems, and this need may extend over the system lifecycle[1];
- Complicated feedback mechanisms and behavior are exhibited that cannot be fully explained by an understanding of the component parts—the formal hallmark of a mathematically "complex" system;
- The system involves processes with differing scales, granularity, and/or mathematical nature;
- The applications are of critical importance to national priorities.

4.1 Fossil energy power generation

The DOE Office of Fossil Energy has the mission of "ensuring that we can continue to rely on clean, affordable energy from our traditional fuel resources" [17]. Among the major responsibilities of this office are development of a new generation of environmentally sound clean coal technologies and the FutureGen project [8], intended to design and build a pollution-free plant to co-produce electricity and hydrogen. The Office of Fossil Energy also operates the National Energy Technology Laboratory (NETL), the only national laboratory dedicated to fossil energy [12]. Stephen Zitney, leader of the NETL Collaboratory for Process and Dynamic Systems Research, presented a talk on "Mathematical Research Challenges in Optimization of Fossil Energy Power Generation Systems", co-authored with Lorenz Biegler and Ignacio Grossmann from Carnegie Mellon University.

[1]A system "lifecycle" includes birth, analysis, design, implementation, testing, deployment, usage, maintenance, termination, and disposal [23].

Today, fossil fuels provide approximately 85% of the total U.S. energy supply. However, concerns about environmental impact and energy security, combined with the aging of the existing fossil energy infrastructure, have created unique transition challenges for the industry and for policymakers. Although very little coal generation capacity has been added in the past 20 years, current expectation is for a dramatic surge in coal plant construction over the coming 20 years. Due to improvements in environmental profile and fuel flexibility, much of this new capacity is likely to be based upon technologies such as integrated gasification combined cycle[2] (IGCC) and polygeneration technology.

Future fossil energy power generation systems will consist of plants that individually represent complex, tightly integrated, multipurpose designs. All allowable technologies are required to meet aggressive engineering goals (such as producing near-zero emissions); even so, system planners will need to choose among a wide range of potential plant configurations with differing characteristics. For example, four of the candidate technologies in FutureGen are transport gasification, carbon sequestration, hydrogen production, and fuel cells. Issues to be considered include not only technical requirements but also the need to operate profitably amid cost fluctuations for raw materials, finished products, and energy.

Fossil energy systems are characterized by a variety of mathematical structures and problems. Dynamic process operations arise in analyzing plant startup, shutdown, and transitions, in studying safety issues, and in developing real-time training for system operators. Component models involve differential-algebraic equations—combinations of differential equations describing dynamic behavior such as mass and energy balances, and algebraic equations enforcing physical and thermodynamic relations. Both predictive and adaptive control problems need to be solved when assessing the future performance of a plant and in developing strategies for operating IGCC, FutureGen, and polygeneration plans. Finally, "enterprise-wide" problems at the highest levels need to be addressed to enable system-wide planning of capacity expansion, production, and distribution.

The fossil energy industry has already invested to excellent effect in research on modeling and advanced optimization methods, but many challenges remain. Significant nonlinearities as well as a mixture of continuous and discrete parameters feature in realistic models of plant planning, scheduling, operations, supply, and process synthesis and design. There is little mathematical theory about existence and uniqueness of solutions for general mixed-integer nonlinear optimization problems. Furthermore, current problems are limited in practice to simplified models with many fewer degrees of freedom than in a realistic system.

An additional set of mathematical challenges arises because of the non-convex formulations that occur in current models, which result in the possibility of nonunique solutions. Despite progress within the past decade in "global optimization" methods (which find the "best optimum" when multiple local solutions exist), current techniques

[2] "Integrated gasification combined-cycle technology uses a coal gasifier in place of the traditional combustor, coupled with a key enabling technology .... Integrating gasifier technology with a combined cycle in this way offers high system efficiencies, low costs, and ultralow pollution levels."[7, page 219].

are often unacceptably expensive for large problems. One possible strategy for ameliorating this difficulty is to develop improved models that exploit the sparse structure of the system interconnections to narrow the range of acceptable solutions.

Finally, an obvious ingredient in fossil energy applications is the presence of significant levels of both uncertainty and risk. (See the discussion of these terms in Section 2.)

4.2 The nuclear fuel lifecycle

Although largely dormant in the United States in recent years, nuclear energy is enjoying a resurgence of interest due to its lack of emissions and the domestic availability of nuclear fuel. A major part of the mission of the DOE Nuclear Energy program is to advance civilian technologies for creating a new generation of clean, safe nuclear power plants. Some of the mathematical challenges in this application domain were addressed in a joint talk on “Advanced Fuel Cycles: Modeling Needs” given by two nuclear energy experts from the Idaho National Energy Laboratory—Phillip Finck (Associate Laboratory Director, Nuclear Energy) and Dana Knoll. Physics-based simulations of nuclear power systems were the subject of a recent DOE-sponsored workshop [19]; accordingly, this report will consider only the complex systems aspects of the nuclear fuel lifecycle.

A nuclear plant, like the fossil energy plants discussed in the preceding section, is itself an extremely complicated engineering system, and a prospective system of nuclear power plants is still more complex. At an even higher level, the nuclear power system does not exist in isolation; its components operate within a broader framework involving other forms of energy, transportation links, and (because of public worries about nuclear energy) issues of policy, safety, and security. Thus mathematical research challenges arise from the complexity of the full nuclear fuel cycle as well as the simultaneous goals of promoting energy sustainability, reducing the impact of waste management, and minimizing the potential for nuclear proliferation.

Some of the mathematical issues related to the nuclear fuel lifecycle are:

- Any decision to build new nuclear power plants in the United States will involve analysis of serious policy issues concerning not only internal safety of the plant itself, but safety for the public and potential risks from external factors such as terrorist attacks on the plant. It will be essential to measure safety effectively and convincingly in the face of multiple risks and public anxiety;

- Policy regulations require assessment not only of risks (including the risk of policy changes), but also of estimated costs;

- Remote processing of spent fuel, one of the recycling options, necessarily involves transportation, which needs to be managed in a cost- and safety-effective manner;

- Siting a nuclear plant that will produce electricity must be done based on weighing proximity to customers, public concerns, and safety/security questions;

- Deciding *when* to begin building plants based on certain technologies is difficult because of long construction times and the need for minimal disruption of the overall system during transitional periods.

The associated mathematical challenges have many similarities to those discussed for fossil energy systems in the preceding section. Various control and process applications involve nonlinear optimization with a mixture of continuous and discrete variables. Formulating a full system model produces multi-objective problems as well as problems whose variables are constrained to satisfy partial differential equations.

Of particular note is the importance of realistic risk assessment in settings ranging from public discussions of nuclear plant safety to economic decisions about safe transportation of spent fuel. The impact of risk is greatly magnified by the long lead times for introduction and assessment of new technologies, the effects of construction time variations, and societal and political reactions to deployment.

4.3 Control and optimization of the electric power grid

The mission of the DOE Office of Electricity Delivery and Energy Reliability involves leadership of efforts to modernize the U.S. electric grid, enhance security and reliability of the energy infrastructure, and facilitate recovery from energy supply disruptions [26]. The portion of this mission dealing with transmission of electrical power poses a host of mathematical challenges, which were described by Robert Thomas, a professor in the Electrical and Computer Engineering Department at Cornell University, in a talk entitled "Power Systems Problems".

Power grid optimization comprises combinations of planning, control, operations, contingencies, market dynamics, policy, and socially imposed constraints, all in an environment characterized by enormous uncertainty and significant risk. Mathematical models of the power grid involve some or all of the following elements:

- Functional equality constraints rooted in physics, including algebraic, ordinary differential, and partial differential equations;
- Operational constraints, such as equilibrium conditions based on economic realities or desired properties;
- Game-theoretic elements arising from the current deregulated environment;
- Inequality constraints based on properties of existing systems, plant operating staff, economic or political externalities, and business conditions;
- Severe nonlinearities, in some cases bordering on discontinuities;
- Non-robustness, i.e. extreme sensitivity to small perturbations;
- A mixture of continuous and integer variables;
- Substantial, poorly understood, and difficult-to-predict levels of uncertainty;
- Large numbers of variables—e.g., the North American network has between 10,000 and 100,000 nodes or branches, and 100 control centers;

- A huge range of scales in both physical size (from individual components to continental-size grids) and time (from microseconds to hours);
- Nonunique solutions, with little insight as to how to characterize the most physically reasonable result.

Numerous problems in power systems are, by longstanding practice, formulated mathematically and solved in terms of optimization. For example, the unit commitment problem is to plan power generation over time by determining a minimum-cost dispatch schedule of a variety of generating units to meet a load demand while satisfying operational constraints, where the units have very different characteristics (e.g., thermal, hydro, nuclear, wind, and so on). The generic optimal power flow problem (OPF) is, broadly speaking, to optimize economic benefit (typically, the production cost of real energy) subject to an array of constraints that define operating conditions, such as load, network topology, outages, and so on. Generalizations of the OPF are used to analyze how to keep the system running when some of its components fail. For example, the security-constrained OPF includes additional constraints that represent contingency scenarios, assuming that at most a specified number of components fail.

Since 1992 (the advent of deregulation in the electric industry), the emergence of new electricity markets has substantially increased the difficulty of formulating as well as solving the OPF. In a regulated system, the OPF involves minimizing system cost based on smooth predetermined quadratic cost curves. In the deregulated market, by contrast, the core pricing mechanism for electricity trading requires discrete bids and offers that change on an hourly basis. A next-generation OPF needs to perform real-time full-system calculation of locational marginal prices (which reflect the value of energy at the specific location and time of delivery), subject to an accurate representation of current bids and offers, an explicit set of credible contingencies, and consistency through different time horizons.

Both planning for and operating the power grid are complicated by the need to work with a legacy system that is not operating under the conditions for which it was designed. Today's planning requires forecasting of energy costs and availability, as well as predictions of demographic and industrial changes in demand, subject to obvious uncertainty in all of these elements. Regulatory regimes have changed dramatically and unpredictably—another instance of risk—in recent years and environmental concerns have grown as well. Both of these factors have led to a reduction in excess transmission capacity, increasing system risk and vulnerability. Improved models for studying market designs could help to design regulatory regimes without unintended consequences.

A final mathematical challenge in power systems is to use the vast quantities of data collected in real time by Supervisory Control and Data Acquisition (SCADA) sensor systems to provide better automated control of transient events and as well as serious contingencies.

4.4 Cybersecurity

Cyberspace is a human-made system whose smooth and secure functioning is crucial to national well-being. Cybersecurity is also of great interest to the Department of Energy, which manages complex communication systems serving not only DOE employees but the international scientific community as well. The final workshop applications talk, "Challenges in Cyber Risk Assessment", was given by Dwayne Ramsey, Manager of the Integrated Safeguards and Security Program and Computer Protection Manager at Lawrence Berkeley National Laboratory.

A feature that cybersystems have in common with the other complex systems discussed at the workshop is that they involve large numbers of components with different mathematical structures and/or scales, ranging through individual machines, a local network, the network at a DOE lab, and the full Internet. For example, the computer system at Lawrence Berkeley Lab has approximately 13,000 devices on its internal network and serves thousands of transient non-employees. As in the other applications, understanding, assessing, planning for, and predicting risk are central elements in cybersecurity, including factors such as cost, impact, policy, and privacy.

The challenges posed by mathematical modeling of cybersystems—for example, to achieve an acceptable level of security—are inherently different from those that arise in modeling systems whose components are physical objects. There is no "ground truth" in the cyber world, and hence validation of system models is problematic, especially since the furious pace of change in the cyber environment means that today's models become obsolete very rapidly. An added difficulty in cybersecurity is that external factors—notably, resources not under central control—can play a major role in system behavior. Perhaps the most important factor is the wide variation of human behavior, including contrariness, which complicates attempts to develop predictive models. In particular, a worry in cybersecurity modeling with no counterpart in physics-centered systems is that some of the humans who have been modeled can decide to change their behavior to contradict the model's assumptions.

Risk assessment of cybersecurity policy is an obvious arena in which mathematics could be helpful. A first and very difficult step is to model the tradeoffs among the potential damage from security breaches, the openness needed to support a wide range of scientific collaborations (which include international and non-DOE colleagues), and the privacy and freedom that most users prefer. (If users changed their passwords every day, the risk of break-ins by outside hackers would be greatly reduced; but it is often difficult for systems managers to force users to change their passwords even once a month.) Realistic models of security regulation systems accordingly need to include not only financial costs such as staff and infrastructure expenses, but also factors such as user inconvenience and unhappiness that are much less easily quantified and may vary with context. In protecting highly classified data, for instance, the convenience of users will naturally be seen as less important than in an open scientific environment.

A further clear mathematical challenge in cybersecurity is making sense of the vast quantities of data from transmission traffic in order to identify and correct potential problems. Since most data traffic is innocuous, cyberdata analysis faces the "rare event" problem of detecting a very rare condition in a huge set of data without generating a large number of false positives. In addition, the mathematical approaches used in analyzing real-time data are likely to be different from those appropriate for a more leisurely study of archived information.

Beyond coping with an avalanche of data, security procedures based on predictive and adaptive control will need to take careful account of high levels of uncertainty, particularly when the available policy choices are small in number but radically different in nature. For example, a decision to impose the stringent lab-wide measures appropriate for a major security breach should include consideration of the probability that the breach was mis-diagnosed—but it is not clear how a decision-maker in such a position can be informed most effectively. Given the lack of clarity about this and similar decisions, obtaining a precise definition of the questions in cybersecurity may be among the most difficult mathematical challenges.

5 Mathematical Research Challenges

The research challenges described in this section range widely over several dimensions, from relatively specific to very general, and from "likely to succeed" to "blue sky". We regard this richness in nature as one of the best outcomes of the workshop. "Blue sky" ideas are essential because mathematicians have a track record of producing unexpected and novel insights that lead to "step changes" in our ability to understand and/or solve previously intractable problems.

We have deliberately not framed all the mathematical challenges in terms of algorithms; some focus instead on qualitative features of the solution such as existence, uniqueness, and sensitivity.

In several instances, progress on a particularly difficult problem class is likely to begin by focusing on important subclasses with specific mathematical structure. Thus the research challenges may concentrate on mathematical properties (such as network structure, linearity, partial separability, or strict convexity) that are common to large numbers of diverse applications.

5.1 Modeling

Construction of a mathematical model—a mixture of science, engineering, and art—is the first step in trying to understand a complicated system. A well crafted model is possible only if the behavior and interactions of the systems are carefully deciphered and understood, and so principled scientific methods must be followed. But models are only idealized approximations to the real world, and necessarily describe some, but not all, details of the system's behavior. For this reason, a model must be constructed with an understanding of its range of applicability and the kind of questions that it will need to answer. This process involves both complex tradeoffs and expert judgment.

Challenges in modeling complex systems. Scientists and engineers have long used mathematical and computational models for analysis and design of physics-centered systems, such as those involving fluid flow or combustion. In these domains, there is an underlying "ground truth", often described by a system of partial differential equations, and sophisticated methodologies have been developed to translate physics into mathematical and computational models.

For the kinds of complex systems motivating this workshop, the underlying "truth" is elusive or even non-existent. The following list summarizes system properties that further complicate the modeling process:

- An array of heterogeneous system components with multiple time and length scales, interacting through complicated feedback mechanisms;
- A mixture of variable types, including continuous, discrete, and categorical[3] variables, connected in some cases by a network structure with discontinuous or highly nonlinear behavior;
- Risks and uncertainties from many sources, including economic, social, political, technological, and behavioral.

Without underlying physics, it is difficult to evaluate such models because of questions like the following three: Are there any limiting cases to test the model's asymptotic behavior? What is the range of model validity? How sensitive is the model to parameter changes, particularly those which affect discrete or categorical variables? (Further comments on these issues appear in Section 5.3.)

A variety of approaches, including aspects of game theory and agent-based models, have been proposed for describing the interplay of social and behavioral factors. Components of these and related techniques are likely to be necessary for building useful models for DOE applications that include policy issues.

Models can be used in many ways and for many purposes, and different kinds of models will be appropriate in different settings. When used to make or support decisions in real time, models must be simple enough to run as quickly as the phenomena they are describing. More sophisticated and higher-fidelity models are called for in settings that are not time-critical. Models for designing systems can thus be much more computationally intensive and should include stochastic components and uncertainties. To inform policy decisions, models of economic behavior, including serious attention to characterizing and analyzing risk, can be used in the design of market mechanisms.

A "science of modeling" is a blue-sky goal, particularly for applications with heterogeneous components that extend beyond physics-centered systems, but any progress in this direction would be extremely beneficial to all the workshop applications. A mathematical *education* challenge is to create pedagogical materials drawing on fundamental mathematical principles as well as the experience of practitioners to accelerate the field and inform the modelers of the future.

[3]Discrete variables correspond to integers. Categorical variables also have an integral number of states, but without an inherent ordering. For example, the choice between coal and nuclear energy does not correspond to an ordered pair of integers.

Model reduction; reduced-order models. The broad motivation for model reduction, which produces reduced-order models, is to define a "simplified" (e.g., smaller and/or lower-order) model that adequately captures the behavior of the more complicated original system. In some contexts, reduced-order models are intended to provide low-error representations of more complicated models; in other instances, the reduced-order model is intended to "act like" the original model during optimization, but to be much less expensive to evaluate. Reduced-order models are likely to be necessary in several of the workshop applications—for example, system-wide coal plant design and management of the power grid.

Model reduction for problems with similar mathematical features is sufficiently difficult to qualify as an important research challenge. A (very) long-term goal in model reduction is to produce reduced-order models *automatically*, without knowledge of the mathematical nature of the underlying system (see [11]).

Further research themes identified during the workshop include analysis of robustness (does the reduced-order model accurately represent the full system if small changes are made in system parameters?) and theory and algorithms that could enable dynamic or data-driven updating (how can observed data be used automatically to improve the reduced-order model?).

5.2 Optimization

Many problems labeled as "optimization" appear in Section 4. We have deliberately adopted a "big tent" approach, grouping the associated mathematical challenges under a single heading.

Problems with heterogeneous variable types. Many of the complex systems discussed in Section 4 can be represented realistically only if the models include a mixture of variable types—continuous, discrete, and categorical. This requirement leads to huge consequences for research in optimization, since the extreme difficulty of mixed-variable nonlinear optimization problems is well known. (Some mixed-integer *linear* programs cannot be solved today even with state-of-the-art algorithms running on high-end computers.)

There are major mathematical research challenges in determining what can be said rigorously about existence, uniqueness, sensitivity, and solution techniques for mixed-variable nonlinear problems with some or all of the mathematical features characteristic of the workshop applications. Even if theoretical results turn out to be negative (e.g., a solution may not exist for certain problem classes), this knowledge would be valuable in guiding algorithm design, especially in time-critical contexts where there may be a backup layer of less accurate but solvable models.

Both theoretical analysis and algorithmic development are needed to assess the significance for mixed-variable nonlinear problems of techniques that are widely used in combinatorial optimization, such as relaxation/randomization strategies and approximation algorithms. This research domain necessarily involves elements usually associated with operations research and computer science.

Some of the problems presented at the workshop involve not only familiar equations defined by the laws of physics, but also inequalities derived from limitations imposed by strategy, economics, or politics. There is thus substantial scope for research on representing and solving systems of nonlinear mixed-integer *inequalities* in situations where only a feasible (not necessarily optimal) solution is needed.

Theory and algorithms for very large, structured problems. Even extrapolating the capabilities of ultrascale computers a decade into the future, solution of very large-scale optimization problems will be possible only by taking advantage of their structure. This translates into two areas of research: theory examining the mathematical nature of solutions to problems with specified structures, such as network constraints; and development of efficient algorithms for representing and computing with these problem structures.

Research on structured problems is likely to involve, but is not necessarily restricted to, research in linear algebra. An optimization problem can be highly structured when represented in symbolic form, e.g., in a modeling language, even though the associated matrices (such as the matrix of second partial derivatives of the objective function or the Jacobian of the constraints) are not sparse. Furthermore, the evolution of structure during iterations of an optimization algorithm may lend itself to new fast algorithms that exploit the known form of the changes.

Hierarchical, multilevel, and multi-objective optimization. In all four of the workshop applications, decisions made in one system may affect, directly or indirectly, decisions in other systems, with the added complication that the criteria used in making the decisions can vary significantly.

As with "complex system", there is no universal agreement about terminology for describing such problems. In some problems, there is an explicit hierarchy of levels, from highest to lowest—for example, the energy policies of the federal government (the highest level) affect state planning agencies, which optimize their behavior based on the actions at the federal level. The associated *hierarchical* or *multilevel* optimization problems are characterized by decision variables that are partitioned among several levels, e.g., the top level optimizes a function with respect to a subset of the variables, the next-lower level optimizes a different function with respect to a different set of variables, and so on. This kind of problem has also been called "multiscale optimization", and involves efficiently solving subproblems at different levels and aggregating information from different levels.

Multi-objective or *multi-criteria* optimization involves simultaneous optimization of several objective functions (rather than a single objective) subject to constraints. The existence of alternative definitions of "optimality" (see, e.g., [2]) is one of many complications in developing effective algorithms for multi-objective problems, especially when nonlinearities are present.

Because hierarchical and multi-criteria optimization problems are extremely difficult, new approaches to analysis and algorithms are needed to realize their potential in complex nonlinear systems. Even the linear bilevel programming problem, which contains only two levels in which all of the objective and constraint functions are linear, is nonconvex and has an exponential number of local minima; see [3]. Thus there are numerous opportunities for mathematical research in devising fast approximation algorithms based on provably reliable heuristics. Additional mathematical issues involve control of the iterations—how accurately do the subproblems need to be solved to ensure convergence to a reasonable solution?—as well as the extraction of predictive sensitivities with respect to the inputs from the subproblems.

Optimization under uncertainty. Multiple forms of uncertainty were ubiquitous in the workshop applications. Taking the single example of power grid systems, there is uncertainty from nature (when is there a serious windstorm?), from energy users (who uses electricity, and when?), and from technology (when does a power generator break down?). An immediate research challenge is that each of these is likely to require a different mathematical treatment.

One way to deal with uncertainty in these settings is to interpret it as randomness and use stochastic programming, a form of optimization with a mixture of deterministic and random variables (see, e.g., [22]). Unfortunately, classical stochastic programming assumes that the probability distributions for the random variables are known, whereas the forms of uncertainty in the workshop applications are likely to be deduced from sampling. Serious questions about reliability and sensitivity arise when the number of samples is small, as well as questions about how to include and take advantage of adaptive sampling. Other issues related to optimization under uncertainty involve formulation of very large problems with sampled parameters.

5.3 Sensitivity, validation, and uncertainty

As mathematical and computational models play an increasing role in critical decision making, it is imperative to gain a quantifiable understanding of the limits of the models. A standard mathematical tool in this regard is sensitivity analysis, whose goal is to understand the effects on the outputs of a mathematical model of changes in the model's parameters. This understanding helps to evaluate the model's applicability, to predict its behavior, and to determine the likely effects of uncertainties or errors in the parameters.

Sensitivity analysis and model validation are formidable tasks in the best of circumstances, and they are particularly challenging for complex systems. Many of the issues mentioned in earlier sections complicate the needed analysis, including the presence of heterogeneous variable types, the lack of underlying physics-based "ground truth" to justify a model, highly nonlinear behavior, and the often-erratic effects of social, economic, and human factors.

Especially for discrete variables, it is unclear how best to characterize model sensitivity. Uncertain and stochastic inputs only add to the challenges of model validation and sensitivity analysis. Data for model validation—particularly when modeling economic, political, or social forces—will almost surely be difficult to obtain. Hence experimental design and advanced statistical techniques are needed to make optimal use of limited observed and experimental data, since there will rarely be sufficient data to confirm high confidence levels.

Of particular importance in maintaining critical infrastructure is an understanding of extreme, or worst-case, behavior of a model. Unfortunately, the obvious validation technique of comparing the results of a model with observations is inadequate when the model is intended to explore extreme and unobserved situations such as the total failure of the power grid. In some cases, such a scenario can be phrased as an optimization problem, albeit one whose solution is especially problematic. Once tools have been built for these kinds of analyses, they can be used to design systems with improved robustness and efficiency.

The long time periods associated with infrastructure investments pose additional challenges, since traditional methods for propagating uncertainty forward in time are likely to be inadequate. A fresh perspective is needed—perhaps one based on dynamical systems—that emphasizes the phase space of solutions rather than the details of individual trajectories.

Work is needed on representation of uncertainties as well as development of algorithms that trace the propagation of uncertainties through complex models and help to identify the most critical parameters. Uncertainties can be represented in terms of ranges, confidence intervals, data-derived histograms, and probability density functions [10], and each of these forms brings its own challenges.

5.4 Data analysis

Even more than models used for prediction, the mathematical bases for operational decisions must be informed by data. Different applications will have access to very different kinds of data, and decisions will happen on different timescales. But mathematical progress in data interpretation and analysis is crucial to the decision-making or decision support problems discussed at the workshop.

In all of the workshop applications, certain decisions need to be made in real time. In some instances, this process will be entirely automatic—for example, decisions in cybersecurity about individual packets are mostly made using rules drawn from prior data analysis and experience.

In other contexts, data must be organized and presented to facilitate rapid understanding and assimilation to inform higher-level decisions made by humans. Decision-makers who need to react to events in real time, such as operators of power plants, often do so by consulting operational guidelines and/or relying on implicit models in their heads of how the system "should" behave. As systems become increasingly complex, however, especially when levels of uncertainty are high, there is a need for an explicit means of integrating newly acquired data into an evolving system model. This kind of data-driven or data-influenced simulation could significantly augment an operator's understanding and ability to make a good decision. The associated mathematical challenges include development of mechanisms for managing observational data, adaptive mathematical and computational models, and user interfaces to convey the results in a manner that aids the decision-maker.

Removed from the treadmill of real-time decision-making, data can be subjected to a variety of more sophisticated analyses. For cybersecurity, patterns of suspicious and constantly evolving behavior need to be recognized and mitigated. The high volume of network traffic combined with the subtle signatures of malicious behavior suggest the need for sophisticated machine learning capabilities. In power grid management, sensor data can provide forewarning of unusual operating conditions or equipment troubles. For power generation, data analysis drives the supply chain management that is central to cost control.

5.5 Risk

Every application presented at the workshop included elements of risk, some potentially catastrophic in both the short and long term. A list of these can be found on the workshop Web site [25].

This report has already mentioned (in Section 2) the importance of model- and data-based risk analysis in business and finance. Risk analysis is also common in clinical trials of drugs and medical treatments, the insurance industry, and public works. Although the workshop applications have distinct individual characters with respect to the role of risk, they visibly have much in common with applications in the just-mentioned areas. Consider, for example, some of the conclusions of a May 2006 conference co-sponsored by the National Academy of Sciences and the Federal Reserve Bank of New York on "New Directions for Understanding Systemic Risk" [18]:

1. Policymakers play multiple roles that produce important tensions and need careful analysis;
2. Economic behavior displays a large variety of complicated nonlinearities that are not well understood; and
3. The economy is a network of heterogeneous agents.

These observations are highly reminiscent of the workshop applications, leading to the obvious conclusion that important mathematical research challenges—primarily in system modeling and data-driven adaptivity—arise in incorporating risk into the complex systems of interest to DOE.

6 Connections with the Applied Mathematics Research program

As discussed in Section 3.3, the applied mathematics research program in ASCR has traditionally focused on selected topics, guided in large part by their relationship to science applications in the Office of Science. Nonetheless, a 2003 internal ASCR assessment exercise [20] determined that the applied mathematics program contained gaps in five areas. Two of these—multiscale mathematics and ultrascalable algorithms—have since become the foci of new initiatives in ASCR. The three remaining areas viewed as gaps in this exercise were discrete mathematics, statistics, and "multiphysics mathematics", which involves the coupling of disparate physics-centered models.

Echoing these views, the most recent (2004) ASCR Strategic Plan lists "underinvestment in all areas of discrete mathematics" and "underinvestment in statistics" among the weaknesses of the applied mathematics research program [16, page 31]. A "gap analysis" [16, page 32] then identifies program gaps in:

- discrete mathematics, noting its "potential to make orders-of-magnitude gains in the computational complexity of some application areas, including computational biology and homeland defense";
- statistics, because of the need to extract knowledge from the large quantities of data produced by large-scale simulations; and
- multiphysics, because of "the need to formulate complex models of multiphysical systems", either by combining separate subsystems or designing new models that capture a much wider range of physical behavior.

In the above list of gaps, mathematical topics are explicitly linked to and justified by applications in the Office of Science. However, if we focus only on *mathematical* issues and compare this list with that in Section 5, it is immediately obvious that discrete mathematics and statistics permeate many of the research challenges identified during the workshop. In addition, taking a high-level view of the mathematics needs in "multiphysics", the general modeling challenges in Section 5 carry over directly to multiphysics applications. Thus the research challenges independently articulated during the workshop align well with previously identified gaps in the applied mathematics research program that pose impediments to progress in basic science applications from the Office of Science.

7 Summary of Research Challenges

The mathematical research challenges articulated at the workshop fall into the following six broad categories:

1. Modeling of heterogeneous, coupled systems with nonlinear interactions;
2. Optimization of large nonlinear systems with a mixture of variable types (including continuous, discrete, and categorical);
3. Methods for analyzing sensitivity and assessing uncertainty in highly nonlinear systems;
4. Statistical approaches, especially those that use a limited number of observed data, for validating and improving mathematical models;

5. Techniques for integrating models with data to support decision-making and adaptive control;
6. Analysis of how risk should be incorporated into complex systems models.

We believe that sustained investments in these mathematical research areas would make a significant contribution to the solution of many important problems across the Department of Energy. Support for this research is especially timely because recent advances in high-end computing, stimulated by the Office of Science, allow progress far beyond the simplified models and inadequate heuristics previously dictated by computational limitations.

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Appendix A. Workshop Participants

Invited Mathematicians

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14. Tim Kelley
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15. Tamara Kolda
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18. Juan Meza
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19. Jorge Moré
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20. Richard Murray
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21. Cynthia Phillips
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22. Vladimir Protopopescu
    Oak Ridge National Laboratory
23. William Pulleyblank
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24. Roman Samulyak
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25. Radu Serban
    Lawrence Livermore National Laboratory
26. Ellen Stechel (Advanced Scientific Computing Advisory Committee)
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27. Virginia Torczon (Advanced Scientific Computing Advisory Committee)
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