

**Report of the First Multiscale Mathematics Workshop:
First Steps toward a Roadmap**

Transmittal

July 30, 2004

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

Dear Dr. Johnson:

I am pleased to deliver, on behalf of nearly 100 contributing computational scientists from leading universities, Department of Energy laboratories, and other federal agencies, the report *Report of the First Multiscale Mathematics Workshop: First Steps toward a Roadmap*.

There is an urgent need for investment in the area of multiscale mathematics. This report identifies compelling scientific problems from areas as diverse and important to DOE missions as environmental and geosciences, materials, and combustion, to high energy-density physics, and to the biosciences that are facing major roadblocks due to multiscale modeling needs. It then outlines the components of a strategic plan for investment in multiscale mathematics to meet these needs.

It is an exciting time in science and technology. The rapid advances in recent years in understanding and design at the very small scales have the potential to have an enormous impact on the macroscale world in which we live. Yet at present we have no means of translating fundamental, detailed scientific knowledge at the small scales into its effects at larger scales. Without the capability to “bridge the scales,” important scientific and engineering problems will remain out of reach for the foreseeable future.

The Department of Energy has played a pivotal role in developing the scientific computing infrastructure that now enables the routine solution, in academia, government and industry, of a great many problems for scientific discovery and engineering design. The next generation of problems offers payoffs that are enormous, along with a daunting set of challenges. We urge the Department to seize the opportunity!

Best regards,

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Executive Summary

Science and technology are on the brink of a revolution. Physical processes at exceedingly small scales of time and space are becoming increasingly well understood. Technologies for engineering systems at the micro and nano scales are rapidly emerging. Yet in general we have no means of translating fundamental, detailed scientific knowledge at small scales into its effects on the macroscopic world in which we live. Without the capability to “bridge the scales,” important scientific and engineering problems will remain out of reach for the foreseeable future.

Mathematical modeling and computational simulation have reached the point, following 30 years of exponential advances in modeling, algorithms and computer hardware, where simulation of most physical processes over relatively narrow ranges of scales has become an essential tool for both scientific discovery and engineering design. But currently we do not have a mathematical framework and software infrastructure for the integration of heterogeneous models and data over the wide range of scales present in most physical problems. Fundamentally new mathematics and considerable development of computational methods and software will be required to address the challenges of multiscale simulation.

Nearly 100 of the nation’s leading computational scientists gathered in Washington, D.C., on May 3–5, 2004, at a workshop to consider the scientific needs and mathematical challenges for multiscale simulation. The computational scientists participating in the workshop included those who are primarily natural scientists—physicists, chemists, geologists, biologists—as well as computational mathematicians and computer scientists. They were asked to (1) identify the most compelling scientific applications that are facing major roadblocks due to multiscale modeling needs and (2) formulate a strategic plan for investment in multiscale mathematics research that will meet these needs. The results, including the potential impacts for areas of science ranging from environmental and geosciences, materials, and combustion, to high energy-density physics and fusion, and to the biosciences, are summarized in this report.

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1. Introduction

Until recently, most of science and engineering has focused on understanding the fundamental building blocks of nature and on building components “from the ground up.” This effort has been enormously successful. We are now in a position to tackle an even greater challenge: to assemble and integrate this information so that we can reliably predict and design complex real-world systems. The potential payoffs are enormous, but the challenges are daunting. New ways of thinking in mathematics and computation will be required to “bridge the scales.”

The problem of multiscale simulation can be summarized as follows. Science and engineering have reached the point where the ability to simulate processes at very small scales of space and time is essential to furthering our understanding of macroscale processes. In many cases, models of the systems over specific scales have been developed and used successfully. But the ability to simulate *systems* does not follow immediately or easily from an understanding, however complete, of the component parts. For that, we need to know and to faithfully model how the system is connected and controlled at all levels. Currently, we do not have a mathematical framework and software infrastructure for the *integration* of heterogeneous models and data over the wide range of scales present in most physical problems.

The need for a multiscale simulation capability is pervasive in many areas of science and engineering, ranging from environmental and geo-sciences, to materials and combustion; from high energy-density physics and fusion to the biosciences. For example, Figure 1 shows the broad range of timescales—14 orders of magnitude or more—that come into play in modeling a burning plasma experiment for magnetic fusion. Widely different analysis techniques and computational approaches are appropriate for different subsets of the time or frequency domain. An emerging thrust in computational plasma science is the integration of the now-separate macroscopic and microscopic models and the extension of the physical realism of these models by the inclusion of such phenomena as radio-frequency (RF) heating and atomic and molecular physical processes (important in plasma-wall interactions), so as to provide a truly integrated computational model of a fusion experiment. Such an integrated modeling capability will greatly facilitate the process whereby plasma scientists develop 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.

Relevant timescales for a burning plasma experiment

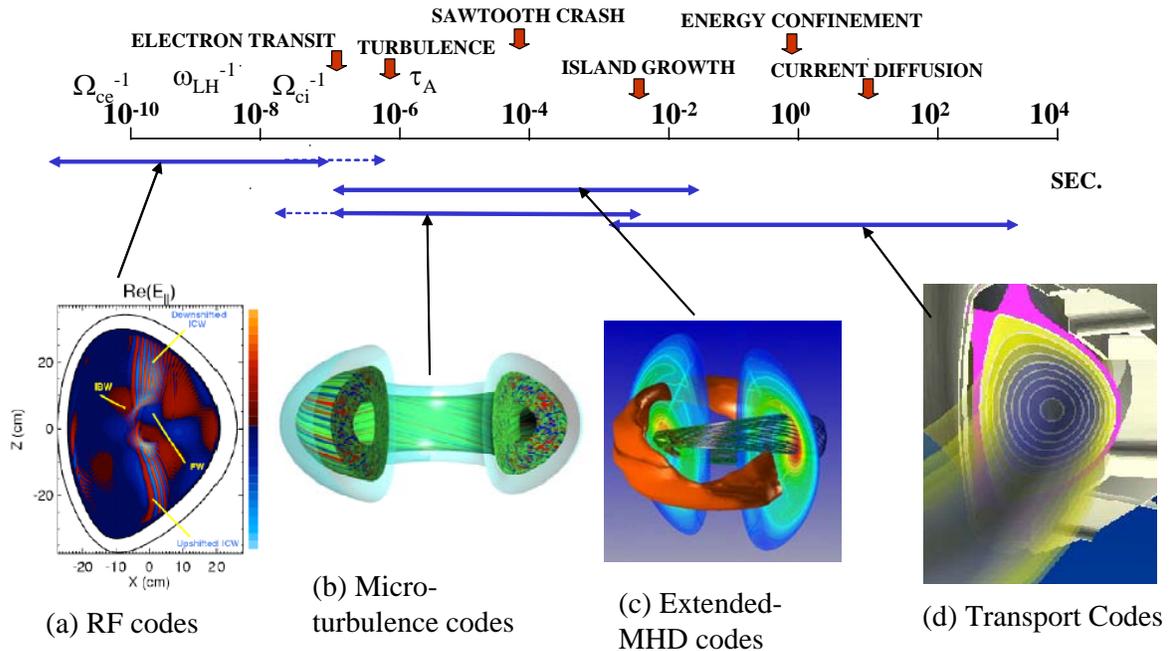


Figure 1. A broad range of timescales are involved in modeling a burning plasma experiment for magnetic fusion. The four parts of the figure illustrate the types of simulation techniques used over subsets of the time or frequency domain.

Another area where a multiscale simulation capability is urgently needed is in environmental science. Figure 2 is a schematic illustration of CO₂ sequestration. This problem involves the removal of atmospheric carbon dioxide and injection of this gas deep below the Earth's surface. The objective is to retard the return of this gas to the atmosphere, thus reducing its atmospheric concentration and reducing the rate of apparent global warming. Quantitative study requires the simulation of multiple fluids, a solid phase, and a complex set of biogeochemical reactions over spatial scales that range from the pore scale to hundreds of meters, and time scales that range from the rapid rate of certain geochemical reactions to the several decades over which the results of such simulations are of interest. The processes at the 100 m scale of surface and groundwater are strongly coupled with land vegetation, ecosystems and surface energy fluxes to the atmosphere (which itself is described using different scales). Once again, the simulations of processes at different scales are based on vastly different physical and mathematical models. Currently, simulations at the various scales use different types of computational methods involving problem descriptions and variables that are relevant only at those scales. In addition, much of this information is uncertain. There exists a great need to properly account for the effect of these uncertainties when simulations are used for decisions that affect public policy.

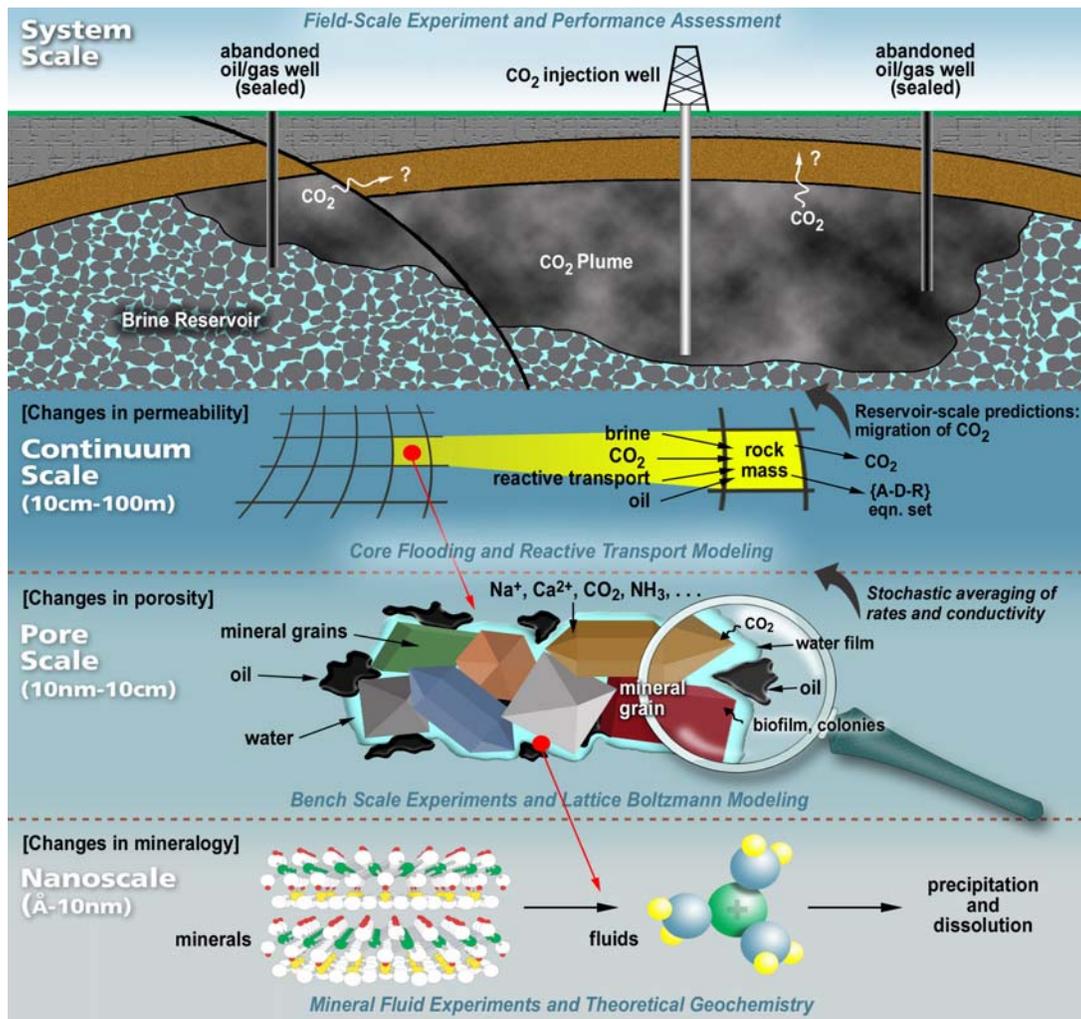


Figure 2. Multiscale nature of carbon sequestration. Simulations of processes at different scales are based on vastly different physical and mathematical models and computational methods. Much of the data at various scales is uncertain, yet decisions must be made that affect public policy. (Figure courtesy of Los Alamos National Laboratory)

Certainly, science and engineering have always involved processes that operate over a wide range of scales. What makes the need for multiscale modeling and simulation so compelling now? The answer lies in the fact that, until relatively recently, in most areas we have been hard-pressed to model processes accurately over even a narrow range of scales. Such a model requires an understanding of the fundamental physical processes operating at those scales, mathematical models that describe those processes, computational algorithms that realize the solution to those mathematical models, and

computing hardware capability that is up to the task. The past 30 years, however, has seen exponential advances in all of these areas. Indeed, advances in computational methods and in supercomputer hardware have each contributed 6 orders of magnitude to the speed of simulation – a total of 12 orders of magnitude! This speedup has been augmented by the development of new mathematical models that enable simulations in regimes that would otherwise still be inaccessible. Considering, in addition, our vastly increased base of scientific knowledge and data compiled over the same period, one can easily see why simulation is now often considered to be a peer to theory and experiment in scientific discovery and engineering design.

Yet even with these incredible capabilities, we are currently able to simulate most phenomena over only a relatively narrow range of scales. In general, we have no means of translating fundamental, detailed scientific knowledge at small scales into their effects on the macroscale world in which we live. Without the capability to “bridge the scales,” important scientific and engineering problems will remain out of reach in the foreseeable future.

Fundamentally new mathematics and considerable development of computational methods and software are required to address the challenges of multiscale simulation. An essential issue in resolving the coupling between models at different scales is how to derive the correct microscopic interface conditions that connect large scales to small scales or that connect a continuum model to a subgrid microscopic model. The coupling is not just a matter of tying together well-developed software at different scales. In many cases, the models and methods available at different scales need to be enhanced in order to provide the information required for informed, adaptive decisions across scales. Although considerable effort has gone into continuum modeling and simulation, often the methods are not equipped with the error estimators and infrastructure for adaptivity required for successful multiscale implementation. At the same time, subgrid models and algorithms are often not nearly as well developed and may require substantial improvements to be effective in the context of multiscale modeling and simulation. Rigorous mathematical analysis is required to quantify modeling error across scales, approximation error within each scale, and errors due to uncertainty in the models, and to address the well-posedness and stability of the overall multiscale model.

Stochastic processes are heavily used in modeling small-scale and mesoscale processes for a wide range of physical systems. These models may be either discrete or continuous. We need to understand how stochastic effects enter a physical system and how and when stochastic effects can fundamentally alter the properties of a system. Traditional Monte Carlo methods are robust but slow to converge, and their accuracy is poor, requiring many realizations to compute high-order moments with adequate resolution. The coupling of discrete stochastic models with continuous stochastic or deterministic models, where appropriate, would enable the simulation of many currently intractable problems.

2. A Multiscale Mathematics Research Program

In this section we discuss the technical objectives and core components 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.

2.1 Approaches

Three major approaches to the multiscale problem have been identified: *multiresolution discretization methods*, which resolve multiple scales within a single model system by dynamically adjusting the resolution as a function of space, time, and data; *hybrid methods*, which couple different models and numerical representations that represent different scales; and *closure methods*, which provide analytical representations for the effect of smaller, unresolved scales on larger scales in a numerical simulation that might resolve only the larger scales.

2.1.1 Multiresolution Discretization Methods

Multiresolution numerical methods include adaptive timestep methods for stiff ordinary differential equations, differential-algebraic systems, and stochastic differential equations; adaptive mesh refinement (AMR) and front-tracking methods for partial differential equations; and adaptive analysis-based methods for integral equations. Such methods are the subject of ongoing development in the mathematics community and have been used successfully on specific multiscale problems. Furthermore, these methods form, in large measure, the fundamental components from which more elaborate multiscale simulations will be built. Open questions in this area include the extension of AMR and front-tracking methods to a broader range of multiscale problems involving complex combinations of multiple physical processes; the development of new multiresolution-in-time algorithms for stochastic differential equations, particularly for the case of pure jump processes; and fast adaptive analysis-based algorithms for integral equations for problems with spatially varying coefficients. With such advances, we will be able to provide new capabilities for solving a variety of timely and important science problems for DOE.

The following are examples of science opportunities involving the development of new multiresolution discretization methods.

- *RF modeling in fusion problems.* Radio-frequency analysis codes calculate the details of heating the plasma as it is exposed to a strong electromagnetic field. Calculations indicate that the regions of high gradients are strongly localized in space; furthermore, the underlying solvers for the integral equations are based on dense matrix representations that do not take advantage of locality. The application of adaptive analysis-based methods to this problem could speed its

solution by 2–3 orders of magnitude and thus decrease the time spent in this phase of the design cycle for fusion reactors by months or years.

- *Supernova simulations.* The extension of the combination of AMR, front-tracking, and low-Mach number models to the case of nuclear burning in supernovas would enable computation of the large-scale, long-time dynamics of those processes which lead to the explosion of a type 1A supernova and are believed to determine its later evolution. For both type 1A and core-collapse supernovae, transport of photons and other particles is an essential component of the physics: it is the mechanism by which we observe and interact strongly with the multiscale structure of the system. However, the development of AMR for radiation is far less mature than it is for fluid dynamics, and new ideas will be required.
- *Stochastic dynamics of biochemical reactions.* In microscopic systems formed by living cells, small numbers of reactant molecules can result in dynamical behavior that is discrete and stochastic rather than continuous and deterministic. Accurate description of such behavior is impossible to obtain through deterministic continuous modeling (e.g., ODEs). Stochastic simulation has been widely used to treat these problems; however, because this procedure simulates every reaction event, it is prohibitively inefficient for most realistic problems. Recently, a coarser-grained approximate method called tau-leaping has been proposed for accelerated discrete stochastic simulation. A theoretical and computational framework for such accelerated methods is needed, along with reliable and efficient means to partition the system so that each reaction and species is modeled at the appropriate level.
- *Analysis-based methods in quantum chemistry.* A standard approach to the calculation of ground states and transitions to excited states is to begin with a Hartree-Fock wave function (a tensor product of single-particle wave functions) and to compute coupled-cluster corrections that represent the effect of interparticle interactions. Current methods for computing these corrections scale like N^6 , where N is the number of particles. 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 scales like N . This would enormously increase the range of problems that could be computed to chemical accuracy with such approaches.

2.1.2. Hybrid Methods

The starting point for the development of hybrid methods is typically an analysis of a general mathematical model that describes the system at all relevant scales. This analysis yields either a hierarchy of models each describing the behavior on a particular spatial scale with some overlap in the range of validity, or a splitting of the unknowns into components corresponding to slow and fast dynamics. Examples include the derivation of fluid equations as phase space averages of a more fundamental kinetic description and

deterministic chemical reaction models as averages over many discrete collisions. In hybrid numerical representations, the averaged dynamics, which are less costly to represent numerically, are used in regions where the deviations from those dynamics are small, while the more complete description is used in regions where the deviations from the averaging hypothesis—large mean-free paths in the kinetic/fluids example or sufficiently low concentrations of reactants in the chemistry case—are sufficiently large to have a substantial effect on the macroscopic dynamics. The assumption is that there is sufficient advantage to hybridizing two or more models, as opposed to using a single model that is more generally applicable.

Several areas of mathematical research arise in the development of hybrid methods. First, we are often confronted with models that were not designed for coupling with models on other scales or were not intended for use in simulations at all. In these cases, we will need to develop mathematically well-posed versions of the individual models and of the coupling between models on different scales. Second, we will need to develop stable and accurate discretizations for the individual models, and for the coupling between scales and models. This activity will almost certainly require the development of new numerical methods. For example, for many models, such as the kinetic models cited above, the finer-scale behavior is often represented by sampling a stochastic process (i.e., a Monte Carlo method). The coupling of such a method to a high-order accurate difference approximation can lead to a catastrophic loss of stability or accuracy, even though the component methods by themselves are well behaved. We also expect that hybrid methods will use the multiresolution methods described above as a source of components, and the need to hybridize them will lead to the development of new classes of such methods.

The following are examples of science opportunities involving the development of new hybrid methods.

- *Reaction and diffusion processes in cells.* A multiscale computational framework for the numerical simulation of chemically reacting systems, where each reaction will be treated at the appropriate scale, is clearly needed for the simulation of biochemical systems such as cell regulatory systems. The framework can be based on a sequence of approximations ranging from stochastic simulation at the smallest scales to the familiar reaction rate equations (ODEs) at the coarsest scales. The coupling is not straightforward, however, and must be done dynamically. Many technical issues are involved in ensuring that the system is properly partitioned, that the models chosen at each scale are sufficient to approximate those processes, and that the hybrid method itself is stable and accurate. Further complicating this problem is the need to incorporate spatial dependence, leading to the coupling of stochastic simulation with PDE models that will eventually need to distinguish and model the highly heterogeneous structures within a cell.
- *Macroscopic stability in tokamaks.* The appropriate description of the macroscopic dynamics of a burning plasma is a spatially heterogeneous

combination of fluid and kinetic models, which operate on time scales ranging from nanoseconds to minutes. To perform predictive simulations for such problems will require the development of a variety of hybrid simulation capabilities. Examples include state-space hybridization of a kinetic description of weakly collisional energetic particles produced by fusion with a fluid description of other species and spatial hybridization of two-fluid and kinetic treatments of localized plasma instabilities with large-scale fluid models.

- *Catalytic surface reactions and the synthesis and oxidation of particulates.* Chemical reactions at a gas /solid interface are not well modeled by continuum equations. Such reactions must be modeled at the atomistic level; and integrating their treatment into a continuum simulation will require hybrid discretizations that couple atomistic and continuum scales. The central issue in developing these hybrids is determining statistical distributions from the atomistic scale that are needed to express the coupling between atomistic and continuum scales.
- *Hybrid models for climate modeling.* The large-scale motions of the Earth's atmosphere and oceans are well described by the hydrostatic approximation, in which the vertical momentum equation is replaced by a hydrostatic balance law. However, as it becomes necessary to resolve ever-larger ranges of scales in climate models, the use of the hydrostatic approximation at the smallest scales becomes physically invalid. Hybrid models must be developed in which the hydrostatic approximation is used for large scales, while a non-hydrostatic model is used to simulate localized small-scale behavior. Some of the components of such an approach include asymptotic analysis of the various fluid-dynamical processes (e.g., compressive/thermodynamic, gravity-wave, vortical) operating at different scales; a systematic understanding of the well-posedness of initial-boundary value problems for hydrostatic and nonhydrostatic models; and carefully designed numerical methods to implement well-posed couplings between such pairs of models.

2.1.3 Closure Methods

An open question for a large class of problems is the derivation of macroscopic models from more-detailed microscopic models, often referred to as *closures*. Such problems include those that lack a strong separation of scales, rare-event problems, and problems involving the reduction of high-dimensional state spaces to a small number of degrees of freedom. We must 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 quantify uncertainty in chaotic or stochastic systems. A variety of new analytical techniques have been suggested that, combined with large-scale simulation, provide new tools for attacking the problem of deriving closures. One such technique is the use of concepts from nonequilibrium statistical mechanics for representing the dynamics of a coarse-grained system in terms of the unresolved degrees of freedom. This technique is less susceptible to realizability problems than are traditional moment closure methods. Markov-chain Monte Carlo methods are also promising for finding near-invariant sets

and the transition probabilities between them and projective integration methods for self-consistently determining macroscopic degrees of freedom and their effective dynamics. These methods provide a starting point for designing new closure models, particularly when validated against direct simulation with all of the degrees of freedom resolved. The resulting multiscale models can then be incorporated into large-scale simulations to, for example, further reduce the size of regions using the costly detailed model in a hybrid method of the type described above.

The following are examples of science opportunities involving the development of new closure methods.

- *Turbulent mixing of a multifluid medium.* In turbulent mixing problems that arise in high energy-density physics, it is necessary to simulate the transition between various regimes: distorted sharp interfaces, macroscopic breakup (“chunk mixing”), and atomic-scale mixing. In addition, it is necessary to develop models of the interaction of the turbulent medium with other physical processes such as radiation transport and nuclear burning.
- *Problems with a small number of degrees of freedom.* In materials science and biology, only a few features of a large molecule may determine its function. This situation can occur, for example, when an associated potential has a few well-delineated minima, with much of the motion confined to the neighborhoods of these minima and an occasional jump from one neighborhood to another. Also in this class of problems are rare events, such as ion exchange and nucleation of defects. In all these cases, the number of significant aggregate degrees of freedom is orders of magnitude smaller than that of the microscopic description, as are the time scales over which the aggregate degrees of freedom change relative to those of the microscopic description.
- *Interaction of turbulence and chemistry in combustion.* Current numerical methodology is able to model the interplay between turbulence and chemistry in laboratory-scale systems, but the resolution requirements for such simulations make them intractable for more realistic flames. Existing methodologies for representing reaction kinetics in a turbulent flame explicitly separate turbulence scales from chemical scales. In most situations, however, turbulent transport and reaction scales are strongly coupled; and new approaches are required to represent the reaction process that respect this coupling.
- *Large-scale subsurface flows.* Simulations in environmental remediation rely on ad hoc closure schemes that have little relation to the microphysics. New closure methods will enable the development of models that systematically represent the effect on the macroscale dynamics of pore-scale physics such as wettability, dynamic relations among fluid saturations, and the behavior of disconnected phases. Simulation of subsurface flow is complicated, however, by the fact that the subsurface medium itself is heterogeneous, with fluctuations on scales two orders of magnitude smaller than those of large-scale flow scales, but whose

presence nevertheless has a substantial impact on transport at those scales. In addition, these fluctuations can be characterized only statistically. Such problems need to be attacked with new closure methods combined with new hybrid stochastic and deterministic models to represent those closures.

- *Hierarchical models.* In materials science, there exists an elaborate hierarchy of models for various length scales: macroscale continuum mechanics, molecular-scale models based on classical mechanics, and various techniques for representing quantum-mechanical effects. While some methods are emerging for coupling these scales, they are not yet on a firm theoretical foundation, and they are not applicable to all systems of interest. Work must be done to establish these foundations and to extend the range of applicability of these methods.

2.2 Cross-Cutting Issues

Several multiscale mathematics issues cut across both the applications and the mathematical techniques described above. We focus here on two issues: uncertainty quantification and the need for numerical analysis and mathematical software.

2.2.1 Uncertainty Quantification

Limitations on knowledge and on the scale, scope, and relevance of observations of physical phenomena inject elements of uncertainty into any computational prediction. Uncertainties arise from errors in data, models, and numerical solution procedures. These uncertainties can sometimes be quite large. For example, in the study of cell regulatory systems in biology, parameters are typically known to widely varying degrees of accuracy, and even the network structure may not be known for certain. In many environmental and geoscience applications, model parameterizations are uncertain and often characterized only statistically. At the same time, there is a need to derive whatever understanding and conclusions we can from the data, as well as to understand the limitations of what we have derived. The quantification of uncertainty plays two important roles in multiscale science and mathematics. The first has to do with the fact that multiscale simulation deals with approximate models and solution procedures across a range of scales. Errors arise from the approximations made at each scale and from the coupling process itself. Accurate estimation of errors is needed for the adaptive decisions inherent in multiscale modeling and software, as well as for providing much of the framework for understanding, refining, and validating the multiscale modeling process itself. Second, simulation is often an intermediate step to another goal such as obtaining a better understanding of the science by identifying which steps or processes are critical; guiding the direction of future experiments, optimal design, or control; or providing information for policy decisions. Uncertainty quantification provides a means for obtaining the required information about the solution, as well as determining the reliability of that information.

In order to enable the quantification of uncertainties in multiscale modeling, new algorithms and software must be developed. In large measure, these are extensions of the ideas developed in the core areas of the program, to permit tracking of uncertainty in the multiscale context. Incorporation of known constraints, optimizations, and nonquantitative information into the characterization and analysis of uncertainty is also an important consideration.

2.2.2 Numerical Analysis and Mathematical Software

The application of multiscale mathematics techniques to science will be chasing a moving target. The starting point will be a set of models that, typically, have a specific range of scales over which they are valid and for which there are well-established discretization methods and supporting numerical software. As we introduce new models and new multiscale couplings between existing models, we will need to modify existing numerical software and develop new software. For example, multiresolution methods for two-fluid plasmas will require the development of a variety of high-performance linear solvers for nonsymmetric positive definite or anisotropic systems on adaptive grids, the design of which is an open research question in numerical analysis. In addition, we will need a robust and flexible toolset of mathematical software components for solving partial differential equations. Typically, these components will be on a granularity significantly smaller than that of integrated applications codes but sufficiently flexible and capable that new algorithmic and modeling ideas can be easily prototyped. Without such a toolset, it will be difficult to experiment with different approaches to representing multiscale models in a sufficiently timely fashion to have an impact on the science.

3. The Science-Based Case for Multiscale Simulation

We focus in this section on six target applications that are important to DOE and will benefit dramatically from multiscale simulation.

3.1 Environmental Sciences and Geosciences

Environmental and geoscience applications of crucial importance to the mission of DOE 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; CO₂ sequestration for reducing greenhouse gasses; reducing particulate emissions into the atmosphere; climate, weather, and air quality modeling; and mitigating natural hazards such as oil spills and wildfires. 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.

Society is both demanding and deserving of vastly improved science, mathematics, and predictive tools to inform policy. 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 staggering as well. Petroleum fuel costs are rising at a rapid rate, 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.

Current models of environmental systems lack predictive capability. The reason is that 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. Operative at these scales are diverse physical, chemical, and biological processes, many of which are not well understood. Naturally open systems, which are in turn coupled to other complex systems, must be considered. Data is 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 CO₂ sequestration introduced in Section 1 provides a good illustration. This problem involves the removal of atmospheric carbon dioxide and the injection of this gas 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. In order to achieve this objective, numerous issues must be addressed. First, description of the bulk fluid and solid behavior requires the solution of

multiphase conservation equations for mass, momentum, and energy. Current formulations rely on ad hoc closure schemes that do not incorporate important pore-scale physics, such as wettability, dynamic relations among fluid saturations, interfacial areas, saturations, crucial model parameters, and the behavior of disconnected phases. Laboratory observations provide abundant support for the notion that current models are seriously lacking in their ability to accurately simulate even the processes involved with multiphase flow for such applications. Adequate resolution of these shortcomings will require new, physics-based, rigorous models that are more fully understood at the microscale. Once these macroscale models are developed, issues involved with heterogeneity at the macroscale in the subsurface must be addressed. Here important parameters are known to vary by orders of magnitude over length scales on the order of meters—far below the hundreds of meters of concern. Study of heterogeneous systems has raised another important scientific issue: the usual situation is that subsurface heterogeneity cannot be described by models with clearly separated length scales. Further, subsurface heterogeneity is virtually never characterized in sufficient detail to allow rigorous, meaningful analysis with certain attractive and available methods, such as mathematical homogenization.

Once an appropriate model is formulated, it must be simulated over large spatial and temporal scales. Resulting solutions often lead to sharp fronts that propagate in space and time and require advanced numerical methods to resolve. Because of the complexity of the subsurface, model parameters are uncertain, necessitating a stochastic model. New methods are needed to efficiently account for this uncertainty, since direct Monte Carlo simulations are currently too computationally intensive for the scope of this problem. To reduce the uncertainty in these simulations requires incorporating multiple sources of data—collected with various means from a range of spatial and temporal scales—into conditioned estimates of spatial properties.

Additional challenges exist with respect to resolving the many biogeochemical reactions of concern, along with changes in porosity, mineralogy, and geomechanics. Issues regarding model formulation, numerical methods, algorithms, stochastic aspects, and data assimilation are involved with each of these aspects as well. Moreover, all of these flow, transport, and reaction processes are coupled with each other and with the turbulent processes of the atmosphere.

3.2 Materials Science

Materials are enabling—and limiting—many technologies with high impact on our society, ranging from energy and the environment to new nano- and biotechnologies. Multiscale problems permeate all of materials science. The following are major scientific areas where the use of predictive multiscale capabilities can potentially lead to new discoveries by computer simulations:

- *Materials to go beyond CMOS technology*, including materials to realize molecular electronic devices and quantum computers

- *Materials for fusion and fission reactors*, including materials resistant to radiation and other harsh 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

Better understanding of fundamental processes such as fracture and failure, nucleation, and electronic and transport phenomena that occur on multiple scales will require new mathematical tools and techniques. These are properties encompassing all of the materials science areas identified above. Table 1 illustrates the connection between the categories and the required developments in multiscale mathematics.

The following are specific examples of materials science problems:

- *Nuclear waste migration* involves transport of a radioactive nuclide, for example, Cs, out of the nuclear wastefrom, for example, a zeolite system, when the wastefrom is in contact with ground water. The chemical process is believed to be cation exchange between the Cs and the Na in the ground water. Simulation of this rare event will involve reaction pathway sampling. Capturing the physics and chemistry that determine the ion exchange process will require coupled quantum-classical-continuum simulations.
- *Nucleation and self-assembly of quantum dot arrays* produces nanoscale systems, but their use in microelectronics and other applications depends critically on achieving uniformity in size, shape, and spacing. Simulation of the initial wetting layer, nucleation and self-assembly will require simulation at the atomistic, single dot, and multiple dot length scales.
- *Design of novel materials with specific sensing and labeling properties* requires the simulation of interfaces between inorganic surfaces and organic matter in the presence of a wet environment and the study of reaction paths between organic molecules and inorganic probes. This will involve atomistic simulations both at the quantum and effective potential level, coupled with continuum description of, for example, a solvent, and the simulation of rare events and equilibrium phenomena over time scales from picoseconds to nanoseconds.

Table 1. Coupling of scales in materials problems. The table illustrates the connection between driving scientific applications and the required developments in multiscale mathematics.

| | Coupling of Length Scales | Coupling of Time Scales | Major Challenging Properties |
|-----------------------------|---|---|--|
| Beyond CMOS | Quantum-quantum (e.g., DFT/QMC) Quantum-classical (QM/MM) | Accelerated dynamics for both classical and quantum molecular dynamics (MD) | Nucleation; electronic and transport |
| Materials for Fusion | Quasi-continuum models for MD | Beyond ns time scales in MD | Fracture and failure, resistance to radiation |
| Soft Materials | Quantum-classical-continuum | Accelerated dynamics for quantum methods | Electronic and transport |
| Nuclear Waste | Quasi-continuum coupled to quantum-classical models | Rare events and beyond ns time scales in MD | Electronic and transport; fracture and failure |
| Clean Energy | Quantum-quantum quantum-classical (QM/MM) | Accelerated dynamics for both quantum and classical methods | Electronic and transport |
| | | | |

3.3 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, NO_x, 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.

Potential concepts proposed to address these issues include developing methodologies for clean burning of coal, lean combustion technologies, and hydrogen-based systems. Realizing the potential of these new technologies, however, requires an ability to accurately predict the underlying combustion processes. Our inability to deal with the multiscale nature of combustion systems is the fundamental hindrance to developing this type of predictive capability. Lean, premixed combustion technology



Figure 3. Low swirl burner prototype. The burner's novel flame stabilization mechanism allows it to operate at lean conditions with very

(see Figure 3) 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 with the flame front whose dimensions are measured in hundreds of microns. This interaction of scales spans six decades in space and an even larger range of scale in time.

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. Often this basic problem is compounded by the need to include additional physical processes. Many fuels are initially liquid, and the dynamics of a liquid spray play a crucial role; often the formation and oxidation of soot particles are a critical element governing system behavior; and some systems rely on catalytic surface reactions. Many of these phenomena are not well understood, and high-fidelity continuum models are not known.

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. The fundamental issues with these approaches are that they are inherently single scale. To provide the simulation capabilities needed for chemically reacting flows, new approaches are required that reflect the multiscale character of these problems.

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. 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.

Another area where new approaches are needed for combustion simulation is the coupling of continuum and atomistic models. Many of the phenomena encountered in combustion systems such as soot formation and catalytic reactions are not understood at the continuum level. The most likely avenue for making progress in understanding these types of processes is performing simulations at the atomistic level. The issue then is how to incorporate the atomistic behavior into large-scale continuum simulations. One approach to dealing with this problem is to view it as a closure problem and to develop methodologies to derive continuum models for these types of phenomena. The structure of the resulting models and the issues in treating them numerically are essentially open questions. An alternative approach is to develop methodologies for performing atomistic simulations along with a continuum model as part of a hybrid simulation. Here the fundamental concern is how to couple the scales and numerical issues arising from the inherently stochastic nature of atomistic simulations on the continuum solver.

Computational tools that address the multiscale nature of reacting flow processes have the potential to accurately model complex reacting flows to predict emissions and faithfully quantify the effect of small changes in the design on system performance. This type of capability will fundamentally transform the design and operation of energy and propulsion systems from the subwatt to the terawatt levels and allow us to meet the stringent performance demands of these types of systems.

3.4 High Energy-Density Physics

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 DOE/NNSA laboratories are concerned with this subject for the obvious reason that high energy-density physics governs energy release in thermonuclear weapons. Astrophysicists are interested in the same subject because Type Ia and Type II (core collapse) supernovae are the source of much of the heavier nuclei in the universe, and because Type Ia are the “yardsticks” that allow us to measure the size and age of the universe, as well as to help constrain the amount of “dark energy” in the 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).

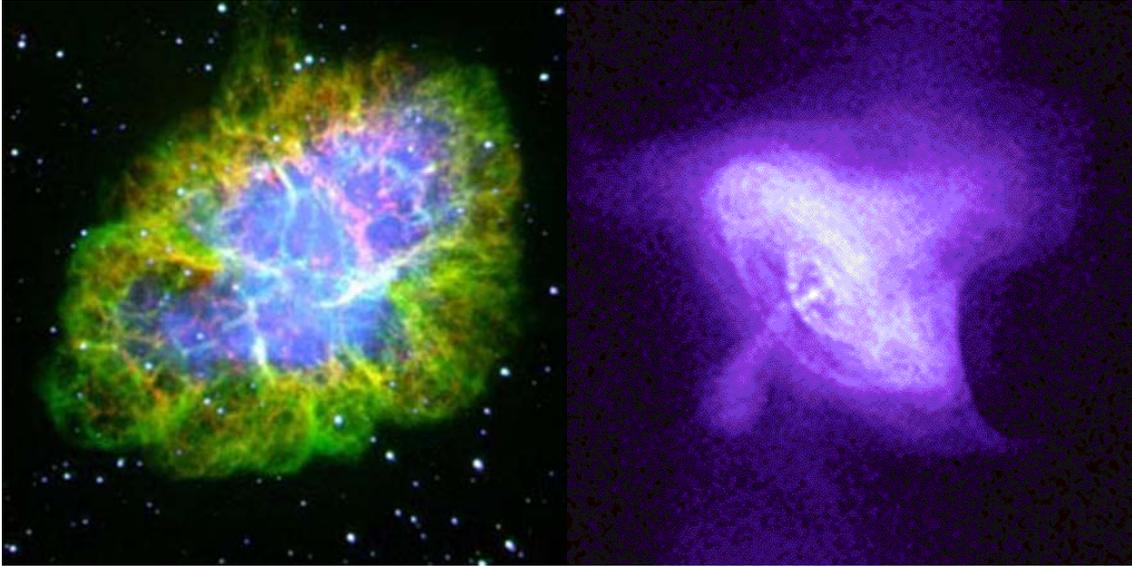


Figure 4: Images of the Crab nebula (seen in the optical; left image) and the core of this nebula, at the site of the pulsar (seen in the X-ray by NASA's *Chandra* X-ray satellite; right image). This supernova remnant, located ~ 6000 light-years from Earth, contains highly relativistic electrons (emitting optical photons on the scale of the nebula, and X-rays on the scale of the extended magnetosphere surrounding the pulsar), together with magnetic fields (which are extremely strong in the immediate surroundings of the stellar remnant of the core collapse supernova explosion of A.D. 1054). 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 played an essential role. (Image courtesy NASA and the *Chandra* Science Center)

A hallmark of high energy-density physics is the prevalence of compressible effects; in many cases, these effects arise in the context of turbulence together with, for astrophysical systems, gravitational stratification. In general, our understanding of such effects is primitive when compared to those of the incompressible case. Thus, better models are needed for compressible turbulence (including reactive and stratified flows) and turbulent mixing. The importance of these models extends beyond the field of fluid dynamics to include photon and neutrino transport, nuclear combustion rates, and relativistic regimes.

Another challenge is understanding how turbulence mixes (e.g., composition, tracers). Modeling turbulent mixing is much harder than the already difficult problem of modeling turbulence; the effects, for example, of “chunk” vs. “atomic” mixing remain to be resolved. Because turbulent mixing between different regions of a star (or of an imploding hohlraum) strongly affects the energy balance via radiation transport or nuclear combustion, and because the emerging radiation and nuclear products are more readily measured, modeling these aspects of the problem gives greater validation capabilities.

Furthermore, in many cases, magnetic fields can attain sufficient strength that they begin to influence fundamental material properties (such as transport coefficients) and exert stresses associated with the Lorentz force. When such fields are externally applied, the problem reduces to computing the material response to these fields; in the more general case, in which magnetic fields are in part generated within the material volume under study, one must solve the magnetic dynamo problem together with the material response to the fields. There is a need to model magnetic turbulence and to include the effect of charged particles.

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 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. Hence, radiation hydrodynamics simulations reside in a high-dimensional phase space.

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 our 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.

A fundamental aspect of high energy-density physics concerns the properties of matter, that is, equations of state (relationships connecting matter pressure and specific energy with density and temperature), and opacities and transport characteristics (such as thermal conductivity and viscosity). These relationships are commonly tabulated for later use in simulations. Ideally the table entries are based on experimental observations. However, for matter that is encountered under extreme conditions, such experimentation is often impossible, so the table entries must be based on computation. Such multiscale calculations starting from nuclear scales to determine macroscopic properties are themselves challenging for a variety of reasons, not the least of which is the fundamental difficulty of directly validating predictions for degenerate or partially degenerate matter.

In some situations, the material under study is not in local thermodynamic equilibrium (LTE). Examples occur in radiation-driven plasmas, such as the photosphere or chromosphere of a star, as well as in laboratory plasmas, where the matter is typically in LTE but the radiation is not. In such situations material properties cannot be tabulated, but must be computed “on the fly.” The small atomic timescales involved in such computations require a multiscale approach. This loss of LTE can occur nonuniformly in space, adding yet another element to the multiscale nature of the underlying problem. In such cases the connection between the “observables” and local physical properties

becomes complex. A clear understanding of the physical models used in simulations is essential in order to understand what is being observed.

3.5 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 twenty-first century. The vast supplies of deuterium fuel in the oceans and the absence of long-term radiation, CO₂ generation, and weapons proliferation make fusion the preferred choice for meeting the energy needs of future generations.

In magnetic fusion experiments, high-temperature (100 million degrees centigrade) plasmas are produced in the laboratory in order to create the conditions where hydrogen isotopes (deuterium and tritium) can undergo nuclear fusion and release energy (the same process that fuels our sun and the stars). Devices called tokamaks (which are axisymmetric) and stellarators (which are not) are “magnetic bottles” that confine the hot plasma away from material walls, allowing the plasma to be heated to extreme (thermonuclear) temperatures so that 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) aim to calculate the details of the heating process when an external antenna produces a strong RF field. These codes work in the frequency domain, as a single frequency is imposed by the oscillator, and the plasma response on these timescales is most naturally formulated in the frequency domain. Although these codes have been used successfully for designing and interpreting many experimental effects, they could be improved in several ways: (1) the actual absorption and mode conversion tends to occur in narrow regions, and it is likely that spatially adaptive methods would provide significant benefit; (2) important localized nonlinear sheath effects occur at the plasma edge that are known to be important but are not being modeled; (3) nonlinear wave-coupling effects sometimes occur that generate different frequencies missing from the single frequency description; and (4) coupling of the background profiles and wave fields is not normally incorporated in a self-consistent manner.

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 (3 velocity + 3 space) to a 5D (2 velocity and 3 space) description. Two approaches have been pursued: continuum, and particle-in-cell methods. This enables code verification by comparing the turbulent fields produced by two very different algorithms. Remaining issues for these computationally intensive codes include validation of code results against experimental measurements of turbulent fluctuations (which will require upgrading the experimental diagnostic capability) and expanding the time and space scales covered by these simulations to encompass the short time ($\sim 10^{-7}$ sec) and space ($\sim 10^{-5}$ m) scales associated with electron microturbulence together with the longer time and space scales associated with ion microturbulence ($\sim 10^{-5}$ sec and 10^{-3} m), and ultimately the transport time and space scales as described below.

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. There are two approaches to the closure problem. The “two-fluid” approach derives analytic closure relations in terms of the fluid variables. The “hybrid” particle/fluid model closes the equations with kinetic equations. Issues in this area are the development of techniques for resolving small reconnection layers in the global simulations, the development of efficient techniques for the inclusion of dispersive waves in the fluid equations (this includes Kinetic Alfvén and Whistler waves), improvements on the closure procedure, and the inclusion of essential kinetic effects on global stability (i.e., those involving wave-particle resonances).

Transport timescale codes (Figure 1d) use a reduced set of equations that have the Alfvén waves removed. These are used for long-time scale simulation of plasma discharges. They require the inclusion of transport fluxes from the turbulence calculations. At present, there is one set of codes for the interior of the plasma (where the magnetic field lines form closed surfaces) and another set for the edge, where the effects of open field are manifested. Improved techniques for coupling these two regions are required.

In addition to transport, edge physics encompasses its own set of turbulence and MHD issues, as well as atomic physics and plasma-wall interactions. The combining of these ingredients presents a number of multiscale challenges. The range of space and time scales is as large as in the core; but some scales—such as radial orbit size and pressure scale length—which are well separated in the core but overlap in the edge, are complicated to treat.

Specialized mathematical models have been developed for other processes as well. One of these models is aimed at describing pellet fueling of plasmas. Here, separate models that describe the detailed ablation physics of the pellet need to be coupled with global models that compute the mass distribution from the pellet once it has been ionized.

An emerging thrust in computational plasma science is the integration of the now separate macroscopic and microscopic models and the extension of the physical realism

of these by the inclusion of detailed models of such phenomena as RF heating and atomic and molecular physical processes (important in plasma-wall interactions). 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. This understanding, and the resultant predictive capability, will be critical in realizing the long-term goal of creating an environmentally and economically sustainable source of energy.

A number of external drivers make this an especially opportune time for accelerating our capabilities in the computational modeling of plasma. The international ITER experiment is scheduled to begin its 10-year construction phase in 2006. There exists a clear opportunity for the United States to take the lead in the computational modeling of this device, putting 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 envisioned in the Fusion Simulation Project is felt to be 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 be evaluating other magnetic fusion energy configurations during this same time period.

In addition to magnetic fusion, there is an active program in Inertial Fusion Energy (IFE) within the Office of Fusion Energy Sciences, which encompasses both driver research and target design. Target multiscale issues can be found in the high-energy-density physics section of this report. Multiscale issues for drivers are also numerous. For example, in order 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 ($\sim 10^{-12}$ sec) to the beam dwell time (up to 10^{-4} sec).

3.6 Biosciences

Biology is perhaps the ultimate laboratory for the application of multiscale modeling. The oxygen that we breathe arose from the earliest single-celled organisms. To this day, our planet'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 base of knowledge regarding 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. Perhaps more important, 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 work that nature has done to produce what are generally very nonrandom systems.

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 energy production.

Figure 5 shows an example of how research focused on many length scales is needed to solve a problem such as carbon sequestration. One needs the genetic information (Box 1) of a typical cyanobacteria such as *Synechococcus* or *Prochlorococcus* (both of which are under study 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 together in an efficient manner.



Figure 5. Multiscale nature of carbon sequestration. 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 ultimate help describe the impact of the cyanobacteria on the global carbon cycle (Box 5).

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 (such as the catalyzation site shown in Figure 6), 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*. If one can incorporate the proper biological constraints, the problem becomes very tractable.

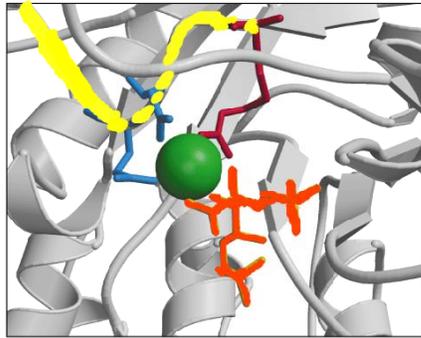


Figure 6. Catalyzation site

The diverse nature of the data that describes 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 protein structure prediction. Experimental data ranges from molecular measurements to gross parameters of an entire system. There is a need not only for researchers to be able to catalog this data, but for modelers to be able to incorporate it in every level of their models and to effectively visualize the different scales of data that experiment and modeling produce.

4. Milestones

Below we present an agenda for research in multiscale mathematics and computation that attacks the fundamental problems of coupling across scales. The plan 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.

Near-term milestones. 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.

- *Development of existing multiresolution techniques for new applications.* In some areas, mature models are already capable of correctly representing the important multiscale behavior. Extensions of existing multiresolution numerical methods will be developed to accurately, efficiently, and stably simulate that behavior.
- *Development of multiresolution and hybrid stochastic numerical methods.* Stochastic models are central to many multiscale science problems. Early development of these new fundamental algorithms will provide a foundation for the later development of the entire program.
- *Mathematical and numerical analysis of the coupling between scales.* A number of areas, such as the coupling between quantum and classical molecular dynamics in materials, plasma turbulence and transport scales in fusion, and hydrostatic and non-hydrostatic scales in atmospheric fluid dynamics, are susceptible to analysis using current state of the art analytical tools, particularly when combined with a robust numerical experimentation capability. Success in analyzing such applications will provide the basis for new multiscale algorithm development, as well as providing new extensions to the mathematical tools.

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 multiresolution and hybrid methods.* This would involve application of the methods described above to scientifically important problems arising in multiscale science.
- *New methods for analyzing multiscale behavior.* New methodologies for closure should be 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, or reduction of high-dimensional state spaces to a small number of degrees of freedom.
- *Algorithms and software for multiscale sensitivity and uncertainty analysis.*
- *Software for core components of multiscale algorithms.*

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.* This would involve the integration of the multiscale methods described above into comprehensive multiphysics simulations.
- *Application of new closure models.* The new models will be used in high-performance simulations to solve some of the outstanding hard problems in multiscale science, e.g., fluid turbulence, protein folding.
- *A new generation of multiscale software.* Robust and adaptive mathematical software will be developed, implementing a new generation of multiscale algorithms for simulation and analysis.