Multiscale Mathematics Initiative: A Roadmap

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Letter of Transmittal

13 December 2004

Dr. Gary M. Johnson
Office of Science
U.S. Department of Energy
Washington, D.C.

Dear Dr. Johnson,

It is both an honor and pleasure to submit this report, *Multiscale Mathematics Initiative: a Roadmap*, on behalf of the computational scientists and mathematicians who attended and contributed to the series of three workshops sponsored by the Department of Energy. My co-organizers and I have done our best to faithfully represent the collective wisdom of this scientific community concerning the needs driving a research initiative in multiscale mathematics.

The broad range of domain experts who attended and presented their work at this conference reflects the extent to which advances in multiscale mathematics can be expected to impact the computational sciences. With mathematics as a common language, experts across domains such as biology, chemistry, and physics were able to share their experiences and insights concerning the underlying computational challenges that we together have a vested interest in solving. We are all faced with outstanding scientific problems that current mathematical methods do not adequately address. As we solve the mathematical problems of multiscale science, we shall also advance science and technology.

Of all the investments that the Department of Energy may choose from, multiscale mathematics offers the greatest payoffs as each step forward will be amplified across the other programs. We urge you to consider the long term returns that a multiscale mathematics initiative will seed.

Respectfully,

Moe Khaleel
Pacific Northwest National Laboratory

On Behalf of Third Workshop co-organizers John Dolbow (Duke University) and Julie Mitchell (University of Wisconsin, Madison)

Executive Summary

Science and technology are on the verge of a revolution. Physical processes at exceedingly large and small scales of time and space are becoming increasingly well understood, and technologies for engineering these systems are rapidly emerging. Yet, in general, we have no means of translating fundamental, detailed scientific knowledge at these micro and macro scales into their effect on the scale of the world in which we live. Without the capability to "bridge the scales," a significant number of important scientific and engineering problems will remain out of reach.

Following 30 years of exponential advances in modeling, algorithms, and computer hardware, mathematical modeling and computational simulation have reached the point where simulation of most physical processes over relatively narrow ranges of scales has become an essential tool for both scientific discovery and engineering design. Further growth, however, is significantly limited by the absence of a mathematical framework and software infrastructure to integrate heterogeneous models and data over the wide range of scales that characterize most physical phenomena. Fundamentally new mathematics and considerable development of computational methods and software will be required to address the challenges of multiscale simulation.

The U.S. Department of Energy (DOE) sponsored three workshops in 2004 to consider the scientific needs and mathematical challenges for multiscale simulation. These meetings were structured to solicit advice from the engineering, mathematics, and scientific communities in developing a roadmap for future investments in multiscale mathematics. The scientists participating in the workshop included primarily natural scientists—physicists, chemists, geologists, biologists—as well as computational mathematicians and computer scientists. The number and location of the workshops was selected to maximize participation from a comprehensive cross section of the scientific community.

The first workshop took place in Washington, D.C. May 3–5, and focused on scientific applications and cross-cutting mathematical issues (http://www-fp.mcs.anl.gov/multiscale-workshop/). Participants were asked to identify the most compelling scientific applications facing major roadblocks due to multiscale modeling needs and to formulate a strategic plan for investment in multiscale mathematics research that would meet those needs. The second workshop took place in Broomfield, Colorado July 20-22, where participants discussed the current state of mathematical methods for multiscale problems and potential directions for development, (http://www.math.colostate.edu/~estep/doe_multiscale/DOE_Multiscale_2.html). The third workshop was held in Portland, Oregon September 21-23, (http://multiscalemath.pnl.gov), where the objective was to emphasize the connection between domain application areas and the multiscale mathematical frameworks, as well as the synergy between domain application scientists and mathematicians, thus completing the process. All three workshops were stimulated by a series of invited lectures and small group breakout sessions.

This report is intended to guide the issuance of a DOE Mathematical, Information, and Computational Sciences call for proposals for the new "Atomic to Macroscopic Mathematics" research initiative. The FY 2005 budget for this initiative, estimated at $8.5 million, is intended to support the applied mathematics research needed to break through the current barriers in our understanding of complex physical processes whose components and processes span a wide range of interacting length- and time-scales. Such research will potentially impact scientific domains including, but not limited to,

environmental and geosciences, climate, materials, combustion, high energy density physics, fusion, bioscience, chemistry, and networks. ***This report represents the important conclusions, themes, and recommendations for DOE investments from all three workshops.***

The recommendations to come out of this series of workshops support research, collaboration, training, and disciplinary infrastructure. Research will be necessary across the spectrum from theory to application: formalisms and frameworks, algorithm development and implementation in software, analysis metrics and tools, and demonstrations of applied principles within specific problem domains. Of particular interest will be: 1) mathematical bridges across levels of type and scale such as stochastic to deterministic, discrete to continuous, interscale coupling; 2) mathematically derived metrics for error, uncertainty, stability, and performance bounds; 3) software development including implementations of new algorithms and problem sets for benchmarking, the transfer of existing software to new problem domains, validation and verification.

Research opportunities should encourage individual efforts as well as highly interdisciplinary teams that partner university scientists with their counterparts in the national laboratories. To spur innovation, a few projects deemed to be high risk should be encouraged. To fully disseminate current knowledge, and to prepare for the rapid dissemination of future research results, multiscale mathematics will require communication conduits including workshops, conferences, travel within collaborative research teams, training programs for young scientists, and educational products such as textbooks.

We expect the Multiscale Mathematics Initiative Roadmap presented in this report to culminate in a new foundation for multiscale mathematics and a new generation of multiscale software applied to comprehensive scientific simulations on problems of importance to DOE.

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1   Introduction

Until recently, most science and engineering has focused on understanding the fundamental building blocks of nature. This effort has been enormously successful but has essentially focused on problems containing one, and occasionally two, space and time scales. The ability to simulate physical processes containing subcomponents that operate in vastly different space and time scales is essential to furthering our understanding of their impact on the scale in which we live. Unfortunately, the ability to simulate complete systems does not follow immediately or easily from an understanding, however comprehensive, of the component parts. For that, we need to know and to faithfully model how the system is connected and controlled at all levels.

Systems that depend inherently on physics at multiple scales pose notoriously difficult theoretical and computational problems. The properties of these systems depend critically on important behaviors coupled through multiple spatial and temporal scales, often without a clear separation between scales, and as such, their description does not fall within the set of classical methods for crossing scales. In such situations, consistent and physically realistic mathematical descriptions of the coupling between, and behavior of, the various scales are required to obtain robust and predictive computational simulations. The physical and mathematical complications that arise in multiscale systems currently present one of the major obstacles to future progress in many fields of science and engineering, including environmental and geosciences, climate, materials, combustion, high energy density physics, fusion, bioscience, chemistry, power grids and information networks.

Multiscale simulations are computationally demanding. Over the past 30 years, advances in computational methods and supercomputer hardware have each contributed speed-up of approximately six orders of magnitude – over a trillion-fold improvement. Yet even with these incredible capabilities, we are currently limited to simulating most phenomena over only a relatively narrow range of scales. For a simple premixed turbulent combustion problem with Reynolds number 10,000 and Zeldovich number 100, direct numerical simulation would require computations that are 10^{12} times greater than what can be solved today. Assuming that hardware and algorithmic performance will continue to improve at the current rate, extrapolation suggests that it will be 40 years before we have sufficient power to simulate this simple model of combustion. Similarly, it will be at least 80 years before we will have the capacity to simulate a crack propagation problem using a molecular dynamics computation for 1 cm^3 of Copper ($\sim 10^{23}$ atoms) over the period of 1 second.

Increasing capabilities in experimental science also contribute to the pressure for the development of multiscale mathematics. New measurement and characterization tools in many fields make it possible to explore spatial and temporal phenomena on an unprecedented range of scales. For systems where such information is available, we have the building blocks to create realistic mathematical models of behavior on a number of individual scales. This increases the need to understand how to combine data and realistic models at different scales to obtain a manageable model of the entire multiscale system.

While several examples exist of successful multiscale simulations, we have neither a mathematical framework nor a software infrastructure to integrate the vast majority of heterogeneous models and data over the wide range of scales present in most physical problems. The ability to build predictive capabilities through simulation will help achieve a deeper understanding of the behavior of these systems and can be used to solve the many problems facing DOE in general. For example, Figure 1 shows the
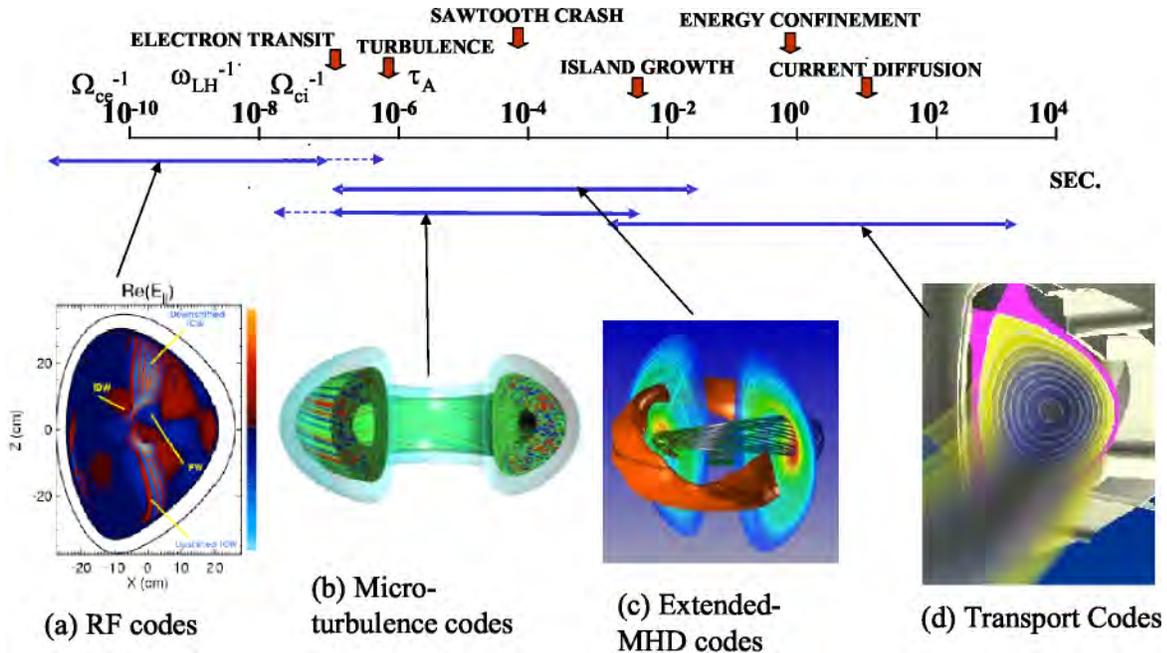
Figure 1. Models for a broad range of timescales need be connected to simulate a burning plasma experiment of magnetic fusion. The four parts of the figure illustrate the types of simulation techniques used over subsets of the time or frequency domain. The predictive capabilities of such a simulation require an ensemble of accurate and efficient multiscale mathematical methods such as multiresolution discretization, hybridization, closure, and model reduction. (Figure courtesy of the First Multiscale Mathematics Workshop report)

broad range of timescales—14 orders of magnitude or more—that come into play in simulating a burning plasma experiment of magnetic fusion (see Section 3.6). Widely different analysis techniques and computational approaches are appropriate for different subregions of the space or time domains. An integrated modeling capability will greatly facilitate the process whereby plasma scientists develop an understanding of and insight into these complex systems. This understanding is needed for realizing the long-term goal of creating an environmentally and economically sustainable source of energy.

The number and diversity of problem domains facing this computational barrier is compelling:

- Simulating the operation of fuel cells, balancing fluid flow, heat and mass transfer, high-heat release non-equilibrium chemical kinetics coupled with catalytic surface chemistry

- Simulating subsurface contaminant transport, balancing advection, diffusion, and reaction in a complex flow environment

- Modeling protein folding processes, coupling physical effects of the fast bond stretching scales to those on the much slower folding scales

- Studying soft matter properties determined or modulated by non-covalent effects, microstructural hydrodynamic coupling, and excluded volume/connectivity constraints

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- Increasing reliance on long-term atmospheric and climate simulations to predict the amount of carbon dioxide in the terrestrial system and determine policy accordingly

- Modeling large-scale graphs and networks representing biological systems, power grids, or communication networks involving hundreds of thousands of nodes coupled through multiple scales in space and time.

Mathematical techniques such as: multiresolution analysis, multigrid methods, multiscale geometric analysis, adaptive timestep methods, adaptive mesh refinement, adaptive analysis-based methods for integral equations, hybrid methods, variational multiscale analysis, variational multiscale method, mathematical homogenization, renormalization group techniques, and operator splitting, among others, have produced significant advances in understanding multiscale problems. However, these techniques have typically been developed and employed in very specific application areas. Consequently, multiscale research remains largely disjointed among physical disciplines, and researchers within each discipline are unlikely to be familiar with more than a few of these methods.

The development of an overall framework of classes of multiscale methods will require circumstances promoting a greater exchange of information among disparate lines of research. We must then expand on this framework to develop new mathematical techniques, computational methods, and software that are both fundamentally novel and built on the foundation of classical methods of applied mathematics if we are to face the challenge presented by DOE mission-critical multiscale scientific problems.

2 Multiscale Mathematics Needs

In this section, we discuss the technical objectives for a multiscale mathematics research program. The goal of the program is to develop scale-linking models and the associated computational methods required to produce simulations that properly account for behaviors occurring over multiple scales. By "simulation" we mean to include predictive computational representations as well as statistics or data-based characterizations of a system. Because the key mathematical and physical issues arising in modern multiscale problems occur across a wide range of scientific and engineering disciplines, the identification and categorization of common issues is an important step in the process of developing a multiscale framework. As an incomplete list, some key simulation issues include:

- Selecting models and model parameters at each scale

- Linking models and information across scales and physical phenomena
  - Determining the form and strength of coupling
  - Representing information transfer across levels of scale and type (e.g., stochastic to deterministic, discrete to continuous, interscale coupling)
  - Resolving model mismatch

- Reducing models
  - Identifying relevant degrees of freedoms
  - Determining necessary and sufficient properties of closure
  - Substituting appropriate approximations (including subscale models, probabilistic representations)

- Understanding and controlling sources of error and uncertainty
  - Quantifying the degree of correspondence between a model and reality
  - Measuring discretization, integration, and basis set errors
  - Determining the propagation of error and uncertainty across scales and physical phenomena
  - Using indicators to adaptively select details and resolution

- Analyzing complex models
  - Understanding how stochastic and rare events alter the properties of a system.

In the following subsections, we summarize the current and emerging mathematical methods being applied to multiscale problems as well as open areas for research associated with each class of methods. Many of the emerging methods will form the foundation for fundamentally new classes of multiscale mathematical methods. Finally, we provide arguments supporting the need for a framework and reaffirm the need for ever-faster hardware and algorithms to meet computational challenges of multiscale simulations.

2.1 Methods

We loosely group the major approaches to the multiscale problem into eight categories. The distinction made in this document is but one among many possible ways that these methods might be categorized. A typical multiscale simulation will require the incorporation of several of these methods:

1. *Multiresolution methods*, which resolve multiple scales within a single model by adjusting the resolution as a function of space, time, and data;

2. *Hybrid methods*, which couple multiple models and numerical representations across different scales (and often, physical phenomena) into a single simulation

3. *Closure methods*, which provide analytical or numerical representations for the behavior of components at much smaller scales than the scale of primary interest

4. *Adaptive methods*, which dynamically control methods, models, and parameterizations so as to minimize the error and uncertainty associated with a simulation or data representation

5. *Error estimation methods*, which characterize and quantify deterministic sources of error associated with analytical and numerical techniques (e.g., discretization, quadrature, and basis set approximations)

6. *Uncertainty quantification methods*, which characterize and quantify sources of uncertainty associated with a model (e.g., geometric idealization, uncertain parameters, statistical representation of microscale fluctuations)

7. *Inverse and optimization methods*, which identify model parameters and control mechanisms such that the behavior of a model matches a desired goal behavior

8. *Dimensional reduction methods*, which reduce models in high-dimensional state spaces to their essential dimensions or fundamental modes in a smaller number of degrees of freedom.

2.1.1   Multiresolution Methods

Multiresolution methods resolve multiple scales within a single model by adjusting resolution and scope as a function of space, time, and data. Many of these methods use information from error metrics to adaptively select numerical parameters. Existing and evolving multiresolution methods include, for example, multigrid and algebraic multigrid, multiresolution analysis (includes multiwavelets), and multiscale geometric analysis. A fundamental need in this category is the development of fast solvers for irregular algebraic systems that naturally arise in multiscale and adaptive resolution processes.

Open research areas include:

- Extension of existing methods to a broader range of multiscale problems

- Extension of multigrid, algebraic multigrid, and other multiresolution methods to include the time domain and to produce coarse model hierarchies, adaptively testing for important fine-scale features

- Analysis and compression of functions and operators by simultaneous multiscale function techniques and multiscale geometry

- Multiresolution-in-time algorithms for stochastic differential and difference equations.

Accurate and efficient simulation and data representation in computational chemistry and many other scientific domains rely on current multiresolution methods, and extending these methods is crucial for extending the range of truly multiscale problems that can be solved.

2.1.2   Hybrid Methods

Hybrid methods couple multiple models and numerical representations across different scales (and often, different physics) into a single simulation over contiguous domains. Individual models in a hybrid simulation may (or may not) use multiresolution methods. The numerical representations and information passing issues that may need to be bridged include discrete to continuum and/or stochastic to deterministic types. Hybrid methods may include closure approximations at the largest and smallest scales. Individual models and/or the hybrid methods for coupling the individual models rely critically on information regarding error and uncertainty to adaptively choose different algorithms or parameters during runtime. Successful implementation of hybrid methods in all cases hinges on the ability to develop error- and uncertainty-based indicators aimed at guiding the selection of the appropriate form and strength of inter-model coupling and identifying regions of space and time where more complete descriptions are required. Existing and evolving hybrid methods include, for example, the quasi-continuum method and hierarchical modeling, and more broadly, information- or parameter-passing methods and concurrent modeling methods.

Open research areas include:

- Hierarchical models, or sequences of mathematical models with increasingly more sophistication with the goal to identify the member(s) of the sequence that are both admissibly accurate and computationally least expensive

- New stable and accurate discretizations for the coupling between scales and models (e.g., coupling statistical sampling of microscale to high-order PDE schemes)

- Derivation of the correct interface conditions to connect large scales to small scales, e.g., continuum model to a subgrid microscopic model.

Several scientific problems urgently demonstrate the need for new hybrid methods including the modeling of chemical and biochemical reaction and diffusion processes in catalysis and bioremediation, characterizing macroscopic stability in tokamaks, materials science, and climate modeling.

2.1.3   Closure Methods

Closure methods provide analytical or numerical representations for the behavior of components at much smaller scales than the scale of primary interest. These approximations can then be used as inputs to simulations resolving the primary scale. Relevant problems include both those that have strong scale separation and those that lack strong scale separation. Closure methods should be designed to both respect the physical integrity of the system and produce computationally efficient schemes. Such methods are a critical component of, for example, mathematical homogenization and renormalization group techniques, as well as more recent advances such as multiscale finite elements, variational multiscale analysis, and the heterogeneous multiscale method. Variational methods exemplify one potential area of promise because they may offer a systematic approach based on decomposition of the

state space into "resolved" and "unresolved" scales, derivation of exact equations for each scale, and identification of scale-to-scale interactions.

Open research areas include:

- Methods that address the non-local and nonlinear effects generated by the interaction between physical models on length and time scales that are not well separated

- New Green's function solutions, which play a major role in many homogenization relations

- Techniques for identifying the terms in closure on which to concentrate error and uncertainty analysis (also critical to embedding closure methods in adaptive methods)

- Stochastic homogenization methods serving as interface filters linking statistics of data across length scales

- Methods for conducting upscaling in systems that have continuously evolving scales of heterogeneities.

Simulating transitions in turbulent mixing problems that arise in high energy density physics, coupling turbulent transport and reaction scales in combustion, accurately representing the effects of microscale physics (pore-scale, cloud-resolved scale) on macroscale dynamics in large-scale subsurface flow models and climate models, and deriving continuum models of large discrete networks are just a few of the scientific areas where new closure methods are needed.

2.1.4 Adaptive Methods

Adaptive methods dynamically control methods, models, and parameterizations so as to minimize the error and uncertainty associated with a simulation or data representation. The method must automatically identify the important features and scales in different subdomains of a model. Such methods seek an optimal trade-off between the efficiency of a coarse scale simulation and the accuracy of an enriched simulation containing a more complete ensemble of scales, models, and data known about the physical system represented by the simulation. Existing and evolving adaptive methods include, for example, adaptive timestepping methods, adaptive mesh refinement and front-tracking methods, and adaptive analysis-based methods for integral equations.

Open research areas include:

- Extension of existing methods to a broader range of multiscale problems

- Fast adaptive methods for integral equations with spatially varying coefficients and fast adaptive algebraic linear solvers that do not require problem-specific tuning

- Methods that adapt the choice of model (rather than mesh resolution) for different subdomains of space and time

- Adaptive timestep selection for stochastic differential equations.

Radio-frequency (RF) modeling in fusion problems, supernova simulations, crack propagation in materials, and stochastic dynamics of biochemical reactions are among the many scientific areas that will depend on new formulations of adaptive methods.

2.1.5   Error Estimation Methods

Error estimation methods characterize and quantify deterministic sources of error associated with analytical and numerical approximations to fundamental models (e.g., discretization, quadrature, series truncation, and basis set approximation errors). While the mathematics community has a long history in development of error estimation, particularly as it applied crucially to adaptive methods, the errors arising from and propagating through information exchange across scales have not been well characterized. Errors transferred across models and scales (including the resolution of model mismatch) and from the coupling process itself must be systematically addressed to guide new adaptive methods. Methods such as variational multiscale analysis, heterogeneous multiscale methods, mathematical homogenization, and equation-free modeling may lead to natural definitions of proper norms for, and derivation of, error estimates and identification of the terms on which to concentrate error analysis.

Open research areas include:

- Natural definitions of proper norms for and derivation of error estimates and identification of the terms on which to concentrate error analysis in adaptive, hybrid, and closure methods

- Development of correction indicators for multiscale adaptation based on error estimates

- Extension of a posteriori error estimates to coupled, nonlinear multiscale discretizations.

Error estimation is a fundamental driver for adaptive methods and a crucial component of all multiscale methods; therefore, research in this area is needed in all multiscale scientific problems of interest to DOE.

2.1.6   Uncertainty Quantification Methods

Uncertainty quantification methods characterize and quantify sources of uncertainty associated with a model due to lack of information about model parameters and the physical fidelity of the model itself, as well as physical processes that are characterized as random (e.g., geometric idealization, uncertain parameters, and statistical representation of microscale fluctuations). The ubiquity of this unavoidable artifact of modeling and observation of physical processes motivates the need to assess their effects on multiscale simulations, particularly if our goals include assessment of predictive capability and computational and experimental resource allocation. A distinguishing feature of multiscale modeling and analysis is the relationship between mathematical models whose states are defined with respect to different measures. Methods are needed to investigate, within an uncertainty context, these transformations of measures and to interface them with mathematical analysis at each of the relevant scales. Coupled with deterministic error indicators, uncertainty estimates are necessary for identifying the proper scale resolutions in adaptive methods. Additionally, new methods are needed to efficiently account for parametric uncertainty, since direct Monte Carlo simulations are currently too computationally intensive for the scope of this problem in multiscale models. Reducing uncertainty, determining reliability, and validating the process itself will require incorporating multiple sources of data—collected with various means from a range of spatial and temporal scales—into conditioned

estimates of spatial properties. Uncertainty quantification and error estimation together provide a means for obtaining the required information about solutions as well as the reliability of that information.

Open research areas include:

- Diagnostics that allow an assessment of how well multiscale models explain data taken on various scales

- Development and coupling of uncertainty indicators for multiscale adaptivity to similar error indicators, to achieve target reliability in predictions

- Reduced order or surrogate models with estimates of error in the model approximation, including statistical learning techniques, to accelerate the convergence of statistical computation algorithms

- Evolution and linking of computational and geometrical statistics, information theory, compatible data compression, and model reduction methods to meet the challenges of interscale information exchange

- Incorporation of Bayesian and other approaches to hierarchical models, classification on multiple scales, and data assimilation.

Uncertainty quantification is critical to solving multiscale problems across scientific disciplines including prediction of subsurface flow, climate, and material properties based on statistical characterization of subscale phenomena, and microbial cell community behavior based on partially known metabolic networks and associated kinetic parameters.

2.1.7   Inverse and Optimization Methods

Inverse and optimization methods seek to identify model parameters and control mechanisms such that the behavior of a simulation matches a desired goal behavior. Parameter identification using standard approaches is expensive with respect to both storage and CPU costs. This cost is increased in multiscale problems because they are typically characterized by a greater number of parameters, each of which may potentially extend over a greater range of values. Since all inverse/optimization methods are characterized by the fact that they must solve the underlying state equations several times before the good approximation of the solution is found, such problems present a huge potential for improving computational performance by careful consideration of the multiscale structure. In the multiscale context, a particular challenge emerges from the fact that many of the underlying models are stochastic in nature or they contain parameters that are the result of uncertainty quantification at the transition between scales. The hierarchical nature of multiscale models offers the promise of obtaining important computational improvement, especially in the early stages of the optimization process, by considering only as much model resolution as necessary to obtain sufficient progress at a given iteration.

Open research areas include:

- Identification of local indicators within the multiscale system response to guide the global selection of parameter subdomains, and development of a theoretical basis for the convergence of sampling methods for parameter selection

- Methods for stochastic multiscale optimization

- Good initial guess and preconditioning strategies for large-scale iterative methods

- Techniques to estimate the difference in iterative improvement between coarse- and fine-scale models.

Improved inverse/optimization methods are critically important to advances in materials science (nanotechnology, composite material design), biological systems (protein network and metabolic pathway elucidation), network analysis, and subsurface remediation problems, among many other multiscale scientific problems.

2.1.8 Dimensional Reduction Methods

The goal of dimensional reduction methods is to simplify models characterized by high-dimensional state or input parameter spaces to their essential dimensions or fundamental modes, with a significantly reduced number of degrees of freedom. Dimensional reduction is used for three reasons: to reduce the computational demands for simulating the system, to identify the most salient components with respect to drivers of model behaviors, and to simplify the process of analysis. Existing and evolving dimensional reduction methods are many and include response surface modeling, statistics-based methods such as principal components analysis, proper orthogonal decomposition, response and statistical surrogate modeling, and dynamic systems-based methods such as center manifold theory.

Open research areas include:

- Methods derived from nonequilibrium statistical mechanics to represent the dynamics of a coarse-grained system in terms of the unresolved degrees of freedom

- Methods to model the dependence between variables using their statistics rather than their mean values

- Methods to explore pattern and structure changes with length scales.

Science domains that will require improved dimensional reduction methods include materials science and biology, where macroscale phenomena depend on rare events such as nucleation of defects, and a few features of a large molecule may determine its function.

2.2 Unifying Mathematical Framework

Beyond research in specific methods and problems, there is also a strong need for abstract mathematical frameworks and a set of benchmark problems within those frameworks for testing and validating new approaches in each of the mathematical areas outlined above. Existing approaches in multiscale mathematics have evolved from ideas and solutions that strongly reflect their original problem domains. As a result, research in multiscale problems has followed widely diverse and disjoint paths. This presents a serious barrier to the application of methods to new problem domains.

A common mathematical framework for multiscale analysis is expected to help identify inconsistencies between model components, formalize the transition process between those components, identify the terms critical for the coupling of those components, and serve as a proof-of-principle and concept for complex, multiscale mathematical models. Rather than consisting of a single unified theory, such a mathematical framework would probably consist of several components tailored toward classes of multiscale problems. Such frameworks should provide a common, rigorous, and systematic language for formulating and analyzing multiscale problems across a range of scientific and engineering disciplines. The creation of frameworks would allow categorization and clarification of characteristics of existing models and approximations in a landscape of seemingly disjointed, mutually exclusive, and ad hoc methods. A framework can ensure a systematic and mathematically sound foundation for validation of multiscale simulations and for uncertainty quantification. Further, such an approach can provide context for both the development of new techniques and their critical examination.

A framework would provide a language to mathematically express well-posed descriptions of the individual models designed for coupling across scales and the coupling between models themselves. A multiscale investigation of uncertainty and error analysis methods within a greater framework would offer scientists, engineers, and mathematicians an opportunity to systematically examine these measures in a manner that is fundamentally different from past approaches, yielding the potential to provide a new path to breakthroughs in modeling and simulation. The ideal framework would also satisfy a fundamental need to build our understanding of where and how small-scale fluctuations affect large-scale dynamics and of how ensembles of simulations might best be used to capture the essential features of fluctuations and quantify uncertainty in chaotic or stochastic systems.

Although it is impossible a priori to describe what such a unifying framework might look like, some well-established techniques present paradigms on which to build. These include, for example, singular perturbation theory and the theory of matched asymptotics, adaptive time-space methods, and variational methods, all of which may allow formulation of some general characteristics of how multiple scales interact.

2.3 Mathematical Software

The methods and framework described in the previous two subsections will need to be implemented in software and widely disseminated to provide utility to all members of the multiscale research community. As with other mathematical software, particular attention should be paid to issues of verification, scalability, and parallelization. By definition, multiscale problems span a much wider range of space and time scales than do single-scale problems. Assuring the scalability of the resulting algorithms to thousands of processors will engender challenges of the highest order. Yet this latter task is crucial—many multiscale problems are unsolvable with today's supercomputers and will require the power and memory of the next generation of machines, and only then in conjunction with advances in models, algorithms, and software. The development of toolsets of mathematical software that are sufficiently flexible and capable so that new algorithmic and modeling ideas can be easily prototyped will be essential. Indeed, without such a toolset, experiments with different multiscale models and solution approaches will be too difficult and complicated to realize the expected impact on the science.

Three categories of multiscale simulation problems illustrate the computational challenges associated with increasing complexity:

- Single Model, Uniformly Multiscale. These problems involve a single model exhibiting behavior on multiple scales that are uniformly distributed in time and space. Examples include homogeneous turbulence, high-frequency wave propagation and Helmholtz problems, various network problems, and more generally, stiff ordinary differential equations (ODEs).

- Single Model, Non-Uniformly Multiscale. These problems involve a single model exhibiting multiscale behavior in different spatial/temporal regions. Typically, the regions of multiscale behavior are not known a priori, and dynamic adaptivity is required. Examples of problems in this class include moving interfaces, shape optimization, molecular dynamics, particle methods, mode conversion of waves, transition to turbulence, material failure, and resolving and tracking shocks and other singularities.

- Multiple Models, Non-Uniformly Multiscale. Problems in this class are described by multiple coupled models describing behavior at multiple scales across space and time. These models may be coupled via interfaces or they may be co-located. Examples of the former include global climate models coupling atmospheric, ocean, and land cover dynamics; atomistic-continuum coupling of material behavior across interfaces; cardiac mechanics models coupling blood flow; and models of solid propellant rockets coupling internal gas flow, combusting propellant, and solid dynamics of the casing. Examples of co-located multi-model multiscale problems include hierarchical atomistic-continuum simulations, macroscopic weather models coupled with mesoscopic local physics, and more generally, problems with complex subgrid-scale models involving; for example, systems of nonlinear ODEs.

It is anticipated that a number of uniformly multiscale numerical algorithms can be made to scale readily to future high-end architectures characterized by tens of thousands of processors. However, for single model, non-uniformly multiscale and multiple-model systems, significant and pervasive challenges lie ahead in addressing the parallel adaptivity, dynamic data structures, load balancing, and synchronization issues. Multiple-model multiscale problems inherit all of the difficulties previously described but are amplified substantially because of the need to manage these problems across multiple vertically or horizontally coupled models.

The numerical and computational difficulties exhibited even by "single-scale" problems—such as ill-conditioning, non-linearity, stiffness, stability, multiple optima, geometric complexity, singularities, localization, dynamic structures, asynchronicity, and long-range coupling—are expected to be amplified significantly in the multiscale setting. Devising numerical algorithms and computer science tools for treating such problems will require a long-term, sustained, and coordinated effort within the scientific computing community (see Figure 2). In additional to the need for advances in high performance computing, there will also be a need for next generation visualization and analysis tools, both for use in software development and for analyzing the results of simulations.
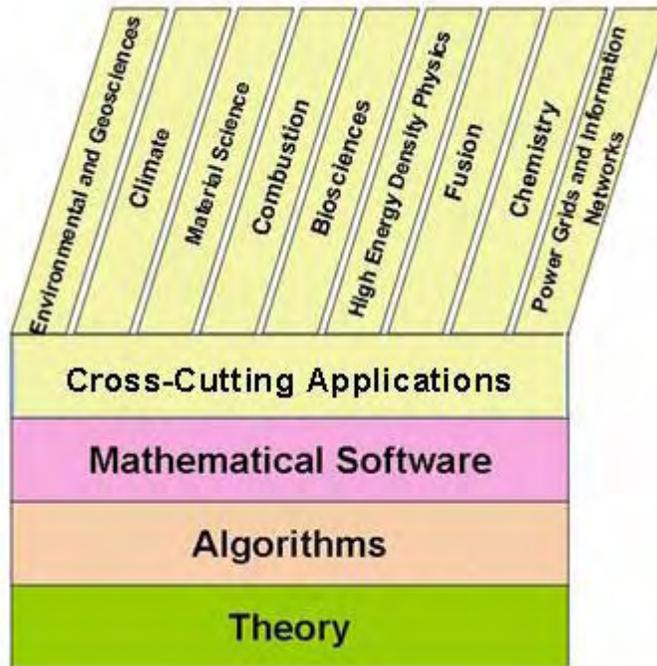
Figure 2. Mathematical software developed for use on high performance computing systems will be critical in the implementation of new algorithms within each of the application domains.

3   The Science-Based Case for Multiscale Mathematics

We focus in this section on nine target applications that are important to DOE and will benefit dramatically from multiscale mathematics. Any such list will be incomplete, and we recognize that other application areas of relevance to DOE may have multiscale issues associated with them. From the perspective of DOE's mission, developing and applying mathematical methods in the context of realistic applications is a critical goal. Mathematics must be informed by scientific and engineering reality in order to obtain physically meaningful information from models to guide action and understanding in the physical world.

3.1   Environmental Sciences and Geosciences

Environmental and geoscience applications of crucial importance to DOE's mission are abundant and provide compelling challenges over multiple time and space scales. Such applications include nuclear waste disposal and environmental restoration of contaminated sites, fuel production and utilization, CO_2 sequestration for reducing greenhouse gases, and mitigating natural hazards such as oil spills and wildfires. The National Research Council in 1999 estimated the cost of subsurface environmental remediation at about \$1 trillion and noted this estimate was highly uncertain. Costs associated with meeting federal Clean Air Act requirements are also staggering. Petroleum fuel costs are rising rapidly, and the sustainable future of our current petroleum-based economy is relatively short. The total cost to the U.S. economy of issues related to these environmental examples alone exceeds \$100 billion per year, and the decisions being made are far from optimal. Because these problems relate to immediate human welfare, their study has traditionally been driven by the need for information to guide policy. Although assessment tools have been developed, their scientific foundation is weak. The development of more effective prediction and analysis tools requires a systematic, multidisciplinary marshalling of basic science, mathematical descriptions, and computational techniques that can address environmental problems across time and space scales involving tens of orders of magnitude.

Current models of environmental systems lack predictive capability because such systems are extraordinarily complex. The scales involved range spatially from the distance between molecules to roughly the diameter of the Earth and temporally from fast chemical reactions to the age of the Earth. Diverse physical, chemical, and biological processes operate at these scales, many of which are not well understood. Naturally open systems, which are coupled to other complex systems, must be considered. Furthermore, simulation is heavily dependent on observed data, which are often sparse and noisy. Hence, development of environmental models that are accurate across the large range of time and space scales remains a major challenge.

The problem of CO_2 sequestration provides a good illustration (see Figure 3). This problem involves the removal of atmospheric CO_2 and its injection deep below the Earth's surface. The objective is to retard the return of this gas to the atmosphere, thus reducing the atmospheric concentration and slowing the rate of apparent global warming. A complete description of this system needs to incorporate surface chemistry (angstroms), pore-scale physics (microns), and subsurface heterogeneity (meters-kilometers).

Current formulations of the mass, momentum, and energy equations that describe subsurface flow rely on ad hoc closure schemes that do not incorporate important pore-scale physics. Laboratory observations provide abundant support for the notion that current models are seriously lacking in their ability to accurately simulate multiphase flow for such applications. Adequate resolution of these shortcomings will require new, rigorous, physics-based models that are more fully understood at the microscale. Methods for accurately upscaling these
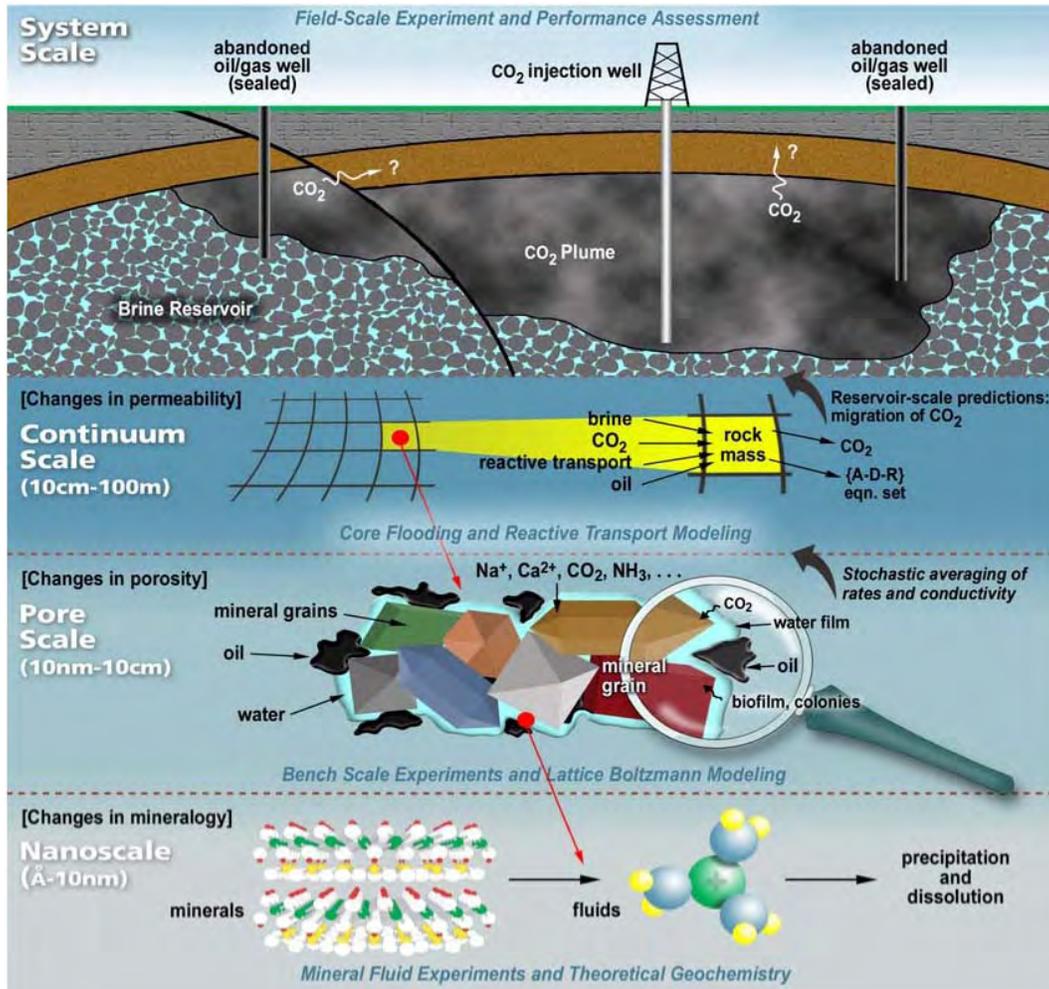
Figure 3. Multiscale nature of carbon sequestration in an atomic to field-scale experiment geophysics model. Models of processes at different scales are based on vastly different physical and mathematical models and computational methods. Much of the data at various scales are uncertain, yet decisions must be made from this data that affect public policy. (Figure courtesy of Los Alamos National Laboratory)

models must be developed along with efficient large-scale parameter estimation technologies that incorporate disparate data at different scales. Additional needs include:

- Developing alternatives to the simulation of bulk surface properties

- Identifying physical properties and parameterizations that contribute the most to uncertainty and variability at the field scale

- Identifying mechanistic, robust, and scalable multiphysics couplings, such as the linkages between groundwater, surface water, and the atmosphere

- Developing efficient schemes for simulating systems with local regime and accuracy based requirements.

3.2   Climate

The problem of global climate change is of particular interest to DOE in its ramifications for the energy economy of the nation. The societal impacts for these efforts are large; it has been estimated recently that a one month increase in lead time for predicting El Nino would save $100 billion worldwide. Climate and weather prediction is also a major component in formulating policy on CO_2 emissions and the generation of particulates and other pollutants. These issues are, in turn, tightly coupled to energy policy.

The realization that human activities can fundamentally impact the Earth's climate has made understanding these impacts a high priority and internationally recognized goal. Coupled model systems have shown steady improvement in capturing global temperature variability and present climate state, but much work is needed to further reduce the uncertainty in their predictions of global climate sensitivities. From the beginning of climate modeling, the job of applied mathematics has been to reduce the range of scales (from centimeters, such as sea spray, to thousands of kilometers, such as the circumference of the Earth) to make the problem solvable on computers. This is one of the most difficult multiscale problems in contemporary science because there is an incredible range of strongly interacting anisotropic nonlinear processes over many spatio-temporal scales.   Contemporary comprehensive computer models are currently incapable of adequately resolving or parameterizing these interactions on time scales appropriate for seasonal prediction and climate change projections.   Both the atmosphere and ocean systems present significant multiscale simulation issues individually, and a complete climate model requires coupling these two systems, adding additional scales to the problem. An example of significant multiscale behavior in the ocean system is thermohaline circulation, which is a global circulation strongly affected by flows characterized by dimensions in the range of ten to hundreds of meters due to the regional overflow (Figure 4).
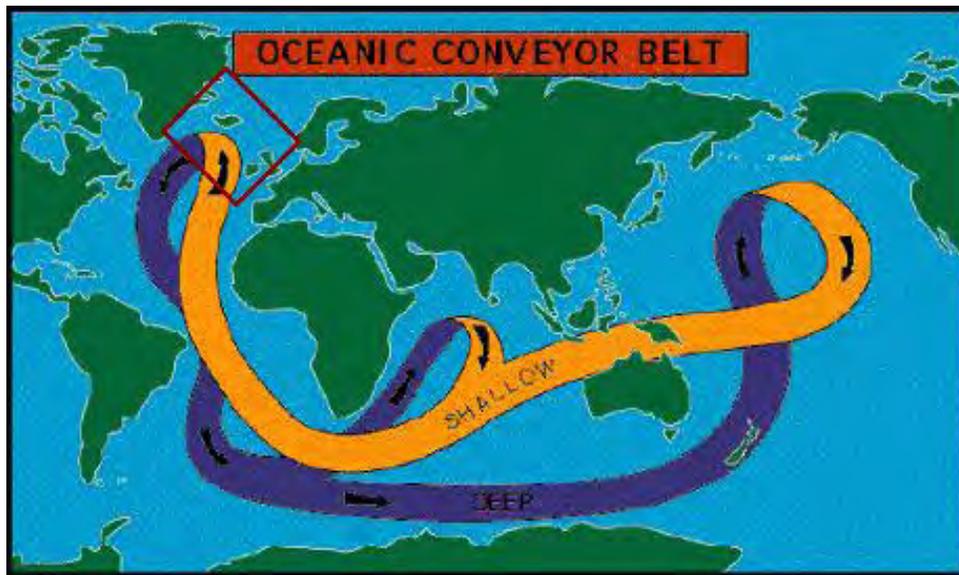
Figure 4. Thermohaline circulation, shown here, is important because breakdowns in thermohaline circulation have occurred during relatively rapid changes in climate. The boxed area in the upper left identifies the Denmark Strait overflow region where three-dimensional, non-hydrostatic effects cause serious drifts from observations in the first 10% of a 1000-year simulation. (Figure courtesy of Los Alamos National Laboratory)

Current mathematical and computational strategies include the following:

- Novel stochastic models for unresolved features of tropical convection.

- Hydrostatic/local non-hydrostatic hybrid models must be developed.

- Embedding cloud-resolving models within global climate model grid cells

- Systematic mathematical methods for low-dimensional stochastic mode reduction in climate.

- Uncertainty quantification in ensemble predictions and loss of information in coarse-grained stochastic models through information theory.

- Adaptive Multifrequency Methods for deriving new sets of adaptive equations. Multiscale, multifrequency decompositions concatenate into a chain of maps depending on successively faster time scales to produce new, hierarchical sets of equations.

Some of the near-term multiscale challenges in climate modeling include:

- Multiscale tropical modeling of cloud circulation and microphysics resolved at scales between 1 and 10 km, coupled with global circulation resolved at scales between 100 and 10,000 km

- The scale up of microphysics models (~nm) to subgrid models (< m) to bulk scale property models (~km)

- The blending of hierarchical Bayesian statistical models for observations and stochastic modeling strategies for practical parameterization

- The use of information theory to quantify information flow among components of comprehensive and reduced models and to quantity their uncertainty.

3.3 Materials Science

The design and control of material properties is a core component of many DOE programs. Materials science plays a central role in nuclear applications, the hydrogen economy, and nanotechnology. A partial list of materials needs of current interest to DOE includes:

- Materials for fusion and next-generation fission reactors including materials resistant to harsh radiation environments

- Soft materials for chemical and biosensors and for actuators (for example, pi-conjugated polymers and self-assembled structures)

- Materials and processes for nuclear waste disposal including ion transport and exchange in cage materials and aqueous environments

- Materials and chemical processes for clean energy sources, for example, materials for hydrogen storage and fuel cells

- Nanoscale-tailored materials for high-strength materials, nearly frictionless surfaces, environmentally friendly materials, field emission flat panel displays, chemical sensing, drug delivery, and nanoelectronics

- Micelles for use in remediation, synthesis, solvent technology, and turbulent drag reduction.

Arguably, the remarkable challenge faced by materials science and engineering in the 21st century will be associated with materials design. The reason is straightforward: development times for introducing new materials into complex systems have become prohibitively long compared with all other components of multidisciplinary optimization associated with engineering design. The consequence has been a reduced driving force for materials innovation except in the most highly constrained problems.

Better understanding of fundamental processes such as deformation, fracture and failure, grain boundary growth and migration, phase changes, and electronic and transport phenomena that occur on multiple scales will require new mathematical tools and techniques. For the design and study of nanoscale materials and devices in microscale systems, models must span length scales from nanometers to hundreds of microns (see Figure 5). Such systems consist of billions of atoms, which is simply too large for molecular dynamics simulations yet too small to be modeled with continuum methods. Hence, coupled multiscale methods are urgently needed to support the design of microscale and future nanoscale systems and processes, and a range of simulation tools must be available to designers just as macroscopic scales are available today. For example, extensions to G-closure and mathematical tools for deriving classes of solutions to inverse problems have been suggested as possible approaches toward revolutionizing composite design. Composite design is a long-standing problem associated with multiscale analysis, and the basic frameworks and capabilities for such multiscale simulation methods and
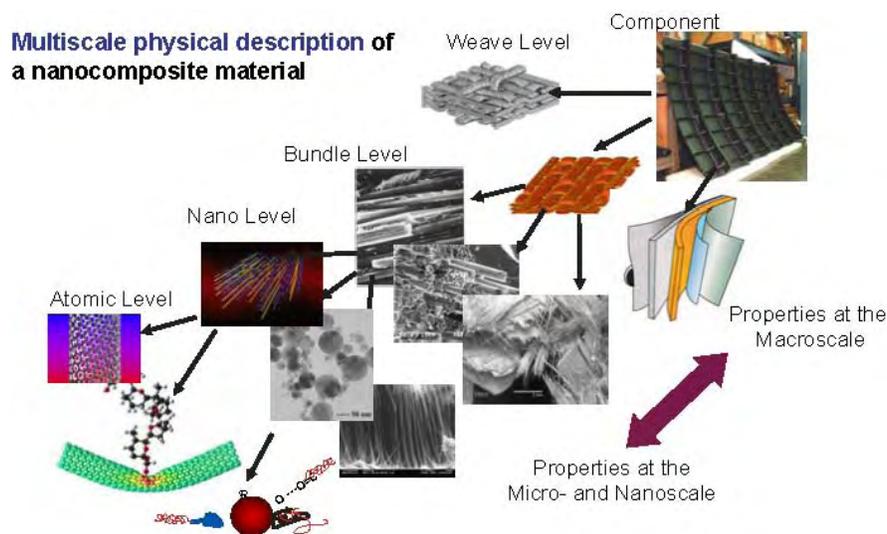
Figure 5. Illustration of scales involved in modeling a nanocomposite material. (Figure courtesy of Mark Shepard)

software are not yet available. Considerable basic research is required to establish the foundations for mathematical frameworks, algorithms, and modeling and their related software.

The basic equations describing the structure, thermodynamics, and transport of many complex fluid and soft matter systems such as micelles, foams, gels, and other self-assembling systems require a significant investment of applied mathematics to advance the science and technology. While progress has been made at each length and time scale of description of these systems, we are still at the stage where simplistic continuum mechanical principles are used at all scale models, e.g., stochastic molecular dynamics, kinetic Smoluchowski equations, mesoscopic scale-up, and continuum mechanical approaches. Dumbbell and multibead-spring idealizations are still the state of the art in stochastic models of long chain polymers in dilute solutions. For nematic polymer nano-composites, the molecules are idealized as rigid, monodisperse, and uniformly dispersed spheroids. All of the approximations inherent in these approaches must be relaxed to model more realistic polymer and nano-composite systems.

While microscale and nanoscale systems and processes are becoming more viable for engineering applications, our knowledge of their behavior and our ability to model their performance remains limited. Furthermore, nanoscale components will be used in conjunction with components that are larger and respond with different time scales. In such hybrid systems, the interaction of different time and length scales will play a crucial role in the performance of the complete system. Computational capabilities that span the scales from the atomistic to continuum need to be developed. These capabilities should include a variety of tools, from finite element methods to lattice mechanics, statistical dislocation dynamics, molecular dynamics, and quantum mechanics, among others, to provide powerful multiscale methodologies.

3.4 Combustion

Combustion of fossil fuels provides over 85% of the energy required for transportation, power generation, and industrial processes. World requirements for energy are expected to triple over the next 50 years. Combustion is also responsible for most of the anthropogenic pollution in the environment. Carbon dioxide and soot resulting from combustion are major factors in the global carbon cycle and climate change. Soot, NOx, and other emissions have important consequences for both the environment and human health. Developing the next generation of energy technologies is critical to satisfying growing U.S. energy needs without increasing our dependence on foreign energy suppliers and to meeting the emissions levels mandated by public health issues.

Figure 6. Low swirl burner prototype. The burner's novel flame stabilization mechanism allows it to operate at lean conditions with very low emissions. (Photo courtesy of R. K. Cheng)

Lean, premixed combustion technology (see Figure 6) provides a simple example of the basic scale issue. We know that if we burn methane near the lean flammability limit we can produce high-efficiency flames that generate almost no emissions. Unfortunately, we also know that a lean premixed flame is much more difficult to control. The stability of such a flame is

governed by the interplay of acoustic waves on the scale of the device with turbulence scales on the order of millimeters and a flame front with dimensions measured in hundreds of microns. This interaction of scales spans six decades in space and an even larger range of scale in time. Although the combustion community has a long tradition of using simulation, current modeling tools will not be able to meet the challenge. The standard Reynolds averaged Navier-Stokes (RANS) methods currently used for full-scale simulations approximate only the mean properties of the system, with turbulent motions and fluctuations modeled across all scales. They are inherently unable to predict the behavior of systems with the fidelity required to develop new energy technologies. Direct numerical simulation approaches that use brute-force computing to resolve all of the relevant length scales can provide accurate predictions, but their computational requirements make them unusable for realistic systems.

One area where new approaches are critically needed is the turbulence closure problem. In nonreacting flows, turbulence is characterized by an energy cascade to small scales where dissipative forces dominate. Large-eddy simulation approaches based on assumptions about scaling behavior and homogeneity of the flow at small scales have made substantial progress in modeling turbulent flows. When the flow is reacting, the closure problem becomes considerably more complex. The turbulent energy cascade again transfers energy to small scales, but these small-scale eddies interact with the flame front to modulate the energy release. This energy release from the combustion process induces a strong coupling to the fluid mechanics. As a result, the details of the small scales play a much more important role than in the nonreacting case. Furthermore, the acceleration of the fluid as it passes through the flame destroys the homogeneity properties implicit in many closure schemes. For reacting flows, what is needed is not simply a turbulence model but a model that also captures the interaction of turbulence and chemistry.

The need to predict the stability and detailed chemical behavior of a turbulent reacting flow for systems spanning a broad range of scale in space and time is fundamental to developing the tools needed to design new combustion technologies. A number of approaches have been presented in the combustion literature for dealing with turbulence-chemistry interaction, but they are typically based on a phenomenological model for the dynamics or implicitly assume some type of separation between the flame scales and the turbulent eddy scales. Developing more rigorous approaches to the turbulence-chemistry closure problem is a daunting task, but the potential payoff for combustion simulation is enormous.

3.5   High Energy Density Physics

The DOE/National Nuclear Security Administration laboratories are concerned with high energy density physics for the obvious reason that high energy density physics governs energy release in thermonuclear weapons. Astrophysicists are also interested in this subject because Type Ia and Type II (core collapse) supernovae are the source of much of the heavier nuclei in the universe. Additionally, Type Ia supernovae are the "yardsticks" that allow us to measure the size and age of the universe and help constrain the amount of "dark energy" in it.

High energy density physics lies at the rich juncture between the physics of the very small (e.g., nuclear and particle physics) and the very large (e.g., the physics of the early universe). The range of spatial and temporal scales on which physically relevant phenomena occur can be enormous. Type Ia supernovae exhibit scales ranging from the dimensions of the parent white dwarf star ($\sim 10^8$ cm) to the thickness of a nuclear "flame" in the deep stellar interior ($\sim 10^{-4}$ cm); similarly, time scales range from millennia (characterizing the slow onset of convection in pre-supernovae white dwarfs) to seconds (the time scale of incineration of an entire white dwarf). Models of these supernovae must include photon and neutrino

transport, nuclear combustion rates, and relativistic regimes. High energy density physics is characterized by many multiscale behaviors including compressible turbulence and turbulent mixing as well as complicated couplings between behaviors such as turbulence and gravitational stratification, turbulent mixing and radiation transport, and couplings between dynamically generated, turbulent magnetic fields and charged particle flows.

In some situations, such as radiation-driven plasmas in the photosphere or chromosphere of a star, local thermodynamic equilibrium (LTE) cannot be assumed. In this case, material properties cannot be tabulated, but must be computed "on the fly," which requires a multiscale approach. Loss of LTE can occur nonuniformly in space, in which case the connection between the "observables" and local physical properties becomes complex. A clear understanding of the physical models used in simulations is essential to understand what is being observed.

Better photon, neutrino, and particle transport simulations are needed. Regions of both large and small optical depth are commonly encountered in the same physical system; in the former, the diffusion approximation is appropriate, whereas free streaming is appropriate in the latter. Of paramount concern is the physical interface between these two regimes where neither limit applies—often a key element in determining the physical behavior of the system. A further complicating factor is that material in stars can become opaque at restricted frequencies while remaining optically thin at others—a situation that can occur even at the same location in space, with orders of magnitude differences in opacities. Better models are also needed for compressible turbulence (including reactive and stratified flows) and turbulent mixing, magnetic turbulence including the effect of charged particles, and turbulent mixing coupled to radiation transport.

For stars, better transport simulations are important not only for getting the physics right in the stellar interior, but for predicting what emerges from the star to affect neighboring objects or to be collected by telescopes, and for properly using the emergent radiation to infer the interior physical properties of the star. A similar argument can be made for laser or particle beam target physics for which radiation acts both as an active participant and as a diagnostic tool for inferring the physics governing the collapsing target.

The extension of the combination of adaptive mesh refinement, front-tracking, and low-Mach number models to the case of nuclear burning in supernovas (see Figure 7) could enable computation of the large-scale, long-time dynamics of processes that lead to the explosion of a type 1A supernova and are believed to determine its later evolution.

3.6 Fusion

The development of a secure and reliable energy source that is environmentally and economically sustainable is one of the most formidable scientific and technological challenges facing the world in the 21st Century. The vast supplies of deuterium fuel in the oceans and the absence of long-term radiation, CO_2 generation, and weapons proliferation make fusion the preferred choice for meeting the energy needs of future generations.

The international ITER experiment is scheduled to begin its 10-year construction phase in 2006. The United States has a clear opportunity to take the lead in the computational modeling of this device, putting
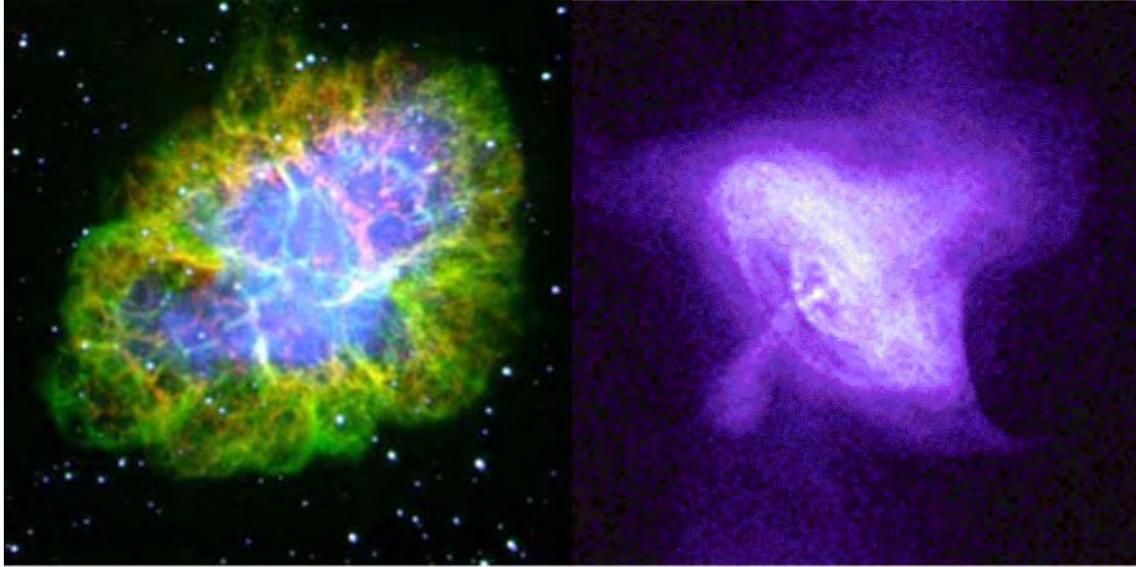
Figure 7. Images of the Crab nebula (seen in the optical, left image) and the core of this nebula at the site of the pulsar (seen in the X-ray by NASA's Chandra X-ray satellite, right image). This supernova remnant, located ~6000 light-years from Earth, contains highly relativistic electrons together with magnetic fields. The X-ray image scale is roughly 40% of the optical image. The pulsar and the surrounding optical nebula are characterized by physical processes that span a dynamic range of spatial scales from ~6 light years down to meters and centimeters and are the consequence of physical processes in which radiation hydrodynamics were essential (Image courtesy of NASA and the Chandra Science Center)

us in a strong position to influence the choice of diagnostic hardware installed and the operational planning of the experiments, and to take a lead in the subsequent phase of data interpretation. Furthermore, a comprehensive simulation model such as is envisioned in the Fusion Simulation Project is considered essential in developing a demonstration fusion power plant to follow ITER, by effectively synthesizing results obtained in ITER with those from other nonburning experiments that will evaluate other magnetic fusion energy configurations during this same time period.

In addition to magnetic fusion, there is an active program in Inertial Fusion Energy within the Office of Fusion Energy Sciences that encompasses both driver research and target design. Multiscale issues for drivers are also numerous. For example, to simulate ion beams in the presence of electron clouds, one must account for timescales ranging from the electron cyclotron period in quadrupole focusing magnets ($\sim 10^{-12}$ seconds) to the beam dwell time (up to 10^{-4} seconds).

In magnetic fusion experiments, high-temperature (100 million degrees centigrade) plasmas are produced in the laboratory to create the conditions where hydrogen isotopes (deuterium and tritium) can undergo nuclear fusion and release energy (the same process that fuels the sun and stars). Tokamaks and stellarators are "magnetic bottles" that confine the hot plasma away from material walls, allowing the plasma to be heated to extreme (thermonuclear) temperatures so a fusion reaction will occur and sustain itself. Calculating the details of the heating process and the parameters for which a stable and quiescent plasma state exists presents a formidable technical challenge that requires extensive analysis and high-powered computational capability.

A high-temperature magnetized plasma is one of the most complex media known. This complexity manifests itself in the richness of the mathematics required to describe both the response of the plasma to external perturbations and the conditions under which the plasma exhibits spontaneous motions, or instabilities, that take it from a higher to a lower energy state. We find it essential to divide the plasma response into different frequency regimes, or timescales, as illustrated in Figure 1. Widely different analysis techniques and computational approaches are appropriate for each of these different regimes.

RF analysis codes (Figure 1a) that work in the frequency domain aim to calculate the details of the heating process when an external antenna produces a strong RF field. Gyrokinetics codes (Figure 1b) solve for self-consistent transport in turbulent, fluctuating electric and magnetic fields. These codes average over the fast gyration angle of the particles about the magnetic field to go from a 6D to a 5D description. Extended magnetohydrodynamic (MHD) codes (Figure 1c) are based on taking velocity moments of the Boltzman equation and solving the 3D extended MHD equations to compute global (device-scale) stability and other dynamics. Transport timescale codes (Figure 1d) use a reduced set of equations that have the Alfven waves removed. These are used for long-time scale simulation of plasma discharges. They require the inclusion of transport fluxes from the turbulence calculations. The edge physics associated with the transport codes presents its own set of turbulence and MHD issues as well as atomic physics and plasma-wall interactions.

These codes could be improved by coupling and expanding the time and space scales covered by the simulations in the gyrokinetic simulations, incorporating spatially adaptive methods in the RF simulations, developing techniques for resolving small reconnection layers and including dispersive waves in the fluid equations for the MHD codes, and coupling the codes for the interior of the plasma with the edge in transport timescale codes. In general, an emerging thrust in computational plasma science is integrating the now separate macroscopic and microscopic models and extending their physical realism by including detailed models of such phenomena as RF heating and atomic and molecular physical processes (which are important in plasma-wall interactions).

Increasingly, it is being recognized that to address some critical scientific issues of fusion research, it is necessary to treat the interactions between different plasma processes and different time/space scales together that previously have been studied as separate subdisciplines of fusion science. The objective is to provide a truly integrated computational model of a fusion experiment that will enable plasma scientists to develop an understanding of these amazingly complex systems.

3.7 Biosciences

Numerous DOE applications require multiscale modeling, given that many of the department's needs in bioscience are focused on understanding the role that bacteria play in affecting large-scale environmental changes such as carbon sequestration, environmental remediation, and production of energy from biomass. Earth's environment is tightly coupled not only to human activity but also to the entire spectrum of living organisms. As we begin to build a large knowledge base of the fundamental molecular processes that drive biology, we wish to understand how the effects propagate through length and time scales to affect the world we live in.

Figure 8 shows an example of how research focused on many length scales is needed to solve a problem such as carbon sequestration up to the cell community scale. One needs the genetic information (Box 1)
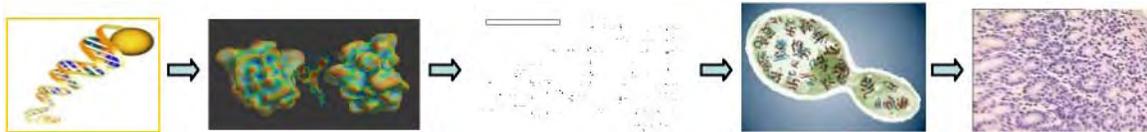
Figure 8. Multiscale models of carbon sequestration from genes to metabolic networks in cell communities. Genetic information from Box 1 (cyanobacteria) drives understanding of the molecular machines driving important cell processes (Box 2), which then drives the creation of metabolic networks describing how the individual molecular machines interact to extract carbon dioxide from the atmosphere and convert it to a simple sugar (Box 3). These networks describe the inner workings of the cell (Box 4). Many of these cells and others working together ultimately help describe the impact of the cyanobacteria on the global carbon cycle (Box 5). (Figure courtesy of the First Multiscale Mathematics Workshop report)

of a typical cyanobacteria such as Synechococcus or Procholorococcus (both of which are being studied in the DOE Genomics:GTL program) to drive the understanding of the molecular machines (Box 2) that drive important processes of the cell. This, in turn, drives the creation of metabolic networks (Box 3) that describe how the individual molecular machines interact to take carbon dioxide out of the atmosphere and convert it to a simple sugar that can be used to drive metabolic processes. Taken as a whole with additional spatial information, these metabolic networks describe the inner workings of the cell (Box 4). But even further, it is the collection of many of these cells and other cells working together (Box 5) that ultimately helps to describe quantitatively the impact of these bacteria on the global carbon cycle. Understanding this overall problem means not only understanding each level but developing methods to couple these different levels efficiently.

In the biosciences, multiscale issues arise not only in the "vertical" sense of processes occurring at different length and time scales but also in the "horizontal" sense within each level. In this horizontal scaling, the variables that span many scales are not strictly time and space variables but are other descriptors that define the phase space of the components. For example, the network that drives the biochemical interactions within the cell incorporates widely differing scales. Molecular machines are very large macromolecules that often have an interaction site that involves only a handful of atoms with many of the scaffold atoms relatively fixed. Even large colonies of bacteria often are most stable with a very large number of one type and a very small number of others. The important unifying theme in all of these processes is that there are only a vanishingly small number of biologically realizable ensembles. Biological science also has a distinguishing characteristic that separates it from other applications. It has a wealth of evolutionary "constraints" that can vastly reduce the potential amount of space that must be explored to find the correct solution to the biological problem at hand. These constraints need to be understood and incorporated at all scales so that we take advantage of nature's work to produce what are generally very nonrandom systems.

DOE's use of microbial communities for metal reduction makes accurate metabolic models over a range of time and space scales a problem of practical importance. A community or ecosystem comprises largely asynchronous processes that are not accurately characterized by the use of sequential programming schemes. Coordination over many timescales will be required to predict long-term behavior. As with many types of multiscale phenomena, the macroscales exhibit regular behavior while the subscales differ dramatically from the average. In particular, the average metabolism of a community

is significantly different from that of any one individual. This is true even among genetically identical populations, as organisms with the same genotype can exhibit different responses to the same environmental stimuli.

The diverse nature of the data that describe biological processes is driving the need for a computational infrastructure that can store and exchange multiscale data. An example is the broad types of calculations (homology, structural similarity, molecular energy minimization) that go into a single problem of predicting protein structure. Experimental data range from molecular measurements to gross parameters of an entire system. There is a need not only for researchers to be able to catalog these data, but for modelers to be able to incorporate it in every level of their models and to visualize effectively the different scales of data that experiment and modeling produce.

Metabolic processes at the finest scales involve specific chemical reactions governed by physics. However, it is not clear whether metabolism at the organism or community level follows directly from first principles. Rather, there appear to be higher-level organizational principles at work. The ability to pose large-scale metabolic behavior as the solution of a non-convex optimization problem is desirable. In addition, effective coarsening and refinement schemes must take into account key microscale phenomena, such as electron transfer, along with metabolic pathway organization. Useful representations should also have the ability to characterize bifurcations and rare events within the macroscale community model.

In microscopic systems formed by living cells, small numbers of reactant molecules can drive macroscale dynamics, requiring discrete, stochastic models. New time-acceleration methods are needed because standard stochastic simulation is prohibitively inefficient for most realistic problems. Reliable and efficient means to partition the system into discrete stochastic and continuous deterministic subsystems are needed, as well as new hybrid models to couple these subsystems in a multiscale computational framework. Additionally, the construction of efficient relaxation techniques that consider the multiscale structure of the inverse problem for biological systems is needed.

3.8 Chemistry

Chemistry is one of the central sciences and a critical element of many of the applications important to DOE, in addition to having its own intellectual merit. An understanding of the structure, interactions, and reactions of molecules is of critical importance to a wide range of phenomena, from the fate of contaminants in the environment through the production of plastics from crude oil to the occurrence and treatment of genetic diseases. By integrating chemical capabilities in the areas of synthesis and characterization with computational modeling and simulation, it will soon be possible to use computation to design molecules that are optimized for both certain preselected properties and the processes used to synthesize them. This will lead to chemicals and materials that are both highly suited to selected applications and inexpensive and efficient to make. Central to these anticipated advances in our computational capabilities are solutions to multiscale mathematical and algorithmic problems that inevitably arise within a discipline that strives to control chemical, electronic, and material processes in complex environments by manipulating the basic building blocks of matter.

Chemistry asks questions at many length and time scales ranging from the electronic and atomic (e.g., plasmas and vapor deposition), molecular (e.g., chemical reactions), to the nano (e.g., nanostructured catalysts and devices, protein folding) and macro (e.g., chemical, biological, and material properties, multiple phases). However, our fundamental understanding exists only at the finest scale—the quantum

theory of matter from which we can directly predict the electronic structure of atoms and molecules as well as chemical reaction dynamics. Thus, the multiscale problem in chemistry requires bridging from the quantum to the classical as well as spanning a wide range of length and time scales. For example, proteins are characterized by a broad range of time scales. Accurate simulations of proteins currently must follow motions that occur on timescales comparable to molecular vibrations thus dictating a timestep of around a femtosecond. However, many of the phenomena of most interest in understanding the biological significance of proteins, such as protein folding, ligand binding, and signaling pathways, often occur on timescales that are many orders of magnitude longer. In between these two timescales are a spectrum of interesting motions consisting of side-chain wags, chain bending, breathing modes, etc. that all contribute to the overall dynamics of the system. At present, there is no clear understanding of how to integrate out these fine-scale motions to obtain accurate predictions of the large-scale behavior at long times.

Similar problems occur in understanding chemical reactions in extended systems such as catalytic reactions at the surfaces of materials (both nano and macro scale). Understanding at a quantitative level requires very accurate computations of the thermochemical and kinetic properties of reactions which have distinct consequences on larger space and time scales as well as on other chemical reactions in the system. The complex interdependencies of reactions involved in different interfaces, such as surface and step faces, are also required to understand how these processes occur in the real world as opposed to the virtual world. Adding additional environmental effects, such as a liquid environment, further complicates the multiscale issues.

Current approaches to solving multiscale problems in chemistry are in the early stages of development. Significant research areas include the search for linear scaling methods for solving ab initio quantum problems, the development of reduced or approximate quantum methods for solving larger problems, and the development of multiresolution analysis for eliminating the use of traditional basis sets in ab initio quantum chemistry. The combination of quantum mechanical calculations with classical atomistic simulations (hybrid methods) is also the focus of much recent work, with the goal of successfully modeling reactions and catalysis in complex environments when only a small region needs to be described quantum mechanically. This is being actively pursued in the area of enzymatic catalysis, cell signaling mechanisms, and the study of reactions in complex environments. The quasicontinuum method is an extension of this approach that seeks to connect atomistic simulations to continuum descriptions. This is being used to model the behavior of defects, the formation of quantum dots, and to develop atomic level descriptions of fracture.

Much work remains to be done in many of these areas. There is a need to quantify error and provide systematic improvement. Better mechanisms are needed for coupling quantum mechanical and classical simulations and understanding the errors associated with the coupling, along with methods for coupling different levels of quantum mechanical theory in a single calculation. The quasi-continuum method must be generalized from the current static descriptions to ones that are applicable at finite temperature. Mechanisms for dynamically switching to an alternate model when assumptions about the current model are no longer valid are needed in a wide variety of reaction simulations. Quantification of uncertainty in a simulation or model also connects directly to the challenge of meaningful simulation of poorly characterized systems. Inevitably, many multiscale simulations involve multiphysics, and we must advance beyond current ad hoc and unsatisfactory models for coupling high- and low-levels of quantum theory and embed these in atomistic and continuum models. Improved methods for sampling rare events

(critical to many chemical processes) need to be further developed, particularly for events in highly anisotropic systems characterized by broad distributions of time scales.

There is also the need for analysis-based methods in quantum chemistry to improve scaling for dimensional-reduction problems such as coupled-cluster corrections that represent the effect of interparticle interactions. The introduction of real-space hierarchical representations of these corrections that represent the smooth nonlocal coupling by an appropriately small number of computational degrees of freedom could lead to a computational method that would enormously increase the range of problems that could be computed.

3.9   Power Grid and Information Networks

Many systems of critical importance to DOE are most naturally or can only be modeled by networks (or graphs). A partial list includes biological systems (viewed at various levels), microbial communities, protein interaction networks, social networks, epidemiology, traffic networks, and designed technological networks (e.g., power distribution, communication networks, sensor/actuator networks, robotic networks, etc.). The behavior of these networks has important implications for energy distribution and consumption, waste remediation, security, telecommunications, and manufacturing.

Descriptive models of network systems have potential value for many problems of interest. However, these models are by no means the only approach to understanding large-scale networks, nor are they always helpful is their study. An alternative, although mathematically equally challenging, class of ab initio models serve an important function in providing the basis for rigorous and profound insights into the behaviors of networked systems. While equations of state are descriptive and can be derived by careful analysis of data collected about dynamic networks, they have the intrinsic limitation that they cannot tell us why the system behaves one way in one phase and another way is another phase. First, principal models of dynamic networks, such as those based on the interplay between entropy and conservation laws, can be an effective way of gaining necessary insights that explain otherwise unfathomable system behavior. These models certainly complement the descriptive equations of state, and indeed, should confirm them by demonstrating their derivation in the most common circumstances. However, ab initio models have the unique advantage of being able to describe how and why network systems behave as they do in the most unusual circumstances where the equations of state fails to accurately predict outcomes. In the context of large-scale engineered networks, this knowledge often is far more valuable, as it is often the surreptitious unusual circumstances (i.e., the rare event that seems outwardly no different that the common) that give rise to catastrophic system failures.

Multiscale issues arise in the modeling, analysis, and simulation of networks with respect to several dimensions: time, space (e.g., topology and geography), state (e.g., queues), and size (e.g., number of nodes, users). In many cases, these systems are dynamic in nature and consist of networks of networks with dynamic interactions. Localized or small magnitude forcing can cause large-scale responses. A noteworthy example is the August 2003 blackout in which an event at a single transmission line knocked out power to much of the northeastern United States and Canada. The mathematical analysis of networks is a relatively new area, and analysis methods are only beginning to be developed and explored. The analysis of these systems will require new methods and also extend ideas from more established areas of multiscale analysis. Mathematical areas that are clearly relevant are graph-based algorithms, combinatorial optimization, discrete event simulation, agent-based simulations, scaling, and ideas developed from continuum modeling of multiscale systems.

One example is communication networks, although many of the issues are also common to other types of networks including power distribution, agent-based, sensor/actuator, and robotic networks. A communication network is a collection of communicating devices connected via communication links. Such devices include computers, phones (wired and wireless), laptops and PDAs, and sensors. Communication networks are multiscale in nature by design. The dominant design paradigm in networking is the hierarchical (layered) architecture. Moreover, the topological arrangement of networks is also typically hierarchical (e.g., the Internet). Finally, general-purpose networks such as the Internet are heterogeneous both in their infrastructural components and in the nature of the traffic that traverses them. All these factors work together to form multiscale phenomena.

Events on networks such as the Internet take place on a variety of time scales. Packet transit times are often in microseconds, file transfers take seconds, routing table updates take minutes, and significant network topological changes may take days. A variety of approaches have been brought to bear on this issue including self-similarity, long-rage dependence, power laws and heavy tails, multifractals, cascades, wavelets, and highly optimized tolerance. It turns out that in the time scale, scaling features are observed. In addition, the topology of the Internet has scaling features. Interest in scaling features like those described above amount to a concern that such features have impact on the design and performance of networks. Within the framework of scaling laws, it is possible to answer questions such as: As the number of nodes in a network increases, how does the capacity that it can support grow? It is also of interest to characterize how different performance metrics are related in scaling laws. For example, is it possible to trade off capacity for delay performance, in terms of scaling laws? These questions have only recently begun to be addressed.

The need for appropriate mathematical models and frameworks has become clear as network researchers struggle to understand the complexity of these manmade systems. While traditional approaches common in networking research have focused on discrete mathematics, continuous techniques have come to the forefront to address issues such as scaling phenomena and large networks. Differential equations (whether ordinary, stochastic, or partial), which are widespread in models of natural systems, are now firmly established in the modeling of manmade networks. This is promising because it opens vast possibilities for many more researchers to contribute to solving the pressing problems in networks. In particular, topics in multiscale mathematics traditionally funded by DOE are now relevant to addressing problems in networking research. The successful marrying of these two areas will involve strategic collaborations and multidisciplinary efforts.

4   Roadmap

The Multiscale Mathematics initiative roadmap presented here culminates in a new foundation for multiscale mathematics and a new generation of multiscale software applied to comprehensive scientific simulations on problems of importance to DOE.

There is no doubt that there are individual projects and individual researchers that can make fundamentally important contributions to multiscale mathematics. Additionally, there is a strong need for new interdisciplinary research models; future progress on multiscale problems requires the efforts of interdisciplinary and multi-institution teams of researchers comprising mathematicians, scientists and engineers, and computer scientists. The success of multiscale mathematics requires appropriate interactions with the science domain experts to ensure the methods are relevant to the physics being modeled. The insight of physical modelers will be crucial in guiding the selection of algorithms within the class of multiscale methods best suited to the scientific questions and the development of multiscale correction indicators and adaptive control methods. Computational and computer scientist and software specialist expertise is needed to ensure that methods meet the demand for software structures that can deal with multiple models and discretizations and can ensure computational efficiency, in particular for adaptive methods as models and discretizations are adapted during the simulations. The demands of algorithms and associated software structures become even more significant when considering that most of these simulations will need to be run on large-scale distributed memory parallel computers. The practical, problem-solving orientation of the DOE mission places it in a unique position to encourage the interdisciplinary activity that is required to get the job done.

<u>Near-term milestones.</u>   Over the first 3–5 years of the program, the principal milestones will be the application of existing techniques to new multiscale problems and the development of new algorithms for stochastic models. Early successes will guide development of new methods.

- Better mathematical understanding of a broad range of multiscale systems. Improved error estimators, stability and robustness analysis, performance metrics (upper/lower bounds).

- Development of existing multiscale techniques that have previously demonstrated correct representation of some important multiscale behavior for application to new multiscale problems, with accurate, efficient, stable simulations.

- Development of multiscale stochastic numerical methods and uncertainty quantification techniques as a foundation for the later development of the entire program. Existing methods for deterministic models require significant modification to apply to stochastic models.

- Mathematical and numerical analysis of the coupling between scales in multiscale problems susceptible to analysis using current state-of-the-art analytical tools, combined with a robust numerical experimentation capability, as a basis for developing new multiscale algorithms and new extensions to the mathematical tools.

- Precisely defined benchmark problem set focused primarily on the mathematics (rather than the physics) of multiscale problems.

- Evaluation of novel, high-risk concepts.

Medium-term milestones. In a 5–7 year time frame, we will see the development of entirely new techniques both in analysis and simulation for multiscale problems as well as the availability of major components of software infrastructure.

- Prototype simulations using the new multiscale methods, developed in the near-term, applied to DOE target problems arising in multiscale science.

- New multiscale mathematical methods developed and used to derive multiscale models for some of the "difficult" cases in multiscale science; e.g., problems without strong scale separation, rare event problems, reduction of high-dimensional state spaces to a small number of degrees of freedom, and discrete-to-continuum physics (identifying the point of transition).

- Algorithms and software for multiscale sensitivity and uncertainty analysis.

- New methods in statistical analysis to identify critical/essential drivers of coupling between scales.

- Software for core components of multiscale algorithms.

- Algorithms that have incorporated improved error estimators, stability robustness, performance metrics (upper/lower bounds). Speedup of multiscale calculations.

- Algorithmic verification.

Long-term milestones. In a 7–10 year time frame, we will see the impact of the program on DOE science applications by means of a new generation of multiscale simulation techniques.

- Comprehensive scientific simulations using new multiscale techniques; models and software in widespread use.

- Application of these new methods to solve some of the outstanding hard problems in multiscale science; e.g., aspects of fluid turbulence and protein folding.

- A new generation of robust and adaptive mathematical multiscale software with metrics to quantify deterministic error and stochastic error (uncertainties).

- Algorithmic validation against complex physical systems.

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