Final Report
Second DOE Workshop on Multiscale Problems
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Contributors

The report of the Second DOE Workshop on Multiscale Mathematics is a collaborative effort by the report editors, session organizers, and invited speakers. The report also includes technical contributions from workshop participants. The workshop participants are listed in Section 1.

Workshop Organizers

Donald Estep
Colorado State University

John N. Shadid
Sandia National Laboratories

Dave Zachmann
Colorado State University

Gary Johnson
Department of Energy

Simon J. Tavener
Colorado State University

Report Editors

Donald Estep
Colorado State University

John N. Shadid
Sandia National Laboratories

Simon J. Tavener
Colorado State University

Session Organizers and Invited Speakers

Todd Arbogast
University of Texas at Austin

Pavel B. Bochev
Sandia National Laboratories

Graham Carey
University of Texas at Austin

Edwin Chong
Colorado State University

Jacob Fish
Rensselaer Polytechnic Institute

Gregory Forest
University of North Carolina at Chapel Hill

Michael D. Graham
University of Wisconsin – Madison

Max Gunzburger
Florida State University

Andrew J. Majda
New York University

Mark S. Shephard
Rensselaer Polytechnic Institute

Eitan Tadmor
University of Maryland

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Summary

The need to understand complex physical systems with interacting behaviors coupled through multiple spatial and temporal scales has increased dramatically over the last decade. Scientists and engineers are seeking to simulate, analyze, and control ever more complex systems. At the same time, the development of new measurement and characterization tools in many fields has made it possible to explore spatial and temporal phenomena on an unprecedented range of scales.

Indeed, the physical and mathematical complications that arise in multiscale systems present one of the major obstacles to future progress in many fields of science and engineering. This has resulted in increasing pressure on the applied mathematics community to develop new methods for multiscale problems. The key mathematical issues are generally described as the need to develop better descriptions of scale representation, scale separation, inter-scale communication and to improve the mathematical analysis and solution techniques for multiscale problems.

Specifically, there is a pressing need to extend existing mathematical techniques, develop new methods, and find innovative ways to combine multiple techniques in order to handle complex systems with multiple scales that may or may not be well separated. Also important is the need to develop and apply mathematical methods in the context of realistic applications with the goal of providing physically meaningful information. Moreover, there is a strong need to develop abstract mathematical frameworks for important classes of multiscale problems. Mathematical frameworks provide the means to categorize and clarify characteristics of existing models and approximations in a landscape of seemingly disjoint, mutually exclusive, and ad-hoc methods. Such frameworks are likely to encompass a variety of analytic and numerical methods.

The overwhelming consensus opinion is that future progress on multiscale problems requires the efforts of interdisciplinary teams of researchers comprising mathematicians, scientists, engineers, and computer scientists drawn from both the universities and the national laboratories. The practical, problem solving orientation of the Department of Energy places it in a unique position to fund the interdisciplinary activity that is required to get the job done.

1. Workshop Participants

Todd Arbogast
University of Texas at Austin
Mathematics and ICES
Austin, TX 78712
Phone: 512-475-8628
arbogast@ices.utexas.edu

Samuel F. Asokanthan
The University of Western Ontario
Mechanical & Materials Engineering
London, ON N6A-509
Phone: 1 519-661-2111 Ext 88907
sasokanthan@eng.uwo.edu

Victor H. Barocas
Biomedical Engineering
University of Minnesota
Minneapolis, MN 55455
Phone: 612-626-5572
baroc001@umn.edu

Lee Berry
Oak Ridge National Laboratory
Fusion Energy Department
Oak Ridge, TN 37831-6169
Phone: 865-574-0998
berryla@ornl.gov

Martin Berzins
University of Utah
SCI Institute
Salt Lake City, UT 84112
Phone: 801-585-1545
mb@sci.utah.edu

Pavel B. Bochev
Sandia National Laboratories
Computational Mathematics & Algorithms
Albuquerque, NM 87111
Phone: 505-844-1990
pbboche@sandia.gov

Steve Bova
Sandia National Laboratories
Thermal/Fluid Computational Eng. Sciences
Albuquerque, NM 87185-0382
Phone: 505-844-6093
swbova@sandia.gov

David L. Brown
Lawrence Livermore National Laboratory
Computing Applications and Research
Livermore, CA 94551
Phone: 925-424-3557
dlb@llnl.gov

Jason E. Butler
University of Florida
Chemical Engineering
Gainesville, FL 32611-6005
Phone: 352-392-2591
butler@che.ufl.edu

Roberto Camassa
University of North Carolina, Chapel Hill
Mathematics Department
Chapel Hill, NC 27599
Phone: 919-962-8476
camassa@amath.unc.edu

Graham Carey
University of Texas at Austin
Institute for Computational Engr. & Sciences (ICES)
Austin, TX 78712
Phone: 512-471-4676
carey@cfdlab.ae.utexas.edu

Chung-Ki Cho
Soonchunhyang University
Mathematics
Asan, Korea 336-745
Phone: 82-41-530-1221
ckcho@sch.ac.kr

Edwin Chong
Colorado State University
Department of Electrical and Computer Engineering
Fort Collins, CO 80523-1373
Phone: 970-491-7858
echong@colostate.edu

L. Pamela Cook
University of Delaware
Department of Mathematical Sciences
Newark, DE 19716
Phone: 302-831-0582
cook@math.udel.edu

Richard Counts
Oak Ridge National Laboratory
Computer Science and Mathematics
Oak Ridge, TN 37831-8264
Phone: 865-574-8264
countsrw@ornl.gov

Lori Freitag Diachin
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
Livermore, CA 84551
Phone: 925-422-7130
diachin2@llnl.gov

Yalchin Efendiev
Texas A&M University
Mathematics Department
College Station, TX 77843-3368
Phone: 979-845-1972
efendiev@math.tamu.edu

Kenneth Eggert
Los Alamos National Laboratory
Theoretical Division
Los Alamos, NM 87545
Phone: 505-667-5200
kge@lanl.gov

Anter El-Azab
Pacific Northwest National Laboratory
Fundamental Science Directorate
Richland, WA 99352
Phone: 509-376-9587
Anter.el-azab@pnl.gov

Donald Estep
Colorado State University
Department of Mathematics
Fort Collins, CO 80523
Phone: 970-491-6722
estep@math.colostate.edu

George Fann
Oak Ridge National Laboratory
Oak Ridge, TN 37831
Phone: 865-576-2374
fanngi@ornl.gov

Petri Fast
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
Livermore, CA 94551
Phone: 925-424-2649
Fast1@llnl.gov

Jacob Fish
Rensselaer Polytechnic Institute
Department of Civil & Environmental Engineering
Troy, NY 12180
Phone: 518-276-6191
fishj@rpi.edu

Joseph Flaherty
Rensselaer Polytechnic Institute
Troy, NY 12180
flahej@rpi.edu

Gregory Forest
University of North Carolina at Chapel Hill
Department of Mathematics
Chapel Hill, NC 27599-3250
Phone: 919-962-9606
forest@amath.unc.edu

Bengt Fornberg
University of Colorado
Applied Mathematics
Boulder, CO 80309
Phone: 303-492-5915
fornberg@colorado.edu

Aime Fournier
NCAR and UMCP
NCAR Institute for Mathematical Applications in the Geosciences
Boulder, CO 80307-3000
Phone: 303-497-1614
fournier@ucar.edu

Laura J.D. Frink
Sandia National Laboratories
Computational Biology & Evolutionary Computing
Albuquerque, NM 87185-1110
Phone: 595-844-1910
ljfrink@sandia.gov

Venkat Ganesan
University of Texas, Austin
Chemical Engineering Department
Austin, TX 78712-0231
Phone: 512-471-4856
vankat@che.utexas.edu

Rao V. Garimella
Los Alamos National Laboratory
Santa Fe, NM 87545
Phone: 505-665-2928
rao@lanl.gov

Roger Ghanem
Johns Hopkins University
Civil Engineering
Baltimore, MD 21218
Phone: 410-516-7647
ghanem@jhu.edu

Michael D. Graham
University of Wisconsin – Madison
Department of Chemical and Biological Engineering
Madison, WI 53706-1607
Phone: 608-265-3780
graham@engr.wisc.edu

Max Gunzburger
Florida State University
Department of Mathematics
Tallahassee, FL 32306-4520
Phone: 850-644-7060
gunzburg@csit.fsu.edu

Jeff Herdtner
Miami University
Electrical & Computer Engineering
Oxford, OH 45056
Phone: 970-491-3148
herdtner@purdue.edu

Michael Holst
Department of Mathematics
University of California, San Diego
La Jolla, CA 92093-0112
Phone: (858) 534-4899
mholst@math.ucsd.edu

Richard Hornung
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
Livermore, CA 94551
Phone: 925-422-5097
horning@llnl.gov

Robert Jacob
Argonne National Laboratory
Mathematics & Computer Science Division
Argonne, IL 60439-4843
Phone: 630-252-2983
jacob@mcs.anl.gov

Stephen C. Jardin
Princeton University
Plasma Physics Laboratory
Princeton, NJ 08543
Phone: 609-243-2635
jardin@princeton.edu

Ken Jarman
Pacific Northwest National Laboratory
Statistical & Mathematical Sciences
Richland, WA 99352
Phone: 509-375-6360
kj@pnl.gov

Yi Jiang
Los Alamos National Laboratory
Los Alamos, NM 87545
Phone: 505-665-5745
jiang@lanl.gov

Richard W. Johnson
INEEL
Idaho Falls, ID 83415-3760
Phone: 208-526-0955
rwj@inel.gov

Ruben Juanes
Stanford University
Petroleum Engineering
Stanford, CA 94305
Phone: 650-725-3312
Ruben.juanes@stanford.edu

Markos Katsoulakis
University of Massachusetts, Amherst
Dept. of Mathematics & Statistics
Amherst, MA 01003
Phone: 413-545-1331
markos@math.umass.edu

Mohammad Khaleel
Pacific Northwest National Laboratory
Computational Sciences and Mathematics Division
Richland, WA 99352
Phone: 509-375-2438
moe.khaleel@pnl.gov

Mi-Young Kim
Inha University
Department of Mathemetics
Incheon, Korea 402-751
Phone: 82-32-860-7633
mikim@inha.ac.kr

Travis King
Colorado State University
Ft. Collins, CO 80521
Phone: 505-845-0522
king_travis@hotmail.com

Peter Kramer
Rensselaer Polytechnic Institute
Mathematical Sciences
Troy, NY 12180
Phone: 518-276-6896
kramep@rpi.edu

William Layton
University of Pittsburgh
Mathematics Department
Pittsburgh, PA 15260
Phone: 412-624-8312
wjl@pitt.edu

Seong H. Lee
ChevronTexaco ETC
Reservoir Simulation
San Ramon, CA 94583-0719
Phone: 925-842-6392
seon@chevrontexaco.com

Steven L. Lee
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
Livermore, CA 94551
Phone: 925-424-5989
slee@llnl.gov

Richard Lehoucq
Sandia National Laboratories
Computational Mathematics and Algorithms
Albuquerque, NM 87185-1110
Phone: 505-845-8929
rblehou@sandia.gov

Randall J. LeVeque
University of Washington
Applied Math
Seattle, WA 98195-2420
Phone: 206-685-3037
rjl@math.washington.edu

Adrian Lew
Stanford University
Mechanical Engineering Department
Stanford, CA 94305-4040
Phone: 650-725-3585
lewa@stanford.edu

Sven Leyffer
Argonne National Laboratory
Mathematics & Computer Science Division
Argonne, IL 60439
Phone: 630-252-4698
leyffer@mcs.anl.gov

Shengtai Li
Los Alamos National Laboratory
Theoretical Division
Los Alamos, NM 87545
Phone: 505-665-8407
sli@lanl.gov

Scott MacLachlan
University of Colorado, Boulder
Applied Mathematics Department
Boulder, CO 80309-0526
Phone: 303-735-3752
maclachl@colorado.edu

Andrew J. Majda
New York University
Courant Institute of Mathematical Sciences
New York, NY 10012
Phone: 212-998-3324
jonjon@cims.nyu.edu

Jan Mandel
University of Colorado, Denver
Department of Mathematics
Denver, CO 80217-3364
Phone: 303-556-4475
jmandel@math.cudenver.edu

Tom Manteuffel
University of Colorado
Department of Applied Mathematics
Boulder, CO 80309-0526
Phone: 303-492-5199
tmanteuf@colorado.edu

Richard M. McLaughlin
University of North Carolina
Mathematics Department
Chapel Hill, NC 27599
Phone: 919-962-9816
rmm@amath.unc.edu

David Moulton
Los Alamos National Laboratory
Mathematical Modeling & Analysis
Los Alamos, NM 87544
Phone: 505-665-4712
moulton@lanl.gov

David Neckels
Colorado State University
Math Department
Fort Collins, CO 80537
Phone: 461-2646
nickels@math.colostate.edu

Don Nicholson
Oak Ridge National Laboratory
Computer Science and Mathematics
Oak Ridge, TN 37831
Phone: 865-574-5873
nicholsondm@ornl.gov

Assad Oberai
Boston University
Aerospace & Mechanical Engineering
Boston, MA 02215
Phone: 617-353-7381
oberai@bu.edu

Bruce Palmer
Pacific Northwest National Laboratory
Computational Science and Mathematics Division
Richland, WA 99352
Phone: 509-375-3899
Bruce.palmer@pnl.gov

Eun-Jae Park
Yonsei University
Department of Mathematics
Seoul, Korea 120-749
Phone: 82—2-2123-4487
ejpark@yonsei.ac.kr

Valerio Pascucci
Lawrence Livermore National Laboratory
CASC
Livermore, CA 94551
925-423-9422
pascucci@llnl.gov

John Red-Horse
Sandia National Laboratories
Validation & Uncertainty Quantification
Albuquerque, NM 87185
Phone: 505-845-9190
jrredho@sandia.gov

Marcus Sarkis
Mathematical Sciences
Worcester Polytechnic Institute
Worcester, MA 01609
Phone: 508-831-5287
msarkis@wpi.edu

John N. Shadid
Sandia National Laboratories
Computational Sciences Department
Albuquerque, NM 87059
Phone: 505-845-7876
jnshadi@sandi.gov

Dongwoo Sheen
Seoul National University
Mathematics
Seoul, Korea 151-747
Phone: 82-2-880-6543
sheen@snu.ac.kr

Mark S. Shephard
Rensselaer Polytechnic Institute
Scientific Computation Research Center
Troy, NY 12180
Phone: 518-276-6795
shepherd@scorec.rpi.edu

Ralph Showalter
Oregon State University
Mathematics Department
Corvallis, OR 97331
Phone: 541-737-5149
show@math.oregonstate.edu

Alexander Slepoy
Sandia National Laboratories
Computational Materials & Molecular Biology
Albuquerque, NM 87185
Phone: 505-284-3650
aslepoy@sandia.gov

T.P. Straatsma
Pacific Northwest National Laboratory
Computational Biosciences
Richland, WA 99354
Phone: 509-375-2802
tps@pnl.gov

Scott Studham
Pacific Northwest National Laboratory
Computational Sciences & Mathematics Division
Richland, WA 99352
Phone: 509-376-8430
Scott.studham@pnl.gov

Rosangela Sviercoski
National Center for Atmospheric Research
Mathematics Department
Tucson, AZ 85721
Phone: 303-497-1758
rosangel@math.arizona.edu

Eitan Tadmor
University of Maryland
Department of Mathematics
College Park, MD 20742-3289
Phone: 301-405-0648
tadmor@cscamm.umd.edu

Meijie Tang
Lawrence Livermore National Laboratory
Physics and Advanced Technology
Livermore, CA 94551
Phone: 925-422-2415
tang7@llnl.gov

Daniel M. Tartakovsky
Los Alamos National Laboratory
Theoretical Division
Los Alamos, NM 87545
Phone: 505-667-0968
dmt@lanl.gov

Simon J. Tavener
Colorado State University
Department of Mathematics
Ft. Collins, CO 80523
Phone: 970-491-1303
tavener@math.colostate.edu

James Thomas
Colorado State University
Mathematics
Ft. Collins, CO 80521
Phone: 970-491-6456
Thomas@math.colostate.edu

Joseph Tribbia
National Center for Atmospheric Research
Boulder, CO 80305
Phone: 303-497-1377
tribbia@ucar.edu

A. Ted Watson
Colorado State University
Chemical Engineering Department
Ft. Collins, CO 80523-1370
Phone: 970-491-5253
atw@engr.colostate.edu

Larry Winter
National Center for Atmospheric Research
1850 Table Mesa Drive
Boulder, CO 80305

Dongbin Xiu
Los Alamos National Laboratory
Theoretical Division
Los Alamos, NM 87545
Phone: 505-665-4976
xiu@t7.lanl.gov

David Zachmann
Colorado State University
Mathematics
Ft. Collins, CO 80528
Phone: 970-231-9579
dzach@math.colostate.edu

2. Introduction

The Second DOE Workshop on Multiscale Problems was held from July 20 to July 22 in Broomfield, Colorado. During these three days, over eighty researchers with expertise in a wide variety of engineering, mathematical and scientific fields gathered to discuss the current state of mathematical methods for multiscale problems, possible future directions for research, and ways in which the Department of Energy could best support such activity. Stimulated by a series of invited lectures in which general overviews of specific problems and solution methods were presented, the participants gathered into technical sessions for focused presentations, detailed discussions, and debate. The sessions were as follows.

Session	*Organizer*
Systematic Multi-Scale Stochastic Modeling and Quantifying Uncertainty in Atmosphere/Ocean Science	Andrew J. Majda
Complex Fluids and Soft Matter	M. Gregory Forest
Variational Multiscale Analysis	Pavel Bochev
Simulation and Modeling of Multiscale Problems	Graham F. Carey
Multiscale Computational Challenges in Soft Materials	Michael D. Graham
Adaptive Modeling and Simulation	Mark S. Shephard
Variational Multiscale Methods and Multiscale Finite Elements for Heterogeneous Porous Media	Todd Arbogast
Simulation and Analysis of Large Networks	Edwin K. P. Chong

In Section 3, we present some general observations and summarize some general conclusions about the current state of multiscale methods and applications. In Section 4, we synthesize conclusions about possible future directions for research in multiscale mathematics. In Section 5, we present some detailed suggestions for ways to support research in multiscale mathematics. Finally, the reports from the individual workshop sessions comprise the bulk of this report and are presented in Section 6.

3. Multiscale Problems: Past and Present

3.1 Observations about the history of mathematics for multiscale problems

Nature is replete with systems that encompass interacting behaviors occurring across a range of scales, and attempts to treat the multiscale aspects of such systems have a long and deep history in applied mathematics. We need only to observe the ongoing struggles to model turbulent and reacting fluids, biological systems, and complex materials, to understand how multiscale problems have driven applied mathematics. Classical techniques in applied mathematics for multiscale problems include continuum modeling and averaging techniques, Fourier analysis, asymptotic analysis, singular perturbation theory, and the use of scaling laws and self-similarity, i.e., the building blocks of a traditional education in applied mathematics.

While representing a wide range of mathematics, classical multiscale techniques nonetheless share some common limitations. Chiefly, almost all *classical methods apply to systems in which the important behavior occurs on widely separated scales, with the goal of reducing the mathematical description to a model of behavior on a single scale, while approximating the relevant effects of the behavior on the other scale(s), or even discarding these effects if necessary*. This is illustrated, for example, by the continuum modeling of Brownian motion of molecules, the description of boundary layers via asymptotic analysis, and the characterization of "low" and "high" frequency modes when using Fourier analysis.

Classical methods reflect two different historical limitations. Firstly, it was often physically impossible to gather experimental evidence of the behavior of complex physical processes on the finest scales. Secondly, the limited power of mathematical tools and computers often meant that even if the information on the finest scales had been available, it would have been infeasible to include it in a full mathematical description of the system. In other words, there was really no alternative to an approximate mathematical treatment of the fine-scale behavior. One serious consequence is that scientists and mathematicians have often had to introduce "closures" to mathematical models that are at best empirical and often ad hoc, raising serious concerns about the accuracy of such models.

3.2 A perspective on the current state of mathematics for multiscale problems

The need to address the issue of multiscale behavior in complex physical systems has increased dramatically over the last decade. Indeed, without exaggeration, we can say that 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. The increasing pressure on the applied mathematics community to develop new methods for multiscale problems originates from several sources. Firstly, scientists and engineers are seeking to simulate, analyze and even control ever more complex systems. Consider such diverse examples such as

- Modeling fusion reactors using extended magnetohydrodynamics, balancing plasma flow, wave propagation, electromagnetic effects and resistive dissipation
- 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 , and electrostatics
- Simulating sub-surface 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 such as molten plastic, whose properties are determined or modulated by noncovalent effects such as electrostatic and van der Waal interactions, hydrodynamic coupling between elements of the microstructure, and the constraints of excluded volume or connectivity
- Increasing reliance on long term predictions from atmospheric and climate models, to predict, for example, the amount of carbon dioxide in the terrestrial system in order to determine policy with far-reaching financial and social effects
- Modeling large-scale complex graphs and networks that can be used to represent biological systems
- Modeling complex information and communication networks involving tens and hundreds of thousands of nodes coupled through multiple scales in space and time

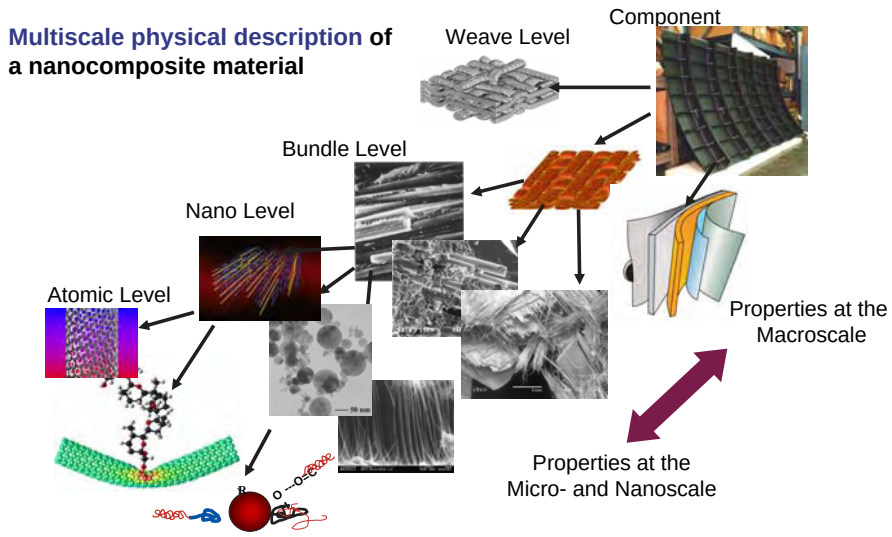

Figure 1: Illustration of scales involved in modeling a nanocomposite material. (Figure courtesy of Mark Shepard)

Many of these problems are of fundamental importance to the mission of the Department of Energy. An examination of the DOE ASC and SciDAC application areas reveals numerous other examples, many of which are highlighted in the report of the First DOE Workshop on Multiscale Problems. The properties of these systems depend critically on important behaviors coupled through multiple spatial and temporal scales without a clear distinction between scales, and as such, do not fall within the classical framework. 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.

Increasing physical capabilities in experimental and computational science also contribute to the pressure on applied mathematics. The development of 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. But, this increases the pressure to understand how to combine realistic models at different scales in order to obtain a manageable model of the entire multiscale system.

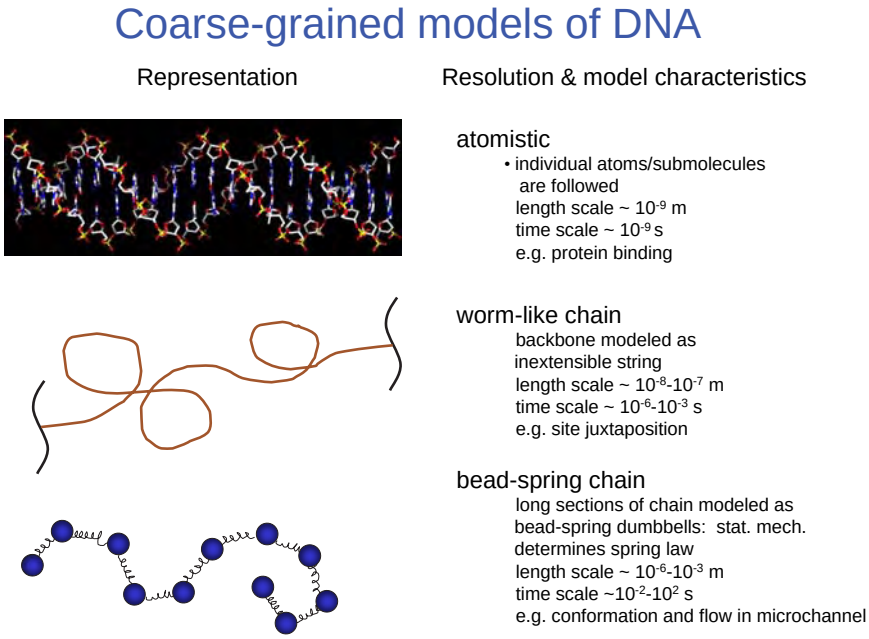

Figure 2: Illustration of scales involved in modeling DNA.
(Figure courtesy of Michael Graham)

Furthermore, simulations of complex, multiscale systems are often just one component of the overall problem. Continuation or homotopy methods to compute steady-state solutions, parametric studies of state solutions, optimization and optimal control problems, and computing feedback control settings in real time, require *many* computational solutions of multiscale systems.

The successes of the past few decades impose their own pressure on applied mathematics. Modern mathematical techniques such as homogenization theory, renormalization group techniques, hybrid numerical methods, operator splitting, variational multiscale analysis, and adaptive discretization and modeling (as an incomplete list), have produced significant advances in terms of understanding multiscale problems, thus supporting the ambition to study even more complex multiscale problems. It is true that most, if not all, of these methods can be traced back directly to classical techniques in applied mathematics. In particular, many of these methods assume a large separation between scales and are commonly applied with the goal of describing the behavior on one scale. Nonetheless, they represent a significant evolution from classical methodology. However, in contrast to classical methods, these techniques have been developed and employed in very specific scientific and application areas, and multiscale research remains largely disjoint among physical disciplines. For this reason, researchers are unlikely to be familiar with more than a couple of these methods, creating the challenge to develop an overall framework

3.3 An argument for the necessity of truly multiscale mathematics

We present a notional discussion based on advances in high performance computing hardware and the development of mathematical algorithms to argue in favor of two points; (1) the development of advanced mathematical solution algorithms during the past twenty five years has provided an effective speed-up that is on the same order as that provided by advances in hardware, (2) the solution of truly multiscale problems based on simulation at the single, smallest scale can

not be used to accurately solve these type of problems, at least not during our research careers. This argument is based on extrapolation of supercomputing hardware advances over the past twenty five years, and the scaling complexity of state-of-the-practice solvers for both elliptic partial differential equations (PDE) and molecular dynamics (MD) calculations.

Over the past twenty five years, there has been a tremendous increase in computing power arising from advances in the semiconductor industry and computer architecture design. The largest-scale scientific computing platforms have transitioned from single processor vector computers and small-scale multiprocessor vector computers (4 to 16 processors) to large-scale massively parallel computers using scalar CPUs (~100 to 10000 processors) and clusters of scalar and vector CPUs (~100 to 4000 processors). The increase in CPU capability and memory capacity represented by these machines is shown in Figures 3 and 4, and represents an increase of 6 orders of magnitude. The data from 1994 (Paragon) to 2003 (Earth Simulator) indicates roughly a doubling of the peak Gflop rate every year. This is faster than Moore's law and includes the additional effects of adding larger numbers of processors and/or more powerful processors in the most advanced machines.

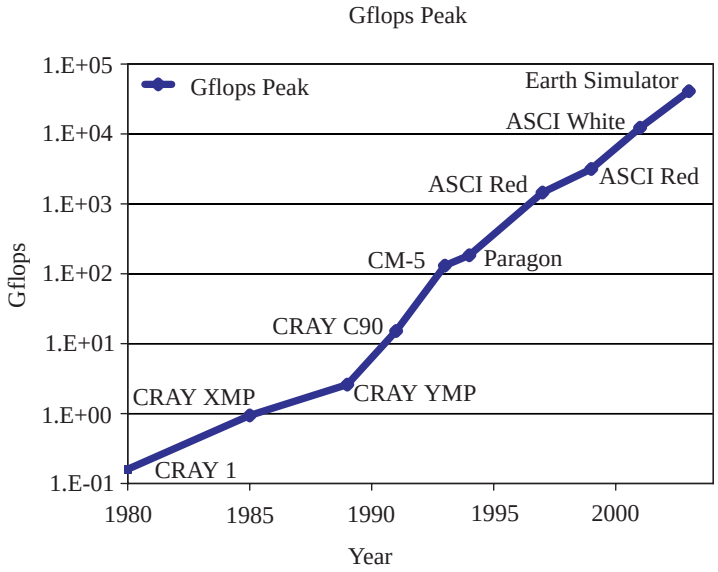

Figure 3: Hardware Performance (Gflops)
(Figure courtesy of S.J. Plimpton and J.N. Shadid)

Simultaneously, there have been developments of mathematical algorithms in several fields, e.g., the solution of partial differential equations and simulation of molecular dynamics, that have kept pace with progress in hardware and we now perform large-scale engineering and scientific simulations that were undreamed-of two decades ago. For example, in appropriate problems, algorithmic developments have decreased the computational complexity of solutions to PDE problems from $O(N^3)$ to $O(N)$, where N is the number of unknowns, by the replacement of direct matrix factorization techniques with iterative solution methods. In Figure 5, we show the approximate increase in normalized speedup due to these algorithmic advances for solutions of a representative elliptic partial differential equation, the Poisson equation, which is a common kernel in many computational elliptic PDE solution methods. Historically the size of PDE simulations has been limited by system memory size and total CPU speed. In this figure, the size of the LINPACK benchmark matrix solve, for a given machine in a given year is used. It should be pointed out that using a sparse matrix algorithm to set the reference problem size would have increased the

expected normalized speed-up of the lower complexity algorithms. Figure 6 indicates the approximate speedup from the brute force $O(N^2)$ algorithm for MD simulations to a lower complexity O(N) method. Simulation sizes have been historically limited by total compute rate (Gflops). In this figure, the largest simulations in 1980 have been scaled by total compute rate to arrive at the problem sizes (number of atoms) that can be simulated on a given machine. This scaling corresponds roughly to the largest simulations that can be run for reasonable total simulation times. Today, these advanced solution methods are often being employed by leading researchers on very large systems and provide optimal complexity for appropriate single-scale simulations. In this context, algorithmic developments have provided commensurate relative performance increases to the strides made in hardware.

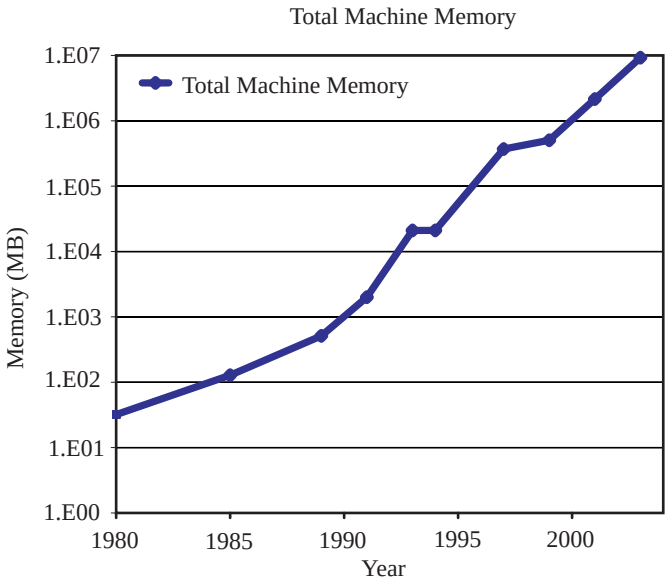

Figure 4: Hardware Total Memory (MB)
(Courtesy of S.J. Plimpton and J.N. Shadid)

Yet, even with extrapolating continuing hardware advances and assuming optimal complexity algorithms, we cannot compute ourselves out of the problem of understanding the mathematics of complex multiscale systems. For example, consider the modeling of a simple premixed turbulent combustion problem with, say, Reynolds number *Re=10,000* and Zeldovich number *Ze=100*. The ratio of the largest length scale, *L*, to the Kolmogorov scale, I_K, is $L/I_K = 10\ Re^{3/4}$ for hydrodynamic turbulence. Further for a premixed turbulent reacting flow problem $L/I_R=10\ Ze\ Re^{3/4}$, with smallest reaction length scale I_R. Therefore a direct numerical simulation (DNS), a single-scale approach, is estimated to require $L/I_R=10^6$ in each spatial dimension while the largest simulations to date solve with $L/l_R < 10^3$. Accounting for numerical stability concerns which limit the time step with respect to the spatial discretization, accurate reacting flow DNS would seem to require computations that are 10^{12} larger than current computations. Extrapolation using current hardware advances and optimal algorithms suggests that it will be 40 years before we see this necessary improvement in computing power. A similar rough computation for a crack propagation problem in 1 cm^3 of Copper ($\sim 10^{23}$ atoms) using a molecular dynamics (MD) computation suggests that it will be at least 80 years before we can perform accurate simulations by a single-scale

solution method for one second. Currently, the largest MD simulations are approximately 10^9 atoms and take 10^5 femto-second (10^{-15}) sized time steps.

These relatively simple multiscale examples demonstrate the limitations of single-scale methods. Clearly, a truly multiscale mathematics and computational approach for modern multiscale problems is required in order to tackle the ever more complex problems of interest to the DOE Office of Science.

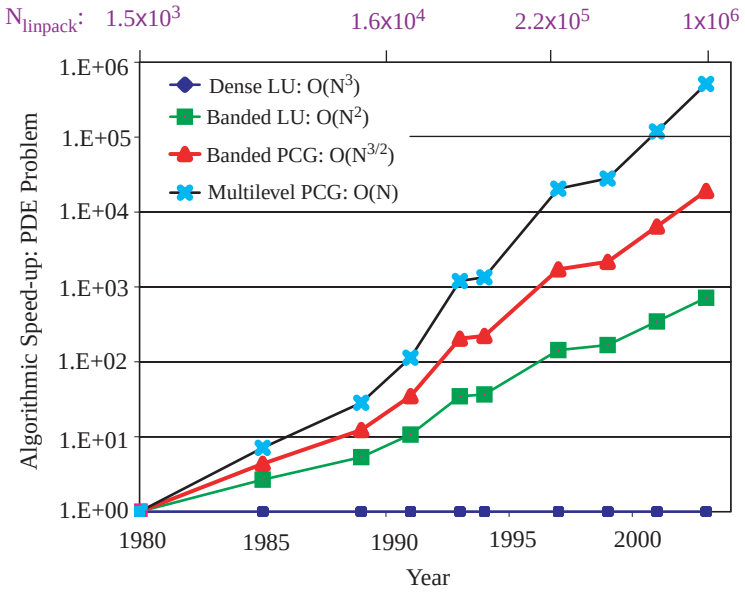

Figure 5: Approximate Speed-up of Solution for PDE Problem (Courtesy of S.J. Plimpton and J.N. Shadid)

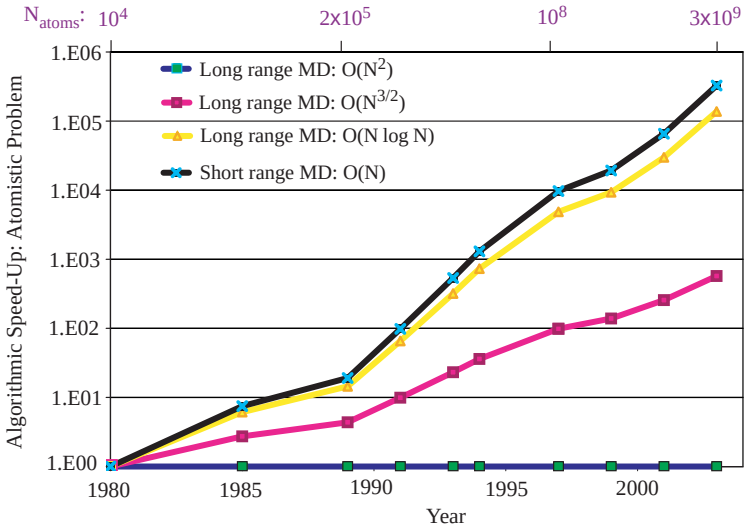

Figure 6: Approximate Speed-up of Solution for Atomistic Problem (Courtesy of S.J. Plimpton and J.N. Shadid)

4. Multiscale Problems: Future Directions

4.1 Mathematical issues arising in modern multiscale problems

The key mathematical and physical issues arising in modern multiscale problems occur across a wide range of scientific and engineering disciplines. Due in part to the historical development of mathematical techniques for multiscale problems, these issues have not been clearly identified or abstracted. The identification and categorization of common issues is an important step in the process of developing mathematical frameworks for multiscale analysis that can guide development of advanced techniques. As an incomplete list, some key issues include:

- Determining the scales to be included over the various portions of the space-time domain and the form and strength of the coupling between scales with regard to the desired information to be obtained from the model. (This basic question of modeling has gained new significance in light of the advances in science in measuring and describing behaviors at different scales.)
- Selecting the appropriate model for each scale that captures the relevant physical behavior. (In many situations, we are still using crude models because of perceived or real limitations in the ability to produce computationally feasible models and to successfully link models.)
- Understanding how to link the information obtained from models at various scales in order to ensure the effects of this linkage are controlled. (As part of this issue, it is important to understand how to ensure models selected at various scales are capable of producing and transferring the desired information to other scales.)
- Ensuring that the errors associated with the transfer of solutions and the approximations or representations used for the component models are adequately controlled. (This is a difficult issue even when we know the basic relations between quantities at different scales.)
- Characterizing the essential properties that a “closure’ model must have to provide physically realistic behavior in the context of a specific multiscale application. (The development of some general multiscale mathematical frameworks for classes of important problems will help to understand this key issue in multiscale modeling.)
- Determining model parameter values needed to exercise each of the models at various scales and quantifying the effect of uncertainty in parameter values as it propagates through the component models at each scale, and by the inter-scale transfer operators, to the quantities of interest. (This is a critical issue in applications to “real world” scenarios. While progress has been made on uncertainty quantification of individual models, much less is known about uncertainly quantification in the context of complex multiscale problems with possibly heterogeneous component scale models.)
- Estimating and controlling spatial and temporal discretization and integration errors. (These classical concerns gain new importance in the context of solving complex multiscale problems where errors from each component and the transfer of information between scales can impact the results from the other scales in both obvious and subtle ways.)
- Developing mathematical analysis tools and producing results for the consistency, stability, convergence and accuracy of complex multiscale methods applied to prototype multiscale problems and challenging applications.

To be brief, we might sum up the key mathematical issues as the development of a more general description of *scale representation, scale separation, inter-scale communication and the ability to apply mathematical analysis to multiscale solution methods.*

4.2 Research directions in mathematics for multiscale problems

On the most basic level, there is pressing need for developing new mathematical methods and continuing work on existing mathematical methods such as

- WKB and renormalization group techniques
- Homogenization theory
- Hybrid numerical methods
- Averaging methods
- Variational multiscale analysis
- Reduced systems
- Model decomposition, e.g., operator splitting and parameter passing
- Adaptive mesh refinement and modeling
- Discrete and continuum modeling techniques for network and graph models
- Uncertainty quantification of single-scale models

in order to address the mathematical issues outlined in §2.1. A critical goal is to combine and extend these methods or develop new methods to handle problems in which there are multiple scales that may not be well separated. The report of the First Workshop and the session reports from the Second Workshop presented in §4 below contain specifics on particular approaches, what is currently lacking, and what might be achieved.

From the perspective of the mission of the DOE, developing and applying mathematical methods in the context of realistic applications important to the DOE is another critical goal. Mathematics must be informed by scientific and engineering reality in order to focus on overcoming the physically meaningful difficulties and obtaining physically meaningful information from models. A reoccurring conclusion that arose during the discussions in the Second Workshop is the need to fund truly interdisciplinary research.

Beyond research in specific methods and problems, there is also a strong need for abstract mathematical frameworks for important classes of multiscale problems. These techniques can provide a common language for formulating and analyzing multiscale problems across a range of scientific and engineering disciplines. 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. The creation of abstract mathematical frameworks would allow categorization and clarification of characteristics of existing models and approximations in a landscape of seemingly disjoint, mutually exclusive, and ad-hoc methods. It is very likely that such mathematical frameworks will encompass a variety of analytic and numerical methods.

5. The DOE Investment in Multiscale Mathematics

The DOE is recommended to pursue a multi-prong strategy in funding research in multiscale mathematics. There is no doubt that there are individual projects and individual researchers that can make fundamentally important contributions to multiscale mathematics, so the DOE should continue to support individual investigator research. But, there is also a strong need for new funding models. In particular, the overwhelming consensus is that future progress on multiscale problems requires the efforts of interdisciplinary teams of researchers comprising mathematicians, scientists and engineers, and computer scientists. Because of differences in funding requirements and culture, truly interdisciplinary research is difficult to fund through traditional avenues. The practical, problem solving orientation of the DOE mission places it in a unique position to fund the interdisciplinary activity that is required to get the job done.

As part of the goal of supporting interdisciplinary research, the DOE should encourage the development of closer ties between researchers at the DOE laboratories and at the universities. DOE funding of research projects should include significant resources to support long term visits by students, postdocs, and faculty to DOE laboratories. The DOE could even go as far as creating a DOE Postdoc program analogous to the NSF Postdoc Program, in which a postdoc would choose co-advisors from a university and a DOE laboratory and pursue an interdisciplinary project that involves periods of residency at both locations.

The DOE should also improve the basic infrastructure among partner universities in large projects by providing funds for the creation of teleconferencing and videoconferencing facilities. In addition continued organization of workshops like the First, Second, and Third DOE Workshops on Multiscale Problems are encouraged. In terms of initiating the creation of an institute(s) focused on multiscale mathematics, the participants of the workshops had mixed reactions and no clear consensus emerged.

6. Specific Reports on Aspects of Multiscale Problems

We next present reports that cover specific aspects of multiscale problems. These reports should be considered as complementing the problems and methods discussed in the reports from the First and Third Workshops.

The Second Workshop was organized into sessions devoted to a particular set of mathematical methods and/or multiscale applications raising mathematical challenges. Each session comprised an introductory overview lecture presented by the session organizer, followed by three shorter talks addressing specific issues in the subject of the session, followed by a group discussion. The session organizers prepared the final reports for their sessions. We also received final reports from two invited speakers who were chosen to add breadth to the meeting.

In presenting the reports, we first arranged them according to whether they emphasized mathematical technique(s) or applications, and then grouped reports that covered similar topics together. It would not be difficult to find other natural arrangements of the material.

6.1 Mathematical Techniques

6.1.1 Adaptive Discretization and Modeling

Session VI: ***Adaptive Modeling and Simulation***

Organizer

Mark S. Shephard, Rensselaer Polytechnic Institute

Contributing Speakers

Victor Barocas, University of Minnesota
C. William Gear, NEC Research Institute
Roger Ghanem, John Hopkins University

Fundamental advances in physical and biological sciences and the development of new measurement and characterization tools have made it possible to understand spatial and temporal phenomena on the atomic, molecular, microscopic, and macroscopic scales. Microelectronics has led this revolution through the development of integrated circuits. Recent progress in nanotechnology and biotechnology has extended the envelope of scales, making it possible to design starting from nanoscale building blocks. The ability to continue to accelerate these advances and to translate them into practice will require the ability to reliably execute multiscale simulations. The effective application of these multiscale simulations will require the development of adaptive methods that apply the appropriate models and discretizations over the space and time scales of the problem.

Multiscale simulation is central to essentially all key DOE applications. A quick examination of the DOE ASCI and SciDAC application areas quickly reveals that each of them involved consideration of multiphysics behavior on multiscales that range over 12 orders of magnitude in space and 15 orders of magnitude in time. All of these applications currently involve scientific investigation at multiple scales from (sub) atomic levels to full scale systems. Increasingly, these applications are expanding their efforts to account for the interactions of the multiple scales in the simulations applied.

The goal of adaptive methods is to control the errors associated with a simulation. In the case of multiscale simulations the sources of error include:

- Scales included over the space/time domain of the problem. Interacting scales of importance range from sub-atomic interactions over femtoseconds to the prediction of long term weather patterns on the global scale. Issues to be addressed include the determination of the scales to be included over the various portions of the space time domain and the form and strength of scale coupling,
- Models selected at each scale. Within any scale how do we select the appropriate model that will capture the physics to be modeled?
- Parameter values used in each model. How well do we know the parameters needed to exercise each of the models at the various scales? How to we account for the variability of these quantities in the prediction of the quantities of interest?
- Scale linking errors. How information from models on different scales is linked together across the scales in a meaningful way and how do we ensure any errors introduced in this process are small enough?
- Solution transfer errors. Even if we know the basic relations between quantities at different scales, how do we ensure that the errors associated with the transfer of solutions on the discretizations used for those models are adequately controlled?
- Equation discretization errors (space, time, etc.). The equation discretization methods used to solve each of the individual mathematical models will introduce their own errors. How are those errors controlled?
- Mismatch of models at different scales. How do we ensure that the models selected at the various interacting scales are capable of transferring the appropriate information between scales? How do we control errors associated with the mismatch that can arise when different models are used to represent the desired behaviors on the various scales?
- Nonlinear equation solution errors. How do we qualify and control errors involved with solving large non-linear systems when they are defined from multiple models interacting over multiple scales?

The desired approach to execute an adaptive multiscale simulation would be to start with a coarse scale model and adaptively enrich it to include the scales, models and discretizations needed to predict the quantities of interest to the desired level of accuracy. This requires effective means to estimate the changes in solution from finer scale models without the application of those models over the entire domain. Although progress has been made on the development of discretization error estimators for this purpose for some classes of mathematical models, such capabilities have not been developed for the other sources of errors. Significant effort will be required to address the questions associated with the development of useful error estimates and correction indicators for the various components of the mathematical framework that is beginning to form for multiscale modeling and analysis.

Central to the development of any adaptive multiscale method is the development of formalized mathematical methods for multiscale modeling and analysis since they provide mechanisms needed for the development of error estimates. An examination of the current efforts on the development of mathematical frameworks for supporting multiscale analysis clearly provides opportunities for the development of adaptive error control. As these methods begin to form an integrated mathematical

framework for multiscale modeling and analysis, specific attention must be given to the adaptive application of the methods included to meet the needs of the many multiscale problems of interest.

The relation of the integrals in variational multiscale methods [7,8] might lead to the natural definition of norms for which error estimates can be developed. Efforts on the development of the Heterogeneous Multiscale Methods [2] should provide the opportunity to apply various mathematical error analyses. The overall structure of the expansions that arise in the application of mathematical homogenization [4] to multiscale analysis immediately identifies the terms on which to concentrate error analysis. Continued generalization of these technologies [3] to include more spatial and temporal scales, including properly represented discrete scales, holds substantial promise for the development of adaptive multiscale methods. Examination of the multiscale extensions to generalized non-linear equation solving technologies being developed in the Equation-Free Multiscale Method [5.9] will also provide mechanisms for the development of multiscale error estimates. Finally, the appropriate quantification and modeling of uncertainty [6] across the various scales is critical to properly account for the stochastic nature of many of the processes that are being modeled.

Some investigators are already beginning to consider the inclusion of adaptive control methods in the multiscale simulations they develop. Adaptive procedures have been added to the quasi-continuum method that locally refine the model to the molecular mechanics level where needed [10]. Basic concepts from multilevel solution methods (e.g., adaptive multigrid) have been used to adaptively control the linkage of continuum discretizations and molecular mechanics models to predict the initiation and growth of atomic level defects [1]. These procedures are guided by two correction indication criterion that attempt to assess the level of non-locality and non-linearity present and adjust the molecular mechanics model, which models these behaviors, where needed.

The development of multiscale simulation technologies will require appropriate combinations of expertise that can only be provided by multidisciplinary teams. At the heart of the development of the methods is the development of the needed mathematical methods to allow the various multiscale modeling methods to provide useful error estimates for the various error contributions. The ultimate success of the development of these methods requires appropriate interactions with the physical modelers to ensure the methods are relevant to the physics being modeled. Since the various mathematical methods for multiscale modeling currently under development have relative strengths with respect to the classes of physical models they are best suited to address, expertise on the appropriate physical models is important for selecting an approach and identifying the parameters of interest to be determined. In addition, the knowledge of physical modelers will provide insights that are useful in the development of the needed multiscale correction indicators and adaptive control methods.

The development of adaptive multiscale methods will also need to engage computational scientist and software specialist. The application of an adaptive multiscale analysis will need software structures that can deal with multiple models and discretizations, and can ensure computational efficiency as the models and discretizations are adapted during the simulations. These software structures and associated algorithms become even more complex when consideration is given to the fact that most of these simulations will need to be run on large scale distributed memory parallel computers.

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Session IV: *Simulation and Modeling of Multiscale Problems*

Organizer

Graham F. Carey, University of Texas at Austin

Contributing Speakers

Steve Bova, Sandia National Laboratory
Donald Estep, Colorado State University
Michael Holst, University of California at San Diego

Methodology

The focus of the session dealt with multiphysics/multiscale problems and adaptive procedures where space and time scales are an issue. The speakers described several representative applications of DOE relevance to illustrate the main ideas and challenges. For example, Steve Bova discussed the problem of multiscale issues that arise in coupled physics problems and the challenge of developing frameworks such as the Sierra framework from Sandia. He provided examples involving heat transfer and thermomechanics to illustrate the ideas. Don Estep described some reaction diffusion problems where the time scales may vary by different orders of magnitude and stressed the need for new algorithms such as operator splitting strategies to treat these more effectively. In his talk, Mike Holst also dealt with some operator splitting strategies to deal with multiscale issues.

It was clear from the discussion that there were still several open issues regarding the appropriate way to deal with different time scales. Most of the discussion of spatial scales considered adaptive mesh strategies as a basic tool necessary to handle boundary layer and similar multiscale problems.

Some related comments:

- Todd Arbogast and Ralph Showalter discussed homogenization and porous media problem. One point that came out is that this technique, like many other techniques, requires a large

separation of scales. There is a need for techniques that work without a large separation or for which there are a number of intermediate scales.

- Graham Carey asked about separating slow and fast times scales. Joe Tribbia discussed weather computations separate fast and slow time scales, but this can be done because they line up with physical phenomena, i.e., convection and diffusion. When the separation does not align with physical effects, it is not clear how this could be done.
- John Shadid ventured the opinion that adaptivity can handle some scale issues, but it generally has to be combined with other analytic methods.
- Don Estep said that an important outstanding problem in adaptivity is developing a theory of optimal mesh selection that allows cancellation of errors in space and time. Existing theories use estimates in which there is no cancellation, so the estimates are orders of magnitude too large. This is especially important in time dependent problems.
- Mike Holst said there should be more theory about convergence of adaptive algorithms. Don Estep countered there should be more theory about accuracy and reliability of estimates as used in practice at the very upper extreme of accuracy (as opposed to the asymptotic, converged limit required for existing results).

Application Areas

The DOE applications are complex. Most of them are nonlinear and coupled. They involve both multiphysics and multiscale challenges. There is a strong synergism between the DOE multiscale objectives of this program and the Lab application activities that should be exploited. This makes a rigorous mathematical treatment very difficult indeed. Usually one can aim for rigorous results such as error estimates, convergence proofs that depend on the multiscale parameters, and so on, in a more limited setting. This is usually accomplished by treating prototype benchmark problems that capture the main essence of the more complex DOE applications. The need for such verification and validation problems and their mathematical analysis was identified as an important area related to the applications component. Mathematical and algorithmic issues concerning modeling error and parameter sensitivity were also singled out. Other issues such as existence and uniqueness results for nonlinear multiscale problems and problems with parameter degeneracy were also mentioned. With respect to homogenization, the general question of a more complete homogenization theory was identified as an important mathematical issue. These problems are shared by a number of applications (for example, in fluid mechanics, heat transfer, solid mechanics), all of importance to DOE.

Some related comments:

- One participant emphasized the common use of operator splitting techniques in the labs and issues related to accuracy and stability of these methods. There is a clear need for more mathematical analysis of the methods in use and for development of new methods.
- A number of applications were discussed: MEMS, thermal problems, reentry vehicles, material properties

The role of a Mathematical Framework

In some sense singular perturbation theory and the theory of matched asymptotic provide the beginnings of a mathematical framework for certain classes of multiscale problems. However, the application of classical perturbation methods is very limited and multiscale today is used in a much broader context, including, in particular, computer simulation. In the latter context, the multiple scales may arise through the mesh sizes of a coarse grid and a fine subgrid problem as well as

through the physical scales (and parameters) of the mathematical models or the scales of underlying microstructures that are homogenized into a macroscopic deterministic model.

There was serious question as to whether a single 'overarching' mathematical framework can be devised. Rather the view of the participants in this discussion was that such a mathematical framework would probably consist of several components tailored towards multiscale classes of problems of interest to DOE. For example, the perturbation analysis mentioned above provides one mathematical framework that encompasses analytical techniques for regular and singular perturbation problems. When such techniques apply they may lead to sequences of perturbation problems with respect to the multiscale parameters and these problems may involve computation. However, such an approach may not accommodate multiscale in the broad sense implied by such issues as homogenization. Moreover, in the case of homogenization, the microscopic problem may encapsulate quite different physics than the macroscopic problems. A mathematical framework for this homogenization component is certainly of interest. On the other hand, variational multiscale methods have also been introduced to incorporate fine mesh effects into a macroscopic model. This is clearly related to homogenization but in variational multiscale the inner scales are more closely allied to the discretization process and a different form of the framework is implied here. Similar points apply to multiscale treatments of transient problems and timestepping. One example of such a mathematical framework might exploit explicit-implicit adaptive timestepping on subregions in conjunction with adaptive mesh libraries. A more general approach might involve adaptive space-time elements.

Funding Initiative

Several avenues for funding of the above activities were discussed in the session. These range from targeted research on specific multiscale questions (in modeling, mathematics, methodology, algorithms and applications) to the funding of centers or academic initiatives for graduate students.

The idea of networking the research regionally and nationally was also discussed. It was felt that teleconferencing and videoconferencing capabilities provide a good mechanism to facilitate integration of work and interaction. If the prime research targets and questions are identified as a result of the workshops then that would certainly provide an opportunity for individual researchers and research partnerships to address key issues. The advantage here (as opposed to funding a more localized large center) is that the most expert people in the country can be brought into the program irrespective of the institution. Such a program does involve a coordination challenge which might be addressed by an annual workshop and program review of participants similar to this present DOE workshop. There is currently an inclination to offer larger grants from single institutions or a consortium of institutions. Such an activity would work best if appropriate participants at the modeling, mathematical and computation level with a good track record of working together, could participate. This would involve a larger level proposal. While the increase in the DOE applied mathematical budget is significant in a percentage sense, it is not a large dollar amount that could support a large multi-university program of this type and still provide adequate resources to involve top researchers not in the institutional consortium. Finally, last but not least, the need for DoE to have a close linkage of university and Lab activities strongly suggests a significant program in which students at universities spend part of their time at the Labs. Hence a fellowship activity of this form should be strongly considered.

Some related comments:

- There appeared to be lukewarm reception for the idea of an institution as the most effective way to address these issues.

- There were similar feelings about the regional network idea that G. Forest described in his keynote lecture.
- Don Estep proposed a DOE series of graduate texts on multiscale mathematics, with DOE providing support to faculty that write such a text.

6.1.2 Variational Multiscale Analysis

Session III: ***Variational Multiscale Analysis***

Organizer

Pavel Bochev, Sandia National Laboratories

Contributing Speakers

El-Azab Anter, Florida State University
Kenneth E. Jansen, Rensselaer Polytechnic Institute
Asad Oberai, Boston University

Introduction

Variational multiscale analysis (VMA) is a systematic approach for modeling of multiscale phenomena in computational sciences. VMA is based on decomposition of the state space into "*resolved"* and "*unresolved"* scales and a subsequent derivation of *exact* governing equations for each scale. In conjunction with appropriate modeling assumptions, these equations serve to provide the basis for variational formulations capable of representing multiscale phenomena. Most notably, the VMA framework allows one to identify readily the appropriate scale-to-scale interactions and to replace interactions that depend on unresolved physics by suitable model terms.

The VMA formalism is applicable to a broad class of multiscale phenomena, ranging from problems where scale separation is induced by choice of a discrete space ("*resolved"* scales), to problems where resolved and unresolved scales may represent concurrent mathematical models of the physical process, operating at different space and/or time scales. In the former case, scale separation reflects computational choice, while in the latter; it is governed by the need to employ different mathematical descriptions of the physics in order to achieve certain modeling and simulation goals. Successful applications of VMA include

- Turbulence, shear banding in plasticity
- Flows in porous media
- Dynamic parameter identification in models
- Atomistic to continuum bridging

These are complex and non-trivial applications where VMA has helped to obtain reliable and accurate results. For example, in turbulence modeling VMA has led to formulation of methods that are comparable in accuracy with DNS calculations. This is illustrated by the plots in Figure 1, where several turbulence models, including a VMA approach, are compared with DNS results (Coleman, Kim and Le, 1996).

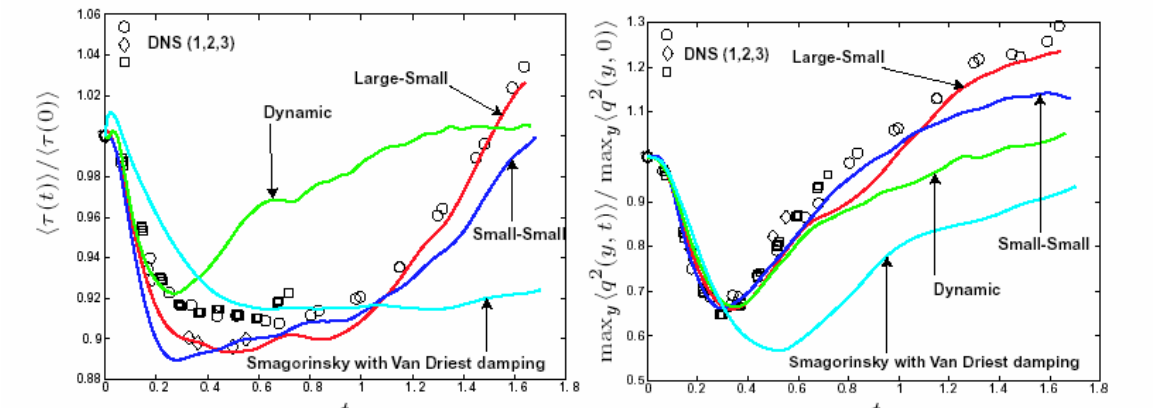

Figure 1: Non-equilibrium channel flow at Re=180 (Hughes et al 2003)

Why a framework is needed

There are several compelling reasons to seek a framework that provides an abstract setting for modeling and simulation of a broad class of multiphysics and multiscale problems. Existing approaches in multiscale science and engineering have evolved from a range of ideas and solutions that are reflective of their original problem domains. As a result, research in multiscale science has followed widely diverse and disjoint paths, which presents a barrier to cross pollination of ideas and application of methods outside their application domains. For instance, multiscale problems characterized by discrete-to-continuum and continuum-to-continuum connections have relied on statistical mechanics and homogenization theory, respectively, to enable inter-scale coupling and transfer. The new challenge lies in the need to have mathematical models of the physical phenomena that incorporate multiple scales rather than just two principal scales. For example, in the context of atomistic-to-continuum bridging, a mix of ODEs and PDEs governs the discrete and the continuum scales, respectively. While computational and theoretical tools exist for each model, coupling of discrete and continuum variables underscores the need for a new mathematical formalism that can handle them simultaneously.

Consequently, the status of the research environment calls for an abstract mathematical framework that can provide a common language to formulate and analyze multiscale problems across a range of scientific and engineering disciplines. In such a framework, critical common issues arising in multiscale problems can be identified, explored and characterized in an abstract setting. This type of overarching approach would allow categorization and clarification of existing models and approximations in a landscape of seemingly disjoint, mutually exclusive and *adhoc* methods. More importantly, such an approach can provide context for both the development of new techniques and their critical examination. Furthermore, notwithstanding the richness of multiscale problems, the key mathematical and physical issues arising in multiscale problems: scale representation, scale separation, and inter-scale communication are ubiquitous, and occur across a wide range of scientific disciplines. Consequently, there is a need for a mathematical framework that unifies these common principles and helps to analyze multiscale problems in a rigorous and systematic way. Such a common mathematical framework for multiscale analysis can:

- Identify inconsistencies between the components of the model;
- Formalize the transition process between the components;

- Identify the terms critical for the coupling of the components and focus on their mathematical and physical properties;
- Serve as a proof of principle and concept for complex mathematical models.

In doing so, such a framework will enable advances that address the following main challenges in multiscale modeling and simulation:

- Coupling of models with different physics and/or operating on different scales
- Bridging the scales
- Inter-scale transfer operators
- Incorporation of uncertainty quantification

Availability of a common framework can provide further insight into key issues such as

- Selection of scale separation: artificial vs. problem driven?
- How to incorporate existing tools from, e.g., statistical mechanics or kinetic theory?

Finally, a framework can ensure a systematic and mathematically sound foundation for validation of multiscale simulations, and uncertainty quantification.

The role of VMA

VMA is an extremely flexible modeling and computation tool that encodes structures ubiquitous in both physical models and computational methods. For instance, problems ranging from turbulence modeling and Dirichlet-to-Neumann maps, to computational techniques such as multigrid, Domain Decomposition, hierarchical bases, and mortar elements, can all be developed using the principles of VMA. Since VMA allows formulating general characteristics of how multiple scales interact, VMA can provide the means necessary for a unified and systematic description of multiscale models and their numerical solution. The VMA approach allows one to identify readily scale-to-scale interactions and to replace those interactions that depend on unresolved physics by appropriate model terms. Theoretical properties of the interaction of modeling assumptions on the various scales can be developed by use of variational equations, the properties of the spaces and the associated projection operators. Of course, the particular choice of basis functions used to represent the solutions as well as the number and partitioning of this basis are critical numerical algorithmic design issues that will change from application to application. What is important, however, is that VMA is flexible enough to accommodate a wide range of representation techniques, including multiscale enrichment, partition of unity, and hierarchical decompositions, to name just few.

The roadmap

The state of research in multiscale science and engineering has progressed to the point where there is a definitive need for an overarching mathematical framework that unifies common principles across disciplines in a systematic and rigorous fashion. To this end, the variational multiscale analysis has been identified as a viable candidate for such a mathematical framework, a fact supported by both theoretical considerations and practical successes. However, as with any modeling technique, VMA requires physical inputs and will not provide the correct responses unless it incorporates the correct physics. Therefore, to exploit the power and promise of VMA, it is of paramount importance to develop a careful understanding of the physical phenomena and how a mathematical separation of scales interacts with a physical based view of scale separation. Mathematicians can be instrumental in the identification of classes of problems for which the framework is applicable. Development, validation and subsequent computational modeling will require close collaboration between mathematicians, physicists, computational scientists and

engineers. Therefore, a viable funding strategy to achieve the desired advances in multiscale modeling and simulation is to support interdisciplinary collaborative research focused on a set of applications that are relevant to the DOE Office of Science.

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Session VII: *Variational Multiscale Methods and Multiscale Finite Elements for Heterogeneous Porous Media*

Organizer

Todd Arbogast, University of Texas at Austin

Contributing Speakers

Yalchin Efendiev, Texas A&M University
Seong H. Lee, Chevron-Texaco Petroleum Technology Company
Juanes Ruben, Stanford University

Overview

Multiscale (i.e., "generalized") finite elements were introduced by Babuska and Osborn in the 80's, and they have seen a reemergence for handling problems with natural heterogeneities. The method involves solving the overall partial differential equation on a course grid by incorporating system microstructure directly into the finite element basis itself. This is accomplished by solving local or subgrid problems that resolve the microstructure. In this way, one can improve the overall resolution of the finite element approximation. Multiscale and variational aspects of the method have recently been put on a sound theoretical foundation. This session will explore various developments that have tailored such methods to solving problems in simulating flow and transport in porous media.

Variational Multiscale Methodology

Variational methods have revolutionized the study and approximation of partial differential systems. They allow an analytical approach: one can "test" or sample a differential equation in various ways to separate effects and competing behaviors. Variational methods also gave rise to

the finite element method, and further refinements such as finite volume methods, and they shed considerable light on existing numerical methods such as finite difference, spectral, and collocation methods.

The Variational Multiscale Method (VMM) or framework is a refinement of the variational method that allows one to consider modeling the part of the system that is traditionally unresolved in more classical approaches. One separates both the solution and test functions into coarse and fine (or "subgrid") pieces. By restricting the test functions to either the coarse or fine scale, we have a natural scale separation of the dynamics of the system. Traditional analysis simply drops the fine scale parts as being unresolvable. In the VMM, one tries to either directly approximate these parts of the system, or model their effects in some reasonable way. The beauty of the VMM is that, as a variational method, it naturally allows one to develop multiscale models that both respect the physical integrity of the system and produce computationally efficient schemes.

The method is particularly well suited for elliptic partial differential systems, such as second order elliptic systems and Stokes or Navier-Stokes flows. In this session we concentrated on second order elliptic systems, which govern the Darcy velocity of flow in a porous medium. A major issue here is to handle the fine scale heterogeneity of the medium, i.e., the permeability, which is the main coefficient of the partial differential equation. The permeability can vary over several orders of magnitude over very short spatial scales, which gives rise to fine scale features in the flow field.

The Multiscale Finite Element Method (MsFEM) approximates the solution of the variational problem by using coarse-scale finite elements that incorporate the fine scale details of the flow into their definition, that is, the microstructure of the permeability determines the finite element basis functions that one uses. MsFEM fits naturally into the VMM framework, because we can view the coarse-scale MsFEM basis as arising from the solution to the fine scale part of the VMM system. However, the VMM framework is more general than MsFEM, since it allows greater flexibility in the modeling.

The VMM can be viewed as an upscaling procedure. The scale splitting allows one to remove explicit reference to the fine scale. In this form, it is easy to see that the upscaled variational problem remains elliptic, but the form of the ellipticity is not the same as in the original system. The fine scale influence is nonlocal, anti-diffusive, and contains an affine correction. Much

upscaling work makes the erroneous assumption that the upscaled equations will be elliptic of the same form, and result in upscaled systems that are too diffusive. It appears that virtually all attempts at upscaling, except the VMM, miss the affine correction terms in the equations. This is significant, as they are related to the source/sink terms. For subsurface flows, sources and sinks are often quite small (e.g., wells or relatively small leaking storage tanks), providing another fine scale feature that must be upscaled in the equations.

The VMM or MsFEM can be used to produce flow fields defined on the fine scale. The method does not fully resolve all of the fine scales of the flow, but it does a good job in capturing the main fine scale features, and we do not see degradation in time for transient problems. Moreover, this increased level of resolution then naturally allows us to couple results to other parts of the system. This is especially important in nonlinear problems, where simply knowing the average behavior is insufficient to determine the nonlinear effects.

The VMM or MsFEM is computationally very efficient. The construction of the multiscale basis requires the solution of a series of small local problems. These can be solved easily, even by direct methods, and, since the local problems are independent of each other, they naturally parallelize. One is then left with a global problem defined on a coarse grid, which is much easier to solve than

a fully resolved global fine grid problem. Similarities were noted between VMM ideas and various multigrid techniques, such as the operator based and Shur complement methods. Additional research in this area could result in improvements to both techniques. It was noted that grid adaptation and non-nesting of coarse and fine space grids has not been considered. Additional research in these areas should complement and improve the VMM. Finally, it was suggested that the VMM should extend to the more general context of variational inequalities.

Variational Multiscale Application Areas

In this session we concentrated on finding the Darcy velocity of flow in a porous medium. The main difficulty is to handle the fine scale heterogeneity of the permeability, which can vary by several orders of magnitude over very short spatial scales, and the fact that wells are very small. The session considered extension of the VMM and MsFEM to nonlinear problems, finite volume discretizations, and multiphase flows. Additional research is needed to model long range coherent heterogeneities. Random heterogeneities tend to cancel themselves out over space, and so many methods model these quite well. The VMM is well suited for coherent structures which do not cancel out over space, but rather the fine scale details of the permeability give rise to large scale flow behavior. Channeling is one important example that needs more research. Resolving high permeability channeling effects is difficult, as it is very sensitive to the details of how one localizes the computations (which is necessary in practice to make the method practical), that is, to the local boundary conditions that one uses. Conversely, we have low permeability "barriers." It was reported that different implementations of the VMM ideas have varying success with channeling and barriers, some working relatively well and some not.

The VMM needs further development to handle additional problems and multiscale features. One such area is reactive flow modeling, which have multiple time-scales as well as multiple spatial scales. The modeling of transport is also an interesting possibility. The VMM has been used to incorporate the fine scales as regards numerical stability on coarse grids, but it so far has not been found to be useful in improving the resolution of the solution itself. Hysteresis, well modeling, and various additional physics have not yet been considered.

The VMM should be applicable to the more general problem of reservoir characterization and quantification of uncertainty. The handling of fine scales, appropriately in this case in a simplified way, should improve our understanding and use of the sparse data we are able to collect regarding subsurface environments.

Benchmark problems are always an asset to numerical modeling, and would be helpful in this subject area. The 10th SPE comparative solution project does provide some benchmarks, but the problems are quite large and cannot be solved so easily by researchers without production quality code and, especially, linear solvers.

Areas of application of interest to the DOE include most all systems that include large porous media. We list just a few potential application areas. Perhaps paramount are subsurface environmental remediation, contaminant containment, and waste repository design. Many proposed methods of sequestering CO2 involve large porous media. The production of oil and gas from petroleum reservoirs is a natural application critical to the economic health and national security of the nation. Living tissues are often modeled as porous media, so medical research on cancer, heart disease, and drug delivery could potentially benefit.

The Role Of A Mathematical Framework

The framework of the VMM and the concept of the MsFEM is a modeling tool that has been applied across several disciplines, as was noted in this session and in the session organized by

Pavel Bochev. The common terminology, notation, and approach aide in the development in each field, and allows teams of researchers to better communicate about the multiscale issues involved in their particular application. Because the VMM and MsFEM are multiscale variants of by now well established techniques (variational and finite element methods), it is relatively easy for researchers unfamiliar with either the field or with the particular application to begin considering the ideas. Of course, every problem has its own unique multiscale behavior, and the details of the VMM treatment become quite problem-specific, but this overarching framework helps to keep the details within a solid theoretical foundation.

Funding Initiatives

It was agreed that much more research in the area multiscale modeling and numerics was needed, including research regarding the VMM.

Progress in modeling multiscale systems requires expertise in the areas of the application, mathematics, and computation. The DOE can promote such progress in at least two ways. First, interdisciplinary teams of experts need to be funded to collaborate on the issues. This would be the most usual case. Second, after a few decades of emphasizing multidisciplinary research, many researchers have become quite broad in their expertise, and can make substantial progress in smaller groups or even individually. It is therefore recommended that the DOE also fund individual investigator research as appropriate.

The possibility of the creation of an institute for multiscale modeling was discussed. It was generally viewed to be inappropriate for several reasons. First, the total funding in this area is viewed as insufficient to fund all the interesting and DOE relevant multiscale research, much less that and an institute. Second, institutes tend to develop a heavy bureaucracy of their own which does not directly contribute to scientific progress. Third, institutes tend to develop an inertia all to themselves, which makes them unable to keep pace with a rapidly developing and changing field such as multiscale modeling. Finally, and perhaps most importantly, it was noted that there are existing institutes that can be used to bring diverse sets of researchers together without a need for a dedicated institute, such as the Institute for Mathematics and its Applications (IMA) at Minnesota, the Banff International Research Station (BIRS) in Canada, and the DOE laboratories themselves.

6.1.3 Discrete to Continuum Bridging

Invited Report: ***Discrete-To-Continuum Bridging: A Top-Down Perspective***

Author

Jacob Fish, Rensselaer Polytechnic Institute

The talk overviewed state-of-the-art discrete (atomistic) to continuum bridging methodologies and emphasized challenges we are facing in developing a unified multiscale mathematical framework. It appears that a variety of scale bridging methods can be housed under the umbrella of hierarchical mathematical models. Hierarchical models are a sequence of mathematical models, which include increasingly more sophisticated effects. The most-comprehensive member of the sequence is based on the “first principles”, such as Density Functional Theory, which evaluates the system energies by tracing the ground states of the electrons. The modeling error associated with any other member of the sequence (discrete or continuous) is assessed by comparing it to the most-sophisticated member of the hierarchical sequence. A member of the sequence is considered to be admissibly accurate if the modeling error in the data of interest is sufficiently small. The goal is to identify an

optimal member of the sequence, which is both admissibly accurate and computationally most inexpensive.

One of the main challenges is to transfer the appropriate information between various hierarchical models, in particular those stated at discrete and continuous scales. Discrete-to-continuum bridging approaches can be classified into two main categories:

1. Information-passing (other names: sequential, serial, parameter-passing)
2. Concurrent (other names: embedded, integrated, hand-shaking)

Information-passing approaches are designated for problems and processes where different scales are weakly coupled. For weakly coupled multiscale problems, diverse length and time scales can be bridged in a two-way sequential manner, i.e., calculations at finer scales, and of high-computational complexity, can be used to evaluate *equivalent constitutive properties* (using mathematical homogenization theory) or *equivalent elements* (using Variational Multiscale approach) for use in a more approximate or phenomenological computational methodology at a longer length/time scale. Several discrete to continuum information-passing approaches are semi-empirical in nature. One popular example is kinetic Monte Carlo for surface growth, where barriers to adatom motion are computed with density functional theory. Similarly, for discrete dislocation dynamics, mobilities are computed using atomistic simulations. For polymeric materials, the so-called coarse graining procedures are employed to lump several atoms into "superatoms." An example of the information-passing approach in space and time domain is based on *Diffusion Equation Approach*, where diffusion equation is mapped into longer time and larger length scales.

There are many systems, however, which depend inherently on physics at multiple scales. These pose notoriously difficult theoretical and computational problems. Turbulence, crack propagation, friction, and problems involving nano like devices are prime examples. In fracture, the crack tip bond breaking can be described with a quantum-mechanical model of bonding, while the rest of the sample is described with empirical potentials. In friction, it might be necessary to describe surface interaction using quantum-chemical approaches while using continuum elasticity to simulate the contact forces. For these types of problems, multiple scales have to be simultaneously (*concurrently*) resolved in different portions of the problem domain. Various domain decomposition and multigrid-like methods can be used to communicate the information between subdomains represented by different hierarchical models corresponding to different scales.

Successful utilization of the multiscale hierarchical modeling methodology hinges on the ability to develop model error estimators/indicators aimed at guiding the selection of the appropriate member of the hierarchical sequence. For example, the coarse graining procedure for polymers may be controlled by an error estimator based on field gradients. By comparison, the use of KMC may be dictated by an estimator based on the relative rate of the investigated process with respect to the smallest time scale considered in the simulation.

In devising a rigorous discrete-to-continuum scale-bridging framework, the main two barriers are:

(i) Increased uncertainty/complexity introduced by discrete scales as illustrated in Figure 1;

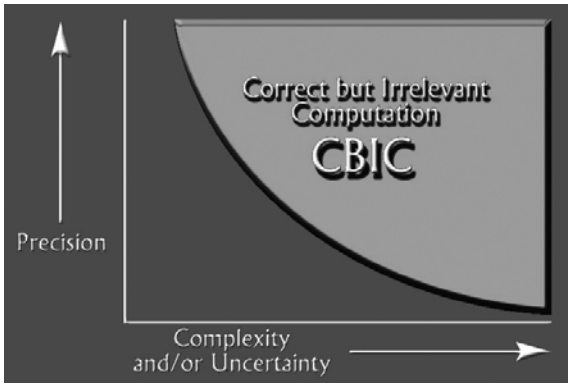

Figure 1: Reduction in precision due to increase in uncertainty and/or complexity

(ii) Multiplicity of physical processes at coarser scales

Increased uncertainty/complexity

As a guiding principle for assessing the need of finer scales, it is appropriate to recall the statement made by Einstein, who stated that "the model used should be the simplest one possible, but not simpler." What is the optimal member of the hierarchical sequence and the need for using discrete scales has to be carefully weighted on case-by-case basis. For example, in the case of metal matrix composites with almost periodic arrangement of fibers, introducing finer scales might be advantageous since the bulk material typically does not follow normality rules and developing a phemenological coarse scale constitutive model might be challenging at best. The behavior of each phase is well understood and obtaining the overall response of the material from its fine scale constituents can be obtained using homogenization. On the other hand, in brittle ceramics composites, the microcracks are often randomly distributed and characterization of their interface properties is difficult. In this case, the use of fine scale models may not be desirable.

Multiplicity of physical processes

Multiple physical phenomena are intimately coupled at the discrete scale. First principle models encompass the whole physics explicitly representing structural, transport, optical, magnetic and electronic processes. Models based at coarser scales represent only one or several aspects of the physics. For instance, atomistic models typically do not incorporate optical, magnetic and electronic information. Continuum models usually represent only one physical process and rarely account for physics coupling. Coupling on continuum scales can be performed either by "equation coupling," procedure in which the PDEs describing a physical process are enriched with coupling terms representing the parallel physics, or by "parameter coupling," in which the system properties entering a PDE depend on the coupled physics. This requires the development of appropriate coupling procedures and specialized error indicators to determine when coupling is required.

6.1.4 Reduced Order Modeling

Invited Talk: ***Reduced-Order Modeling***

Author

Max Gunzburger

Collaborators

In collaboration with John Burkardt, Hoa Nguyen, Janet Peterson, and Yuki Saka (Florida State U.); John Shadid (Sandia); Hyungchun Lee (Ajou U., Korea); Qiang Du (Penn State U.); Lili Ju

(IMA & U. South Carolina). The collaboration with John Shadid is supported by the Department of Homeland Security.

The approximate solution of (nonlinear) complex systems using standard approaches (finite element, finite volume, etc.) is expensive with respect to both storage and CPU costs. As a result, it is difficult if not impossible, to deal with a number of situations such as: continuation or homotopy methods for computing state solutions; parametric studies of state solutions; optimization and optimal control problems (multiple state solutions); and feedback control settings (real-time state solutions). Not surprisingly, a lot of attention has been paid to reducing the costs of the nonlinear state solutions by using reduced-order models for the state. We consider the possibility of approximating a complex system governed by a system of nonlinear partial differential equations using only a handful of degrees of freedom instead of the thousands or even millions of degrees of freedom needed for a finite element, or finite volume, or finite difference, or spectral, etc. approximation. As a result, by paying the up-front cost of solving the full, high-dimensional discrete equations once or perhaps several times, one will be to perform many reduced-order state system simulations at the cost of a single full-order simulation.

A reduced-order method consists of: first, choosing a reduced basis having hopefully very small dimension (determining a reduced basis usually requires perhaps several off-line solutions of the high-dimensional discrete system); then, seeking an approximation to the state in the form of a linear combination of the reduced basis functions; and then, determining the coefficients in the linear combination by solving the state equations, e.g., by a Galerkin method, in the reduced basis space (the cost of such a computation would be very small if the dimension of the reduced basis is very small). There are several potential benefits of using reduced-order models. (We caution that effective reduced-order modeling is not always possible.) In a state simulation setting, a reduced-order method would enable the computation of many states at very little cost. In control or optimization settings, one is faced with multiple state solves or real-time state solves. One can base adjoint or sensitivity equation-based optimization methods on the low-dimensional reduced-order model so that, if the dimension of the reduced basis is small, the cost of each iteration of the optimizer would be very small relative to that using full, high-fidelity state solutions. Compensator, feedback law, etc. design within a feedback control setting can be based on the reduced-order model so that possibly feedback can be affected in real time.

Of course, the key to having any hope of realizing the potential benefits of using reduced-order modeling is having available an “effective” reduced basis. We focus on two types of reduced-order bases: proper orthogonal decomposition (POD) and centroidal Voronoi tessellation (CVT). Both POD and CVT require the generation of a snapshot set from which they remove “redundant” information. The generation of snapshot sets usually requires several solutions of high-dimensional approximations of the state system; the hope is that this perhaps large off-line cost can be amortized over many simulations or optimizations, or enable the real-time, on-line feedback control of the system. Thus, a necessary (but not sufficient) condition for producing effective, low-dimensional reduced bases is the generation of “good” snapshot sets: a POD or CVT basis can be no better than the information contained in the snapshot set on which they are based. Adaptively updating a reduced basis during an optimization or control process is out of the question since it requires the generation of new snapshots which in turn usually requires the querying of the high-dimensional approximate state system; this cannot be done in real-time or is costly to do in the middle of an optimization process. Thus, one is interested in getting all of the information needed or to at least include as much information as one can in the snapshot set before one determines the

reduced-order basis. Snapshot sets should also be obtained as cheaply as possible; one would like to obtain an effective snapshot set using as few runs of the expensive, very high-dimensional simulation code as possible.

Snapshots sets

The state of a complex system is determined by parameters that appear in the specification of a mathematical model for the system; parameters can appear in, e.g., geometrical specifications, initial and boundary conditions, source terms, media-dependent coefficients, etc. Of course, the state of a complex system also depends on the independent variables appearing in the model. Snapshot sets consist of state solutions corresponding to several parameter values and/or evaluated at several values of one or more of the independent variables, most notably time. Thus, elements of a snapshot set can be: steady-state solutions corresponding to several sets of design parameters or a time-dependent state solution for a fixed set of design parameter values evaluated at several time instants during the evolution process or even several state solutions corresponding to different sets of parameter values evaluated at several time instants during the evolution process. Snapshot sets are usually determined by solving a full, very large-dimensional discretized system obtained by, e.g., a finite volume or finite element discretization; experimental data have also been used to determine snapshot sets. A snapshot set itself can sometimes be the reduced basis. On the other hand, snapshots sets often contain "redundant" information; in such cases, snapshot sets can be post-processed to remove as much of the redundancy as possible before they are used for reduced-order modeling; the POD and CVT processes may be viewed as different ways to post-process snapshot sets in order to remove redundant information. At this time, the generation of snapshot sets is an art and not a science; in fact, it is a rather primitive art. The generation of snapshot sets is an exercise in the design of experiments. For example, for stationary systems, how does one choose the sets of parameters at which the state (and perhaps sensitivities) are to be calculated (using expensive, high-fidelity computations) in order to generate the snapshot set? Clearly, some a priori knowledge about the types of states to be simulated or optimized using the reduced-order model is very useful in this regard. The large body of statistics literature on the design of experiments has not been used in a systematic manner. For time-dependent systems, many (ad hoc) measures have been invoked in the hope that they will lead to good snapshot sets. For example, time-dependent parameters (e.g., in boundary conditions) are used to generate states that are "rich" in transients, even if the state of interest depends only on time-independent parameters. In order to generate even "richer" dynamics, impulsive forcing is commonly used. There is certainly the need for developing systematic, rational, justifiable, and effective methodologies for generating good snapshot sets. After all, a POD or CVT basis is only as good as the snapshot set used to generate it. The unintelligent sampling of parameter space can result in "bad" snapshot sets and/or the need to do "too many" high-dimensional state simulations. Unintelligent sampling in time is not so deadly because it does not result in any serious CPU penalties, only storage penalties. One can sample as often as on likes in time with no additional CPU costs; any redundant information included in the snapshot set as result of oversampling in time will be removed by the POD or CVT processes. Of course, if the memory required to store the snapshots becomes an issue, then one should consider intelligent time sampling. Also, the costs of generating the POD and CVT basis depend on the number of snapshots, but this is usually not an important consideration since these costs are small compared to the costs of generating the snapshots using high-dimensional discretization codes

The parameter space sampling needs for snapshot generation are as follows. Perhaps one only knows bounds for the allowable values of the parameters, e.g., $a_i \le \alpha_i \le b_i$, so, we need "intelligent" sampling of hypercubes in parameter space. Alternately, perhaps one knows constraint relations

between parameters, e.g., $\sum_i \alpha_i^2 \leq 1$ so, one needs "intelligent" sampling of more general regions in parameter space. Without any additional information about the parameters, samples should be uniformly distributed. If there is available additional information available about parameters (correlation information, probability distributions, etc.), samples should be nonuniformly distributed. Clearly, properly sampling parameter space is important; remember, one does not want to adaptively update the reduced basis so that we only get one chance to generate snapshots that will be useful throughout the optimization or control process. Also remember that one wants to use as few runs of the high-dimensional simulation code as possible in order to generate the snapshots so that, for the generation of snapshots, one wants to run the simulation code for relatively few values of the parameters. Finally, there may be many parameters appearing in the description the state system that one may want to vary so that parameter sampling may have to be done in a high-dimensional parameter space. Thus, one needs methods for the effective and sparse sampling in regions in high dimensions. There are a huge number of available methods for sampling in, e.g., hypercubes, and a lesser number of methods for sampling in general regions.

Of course, point sampling in regions in R^n is useful in lots of settings. It is the central task in the design of experiments of either the laboratory or computational types. For snapshot generation, one is interested in sampling a small number of points in high dimensions. All types of point distributions are of interest as well, again depending on the application: uniformly distributed points in simple regions (e.g., hypercubes); general regions; nonuniformly distributed points; anisotropically distributed points; and combinations thereof. We caution that sampling methods that are known to be good for a large number of sampling points may not be so good for sparse sampling; likewise, theorems that hold "as the number of sampling points goes to ∞" are useless to us; unfortunately, most sampling methods and the accompanying theorems have been developed for the case of a large number of sampling points. A further cautionary note is that there is a fundamental difference between the design of laboratory and computational experiments: computer experiments are repeatable while, due to noise, laboratory experiments are not exactly repeatable. Thus, sampling methods developed for the design of laboratory experiments (which are biased towards the edges of the parameter bounding box) are not useful for the computational generation of snapshots.

Let us just consider uniform sampling in hypercubes. What makes a point set uniform? For someone that solves PDE's by finite difference methods, a Cartesian arrangement of points would be ideally uniform. For someone that approximates integrals by averaging over sample points, a Cartesian arrangement of points is as bad as it gets! In order to compare different sampling methods, we consider a steady Navier-Stokes problem for which the boundary conditions at several inflow and outflow orifices are determined by 6 parameters; the exact details of the problem description are not crucial. Each of the six parameters are constrained to lie in a bounded interval; thus, after normalization, the parameter space is a 6D unit hypercube. We generate 7 snapshots by sampling 7 points within the 6D unit hypercube and then solving the steady Navier-Stokes equations 7 times, using each of the 7 points to define the boundary data. We then use the 7 snapshots to approximate the solution of the steady Navier-Stokes equations corresponding to other parameter points in the 6D hypercube; the 7D reduced-order approximation is determined by a least-squares projection of the high-dimensional solution of the Navier-Stokes equations onto the span of the 7 snapshots. We use several sampling methods for determining the 7 snapshots: MC - uniform random or Monte Carlo sampling; HAM - Hammersley sampling; LHS - Latin hypercube sampling; CVT - centroidal Voronoi tessellation sampling; LCVT - Latinized CVT sampling; and

CORNER - the six vertices of the hypercube along the coordinate axes and the vertex opposite the origin. We choose 10 random points within the 6D hypercube, solve the Navier-Stokes equations for each of the points, and determine a least-squares approximation for each of these 10 solutions for each set of snapshots. We then sum up the errors over the ten solutions for each of the snapshot sets and provide the results in the table below.

	CORNER	MC	HAM	LHS	CVT	LCVT
velocity error	0.345	0.222	0.333	0.198	0.149	0.157

There are many other opportunities for using statistical methods in snapshot generation. Among these are: screening methods to eliminate unimportant parameters; sensitivity analyses; the incorporation of uncertainty effects; the efficient time-sampling of snapshots (using, e.g., time series analysis); etc.

POD and CVT reduced-order modeling

The reduced-order models we consider start with a set of snapshots: let $\{\vec{\alpha}_k\}_{k=1}^K$ denote the set of points in parameter space that are chosen for generating the snapshots; let Δt denote a time-sampling interval, usually chosen to be a multiple of the time step used in the discretization of the state system; let $\ell\Delta t$, $\ell = 1,\ldots,L$, denote the corresponding sampling times; let $\tilde{S}_{k,\ell}$ denote the solution (e.g., a vector of nodal values) of the discretized (e.g., by a high-dimensional finite element method) state system corresponding to the parameter point $\vec{\alpha}_k$ sampled at the time $\ell\Delta t$; then, a snapshot set could consists of the $N = KL$ vectors $\vec{S}_i = \tilde{S}_{k,\ell}$, $k = 1,\ldots,K$, $\ell = 1,\ldots,L$, $i = (k-1)L + \ell$. (We can (for free) enlarge the snapshot set to include the approximations of the time derivative of the solution of the state system.) Given N snapshots $\vec{S}_j \in R^M$, let S denote the $M \times N$ snapshot matrix whose columns are the snapshots vectors. Let $S = U\Sigma V^T$ denote the SVD of S. The d-dimensional POD-reduced basis vectors $(d < N)$ are the first d left singular vectors of the snapshot matrix S, i.e., $\vec{\phi}_i = \vec{U}_i$ for $i = 1,\ldots,N$. In this guise, POD is closely related to (in fact, it is exactly the same as) the statistical method known as Karhunen-Loève analysis or the method of empirical orthogonal eigenfunctions or principal component analysis. POD is sometimes implemented in terms of the finite element functions (instead of the nodal vectors) in which case the mass matrix enters into the SVD calculation. There have been several variations introduced in attempts to "improve" POD. Suppose one is given a set of points $W = \{\vec{U}_j\}_{j=1}^N$ belonging to R^M and a set of generators $\{\vec{Z}_i\}_{i=1}^d$ also belonging to R^M with $d < N$, let $\{\hat{V}_i\}_{i=1}^d$ denote the Voronoi tessellation of W with respect to $\{\vec{Z}_i\}_{i=1}^d$ and let $\vec{Z}_i^*$, $i = 1,\ldots,d$, denote the centroids of each of the Voronoi regions $\hat{V}_i$, $i = 1,\ldots,d$. In general, $\vec{Z}_i^* \neq \vec{Z}_i$ for $i = 1,\ldots,d$. If it so happens that the centers of mass of the Voronoi regions are the same as the generators of those regions, i.e., if $\vec{Z}_i^* = \vec{Z}_i$ for $i = 1,\ldots,d$, we refer to the Voronoi tessellation as being a *centroidal Voronoi tessellation.* CVT's have to be constructed; there are several algorithms known for constructing CVT's. CVT's have been successfully used in data compression; one particular application was to image reconstruction; therefore, it is natural to examine CVT's in another data compression setting, namely reduced-order modeling. The idea, just as it is in the POD setting, is to extract, from a given set of snapshots

vectors $\{\vec{S}_i\}_{i=1}^{N}$ in R^M, a smaller set of vectors also belonging to R^M. In the CVT setting, the reduced set of vectors is the d-dimensional set of vectors $\{\vec{Z}_j\}_{j=1}^{d}$ that are the generators of a centroidal Voronoi tessellation of the set of snapshots. Both the POD and CVT-reduced bases are optimal (in different senses.)

Once having determined the POD and CVT reduced bases, one can use them to approximate solutions of the full system. For many sample problems, both POD and CVT reduced-order models provide accurate approximations to the solution of the full finite element system. In the table below, we compare the costs of full finite element and reduced-order simulations. This table provides ample motivation for why one wants to develop reduced-order models.

Number of CVT or POD basis functions	Ratio of CVT or POD CPU time and full model CPU time	Number of CVT or POD simulations per full model simulation
4	0.000015	65,789
8	0.000088	11,402
12	0.000391	2,560
16	0.001329	752

A natural question is: should one use CVT or POD? Their accuracy is very similar, but CVT is "cheaper" than POD; POD involves the solution of an $M \times N$ singular value problem, where N is the number of snapshots so that the work is of order $O(MN^2)+O(N^3)$; CVT can be implemented so that the work is linear in M and N so that, in principle, CVT can handle many more snapshots. This is not a big deal because the work of generating either a POD or CVT basis is miniscule compared to the work needed to generate the snapshot set. Fortunately, one does not have to choose between POD and CVT, but can combine the two methods (in several different ways) to define a hybrid CVT-based POD (CVOD) method. CVOD offers the possibility of taking advantage of the best features of both POD and CVT and CVOD is cheaper than POD since it requires the solution of several smaller eigenproblems instead of one large one.

Details and many further references can be found in the papers listed below.

References

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6.2 Applications

6.2.1 Soft Matter

Session II: ***Complex Fluids and Soft Matter***

Organizer

M. Gregory Forest, University of North Carolina at Chapel Hill

Contributing Speakers
L. Pamela Cook, University of Delaware
Richard Superfine, University of North Carolina at Chapel Hill
Qi Wang, Florida State University

Methodology.

The basic equations for many complex fluid and soft matter systems require a significant investment of applied mathematics to advance the science and technology. Since the basic equations remain in evolutionary stage, a careful strategy for building a critical numerical infrastructure for complex fluids and soft matter materials is needed. 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, in stochastic molecular dynamics, in kinetic Smoluchowski equations for the molecular probability distribution function (pdf), in mesoscopic scale-up models for second moments of the molecular pdf, and of course in continuum mechanical approaches. For example, dumbbell and multi-bead-spring idealizations are still the state-of-the-art in stochastic models of long chain polymers in dilute solutions. The spring constants and chain extensibility due to flow gradients are reasonably modeled, but the effects of electrostatic potentials due to polymer-solvent mismatches are not built in yet (cf. M. Graham lecture). In nematic polymer nano-composites, the molecules are idealized as rigid, monodisperse, and uniformly dispersed spheroids. All of these assumptions must be relaxed in order to model realistic polymer nano-composites.

1. Kinetic (molecular scale) modeling for all or part of the coupled fields in complex fluids is a compromise scale of description. Micro-fluidics and nano-fluidics are pushing the envelope where a continuum description of the fluid solvent carrying DNA in micro-or nano-channels is questionable. The solvent itself is typically not a viscous liquid. In nano-composites and nematic polymer materials, extensions of the current theory to include physics not yet resolved (e.g. soft, deformable nano-elements, polymeric solvents, polydispersity, and non-uniform concentrations of nano-elements; charge effects; the chemical interphase between nano-element and polymer matrix). Atomistic numerical technology can be turned into a scale-up predictor, to confirm or suggest revised mean-field potentials of kinetic theory.
2. Scale-up methods (e.g. moment averaging) for a variety of purposes:
3. for numerical parameter sweeps and possible control wrappers (kinetic codes take too long)
4. for analysis of dynamical and spatial scaling laws
5. There is currently no standard for appropriate and hierarchical benchmarks for efficacy of scale-up modeling and simulation.
6. Stochastic differential equations, putatively equivalent to the kinetic Smoluchowski equation, but for dynamical and structure transition-rich systems, there are no robust criteria for knowing when a bifurcation has occurred. Recent results of Kevrekides are a starting point.
7. Self-consistent methods to put stochastic effects into scaled-up models to reflect heterogeneity and scales that are projected out.
8. Homogenization: a priori or a posteriori criteria for when homogenization is valid; i.e. separation of scales tests
9. Sensitivity analysis of parameters, in deterministic systems and stochastic systems

10. Atomistic descriptions aimed at surface physics and chemistry, which are needed to understand the interfaces in mixtures, e.g. nano-composites where the "interphase" between the nano-element and matrix is highly variable and poorly understood.
11. Exploring lattice Boltzmann rules for incorporating elasticity or stored memory.
12. Model stochastic systems, such as polymer blends or polymer solutions, where one has to solve multiple scales (molecular and flow) simultaneously (work of Ganeson and Fredrickson).
13. Investment in carefully chosen model systems for complex fluids and soft materials, and in the combination of analysis, theory, and simulation of these model systems, together with evaluation of the efficacy of these simple models in describing the more complex fluid or soft material. One example of this approach is upscaled mesoscopic models of nematic polymers (Forest-Wang work), or the modeling of worm-like micelles with a continuum viscoelastic model coupled with density fluctuations for the micelles (P. Cook).

Applications of interest to DOE where complex fluids are essential

1. Fuel cells
2. Microfluidics and nanofluidics
3. Micelles and their role in remediation, solvent technology, turbulent drag reduction, all for energy efficiency with friendly environmental impact
4. Particle-laden flows and suspensions where constitutive laws remain primitive
5. Systems biology, e.g. methods for modeling cell membranes (L. Frink)

Investments recommended to DOE managers

1. Numerical infrastructure for small number of identified "universality classes" of non-Newtonian constitutive laws. There is one commercial package available, which is not capable of addressing the broad spectrum of complex fluids and applications. Similarly, a numerical infrastructure for the wide range of molecular architecture models of dilute, semi-dilute and concentrated polymeric systems is needed.
2. Possible requirements to attach to RFPs for the Multiscale Math Initiative:
    a. Research Assistant and postdoc practicum component
    b. DOE postdoctoral fellowships patterned after the NSF Postdoc Fellowships, where there is a faculty mentor and a secondary lab mentor who are part of the proposal
    c. Faculty internships at the labs, and freedom for lab scientists to have sabbaticals in partner academic institutions
    d. Software open source policy
3. Team project proposals should be encouraged in the MMI portfolio, including teams with experimental, modeling & computation components, and resources for experiments included. Leveraging with other programs at DOE should be considered and pursued.
4. Investment in teleconferencing technology at universities to foster team oriented projects and to keep interactions active.

New mechanisms for achieving DOE enhancements from the academic community

The model of single investigator grants submitted by PI's at universities should be retained, yet new models should be strongly considered. If all DOE does with the Multiscale Mathematics Initiative is more of the same, then striking outcomes are unlikely. Some ideas are proposed above, such as teams comprising a full scientific method approach to a targeted application. However, a new concept arises to support regional networks, that link a small group of academic institutions and link that cluster to one or more DOE labs.

Session V: ***Multiscale Computational Challenges in Soft Materials***

Organizer

Michael D. Graham, University of Wisconsin at Madison

Contributing Speakers

Jason Butler, University of Florida
Venkat Ganesan, University of Texas at Austin
Laura Frink, Sandia National Laboratories

Introduction

A wide variety of naturally occurring and manmade materials have properties that lie somewhere between the traditional distinctions of "solid" and "liquid". For example, foams used for firefighting behave like freestanding solids if left alone, but flow somewhat like a simple liquid when subjected to stress. Other important materials, such as molten plastics, display *viscoelasticity:* their response to deformation may be liquid-like or solid-like, depending on how rapidly they are deformed. As a natural example of such a material we point out that inside a living cell resides a cytoskeleton composed of a complex gel of aqueous liquid and rigid and flexible biopolymers; the mechanical response of this gel can be very complex. All of these substances have a nontrivial structure at the microscopic scale, a scaffold of bubbles in the case of a foam, a mass of entangled polymer chains in the case of a molten plastic, and a highly interconnected network in the case of the cytoskeleton.

In contrast to metallic or crystalline solids, the properties of the materials just described are determined or modulated by noncovalent effects, such as electrostatic and van der Waals interactions, hydrodynamic coupling between elements of the microstructure, and the constraints of excluded volume or connectivity. Substances with these characteristics are called *soft materials*. They are important in a tremendous variety of applications in both technology and science, and the science base required for progress in soft materials research is very broad, including: colloid and interfacial science; chemical synthesis; fluid dynamics and transport phenomena; polymer physics; statistical mechanics; sophisticated instrumentation; scientific computing; and applied mathematics.

Soft materials and multiscale modeling

Soft materials have a number of characteristics that provide significant challenges and opportunities for applied mathematics. These include:

- Hierarchies of interacting length and time scales
- Hierarchies of levels of description:
    - atomistic
    - mesoscopic
    - continuum (macroscopic)
- Many-body, long-range interactions
- self-assembly (nontrivial equilibrium microstructure)
- nonlinear dynamics and pattern formation away from equilibrium (e.g. in flow)
- ergodic and nonergodic (glassy) dynamics.

From this list it is clear that development of effective theoretical and computational tools for predicting and understand the behavior of soft materials demands methods that are capable of tackling phenomena that occur on broad spectra of scales in both space and time.

Applications specifically addressed by speakers

- polymer processing:
    - flow instabilities and nonlinear flow dynamics arising from viscoelasticity
    - microstructure development in polymer blends and block copolymers
    - effect of composition variations and polymer-polymer interfaces on the rheology of polymer blends
- turbulent drag reduction by additives
- Micro- and nanofluidics for genomics: dynamics of dissolved genome-length DNA molecules in confined geometries
- biophysics:
    - mechanical properties of biomaterials
    - structure, transport and dynamics related to cell membranes
    - solvation of polymers

Other applications of potential interest to DOE

- Nanocomposites
- Templated self-assembly of materials for photonics, catalysis, separations
- lab-on-a-chip
- liquid crystals and other structured materials/interfaces for sensor applications

Methodologies

- Computational fluid dynamics (e.g. finite element) for macroscopic flows of viscoelastic liquids like polymer solutions and melts.
- Coarse-grained or mesoscale descriptions of polymers in solution – solvent treated as continuum subject to thermal fluctuations, polymer molecule modeled as a bead-spring dumbbell or chain. Two treatments of the solvent dynamics were presented
    - Stochastic ("Brownian dynamics") simulations of bead-spring chain models of polymers in bulk or confined solution: Green's function approaches to hydrodynamic interactions between polymer segments
    - Lattice-Boltzmann approach to hydrodynamic interactions: alternative to Green's function approach involving direct solution of fluid motion in entire domain by solving a discretized Boltzmann equation.

  The relative merits of these two basic approaches are still to be worked out.
- "Micro-macro" methods for computational fluid dynamics, where instead of using a closed form constitutive equation for the stress, a full microstructural (e.g. Brownian dynamics) simulation is carried out on mesh or material points.
- Mean-field (density functional) theory and computations for description of dense inhomogeneous systems such as polymer blends, combined with Brownian dynamics

simulations and continuum mechanics, for treatment of polymer blend interfaces and other dense inhomogeneous soft systems.

Challenges for mathematical analysis and computation

- For computational fluid dynamics applications with highly elastic liquids, no current method is guaranteed to work at high Weissenberg number (ratio of strain rate to material relaxation rate).
    - The PDE for the evolution of microstructure is convection-dominated. Upwind discretization are widely used but still do not guarantee converged solutions at high Weissenberg numbers.
    - Localized regions of high stress arise near corners, free surfaces, stagnation point and other regions of high extension rate. These present significant issues in adaptive meshing.
- Somewhat similar issues arise in the solution of the equations that come from dynamic density functional theories. These equations may contain high-order spatial derivatives or even be partial integrodifferential equations, posing numerical stability problems. Because these methods are specifically intended for highly inhomogeneous systems they require effective methods for resolution of sharp gradients, as are found at interfaces.
- For coarse-grained or mesoscopic models, a wide variety of open issues remain.
    - Long-range interactions, such as those present when electrostatic or hydrodynamic effects are included, often present the dominant computational cost in simulations of colloidal and polymeric solutions. For example, only recently have hydrdoynamic interactions been incorporated into simulations of confined dissolved polymers. It is important to ascertain the relative merits of various approaches (Green's functions, explicit solutions for solvent motion e.g. via the lattice Boltzmann method, dissipative particle dynamics,…) that have been proposed for capturing these interactions.
    - Statistical noise is always an issue for particle-level simulations; methods of variance reduction are needed.
- If a system is to be coarse-grained, what are the correct coarse-grained variables? In more mathematical terms, where does the slow manifold lie? What is the nature of the coupling between slow and fast modes? How does one perform coarse-graining when there is no separation of scales?
    - In general, these questions seem to have received relatively little attention from mathematicians in the context of soft materials. In the engineering and physics communities, this question has largely been addressed on an ad hoc basis.
- A variety of higher-level issues are important as well. Some examples include:
    - Sensitivity of results to parameters – sensitivity analysis for stochastic or other particle-level simulations
    - Parameter estimation for reduced (e.g. coarse-grained) models
    - Arclength continuation and bifurcation analysis using information from particle-level simulations
    - Model based control with atomistic models and data.

Frontiers of physical understanding: some examples

- Interaction of microstructure and flow, e.g. in liquid crystalline, micellar surfactant or block-copolymer systems
- Interfaces:
    - wetting and contact line dynamics
    - polymer/polymer interfaces
    - polymer dynamics near solids surfaces and in confined geometries
    - tribology at the molecular scale
- Very slow or glassy relaxations
- Turbulent drag reduction
- Singularity formation and flow instabilities in free surface flows
- Transport of particles and solutes in sheared colloidal suspensions
- Mechanical properties of biological and biomimetic materials
- Dynamics of polyelectrolytes

Programmatic and other broad issues

- It was suggested in the discussion that a set of benchmark problems for specific computational aspects of soft matter research might be useful. As a specific example, a specific problem in colloidal or polymer dynamics might serve as a benchmark for methods of treating solvent dynamics (hydrodynamic interactions).
- Attention to model problems that are relevant for soft matter systems but at the same time amenable to rigorous mathematical analysis should be encouraged. This might provide a rich and set of issues for mathematical study and at the same time improve the rigorous basis for models and approximation methods used by physical scientists and engineers.
- At the other end of the spectrum, the interaction between computationalists, theorists and experimentalists should also be encouraged. What model experimental systems will allow direct and quantitative comparisons with the leading multiscale computational techniques?

6.2.2 Atmospheric Science

Session I: ***Systematic Multi-Scale Stochastic Modeling and Quantifying Uncertainty in Atmosphere/Ocean Science***

Main Speaker

Andrew J. Majda, New York University

Contributing Speakers

Markos Katsoulakis, University of Massachusetts, Amherst
Peter Kramer, Rensselaer Polytechnic Institute
Joseph J. Tribbia, National Center for Atmospheric Research

One of the grand challenges of contemporary science is a comprehensive predictive model for the atmosphere and coupled climate system. This is one of the most difficult multi-scale 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, GCM's, are currently incapable of adequately resolving or parameterizing these

interactions on time scales appropriate for seasonal prediction as well as climate change projections.

Thus, the multi-scale problems in atmosphere ocean dynamics serve as important prototype problems for developing new systematic multi-scale strategies which are valuable in other scientific disciplines ranging from nanotechnology to macro-molecular dynamics to protein folding, etc. The societal impacts for these efforts are also large; it has been estimated recently that a one month increase in lead time for El Nino prediction would save 100 billion dollars for the world community. Additionally, the problem of global climate change is of particular interest to the DOE in so far as its ramifications for the energy economy of the nation.

Basic questions which drive climate research are the prediction of the weather from 1 to 14 days, the prediction of climate variations on seasonal to yearly time scales and finally, climate change projections on decadal and centennial time scales as well as quantifying the uncertainty associated with these predictions.

One of the striking recent observational discoveries is the profound impact of variations in the tropics on all of these problems. The primary issue in the influence of the tropics occurs through the interaction and organization of clouds into clusters, super clusters, and planetary scale dynamics, an inherently fully nonlinear multi-scale process. For climate change, water vapor is the most important greenhouse gas and the microphysical processes in clouds are a key mechanism for radiative feedback. In fact, only a 4% change in average cloudiness would overwhelm the effects of CO2 in climate change. Current evidence suggests that a few global planetary teleconnection patterns, such as the Pacific North America Oscillation, summarize the weather and climate impact of the tropics for the atmosphere. Since it will be impossible to run resolved coupled atmosphere/ocean comprehensive numerical models for the atmosphere for climate change projections, reduced models involving these basic large scale patterns are of central importance.

Emerging Mathematical and Computational Strategies for Multi-Scale Modeling

A new perspective on several of the issues discussed above for climate dynamics has been developed recently through the paradigm of modern applied mathematics where rigorous multi-scale mathematical theory, the development of prototype model problems and novel computational strategies all interact simultaneously in understanding these complex scientific problems. These emerging mathematical/computational strategies include the following:

1. Systematic multi-scale asympotic modeling for the tropics
   (Majda and Klein, J. Atmos. Sci. 2003; Majda and Biello, PNAS 2004)
2. Novel stochastic models for unresolved features of tropical convection
   (Majda and Khouider, PNAS 2002; Khouider, Majda, and Katsoulakis, PNAS 2003)
3. Systematic Mathematical Strategies for Low Dimensional Stochastic Mode Reduction in Climate (Majda, Timofeyev, Vanden-Eijnden PNAS 1999; Comm. Pure Appl. Math, 2001; Physica D, 2002; J. Atmos, Sci. 2003
4. Quantifying Uncertainty in ensemble Predictions and Loss of Information in coarse-grained stochastic models through Information Theory (Kleeman, J. Atmos. Sci, 2001; Kleeman, Majda, Timofeyev. PNAS 2002; Majda, Kleeman Cai, Math Anal. Appl. 2003; Abramov and Majda, SIAMJ, Sci. Stat. Comp. 2004; Katsoulakis and Vlachos, J. Chem. Phys. 2003; Katsoulakis and Trashorras, J. Stat. Phys., 2004)

Through the serendipity of modern applied mathematics, the issues in (2) have driven new systematic mathematical strategies to course-grain stochastic lattice models with

adsorption/adsorption and diffusion coupled to continuum problems at mesoscopic scales; the result is a new class of coarse grained Monte Carlo methods for material science with simultaneously a speed up of order a billion times in computational labor while retaining fidelity with key features of the microscopic fluctuations (Katsoulakis, Majda, Vlachos, PNAS 2003 and J. Comp. Phys 2003; Katsoulakis and Vlachos, J. Chem. Phys. 2003). In another different multi-disciplinary application, the methodology in (3) has been applied to stochastic immersed boundary numerical methods for microfluid particle suspensions as for example, molecular motors in cellular biology. (Kramer and Majda, SIAMJ, Appl. Math 2003).

The Near Future Agenda for Systematic Multi-Scale Modeling for the Climate

With all of the emerging mathematical techniques and perspectives outlined above, several other important and more complex problems for climate research are capable of being attacked in the near future. Here is a list:

1. Multi-scale tropical modeling of one climate GCM grid box, i.e., a region of order 100 km for a GCM time step of twenty minutes and scale interactions for 1 to 10 to 100 km.
2. The scale up of cloud microphysics models operating on scales smaller than one meter to bulk cloud physics models on scales of one kilometer.
3. The blending of hierarchical Bayesian Statistical Models for observations and the Stochastic Modeling Strategies discussed earlier for practical parameterization.
4. The Use of Information Theory to Quantify Information Flow Among Components of Comprehensive and Reduced Models and to Quantity Their Uncertainty
5. Comprehensive Fluctuation-Dissipation Relations in Various Components of the Multi-Scale Climate System

There are natural emerging partnerships among interdisciplinary university initiatives in applied math and atmosphere ocean science (CAOS at the Courant Institute), the National Center for Atmospheric Research (NCAR), and DOE labs spearheading the climate change initiative (Los Alamos, Livermore).

This is an exciting training ground for a new generation of multi-disciplinary research scientists. This can be nurtured through workshops and special theme years, as well as research finding for Ph.D. students and post docs in a multi-institutional as well as a single investigator framework.

6.2.3 Networks

Session VIII: ***Simulation and Analysis of Large Networks***

Organizer

Edwin K.P. Chong, Colorado State University

Contributing Speakers
Jeffrey Herdtner, Miami University of Ohio

Overview

Many important systems are most naturally or can only be modeled by networks (or graphs). Many of these systems are of critical importance to DOE. A partial list includes, biological systems (viewed at various levels), microbial communities, protein interaction networks, social networks, epidemiology, as well as designed technological networks (e.g. power distribution, communication networks, sensor/actuator networks, robotic networks, etc.). 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. In many cases localized or small magnitude forcing can cause large scale responses. The mathematical analysis of networks is a relatively new area, analysis methods are only beginning to be 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, and ideas developed from continuum modeling of multiscale systems.

Multiscale Phenomena in Communication Networks

Our focus here is on communication networks, although many of the issues are common to other types of networks as well, including power distribution networks, agent-based networks, sensor/actuator networks, and robotic networks. This specific area was the focus of the invited lecture and breakout session talks in the "Simulation and Analysis of Large Networks" session.

A communication network is a collection of communicating devices connected together via communication links. Such devices include computers, phones (wired and wireless), laptops and PDAs, and sensors. Examples of communication networks include the Internet, local area networks (LANs), cellular networks, and wireless ad hoc networks.

Communication networks are multiscale in nature by design. The dominant design paradigm in networking is the hierarchical (layered) architecture. In particular, network protocols are arranged in a hierarchical protocol "stack" (e.g., the ISO OSI architecture). Moreover, the topological arrangement of networks is typically also hierarchical (e.g., the Internet). Finally, general-purpose networks like the Internet are heterogeneous both in infrastructural components as well as the nature of traffic that traverse them. All these factors work together to give rise to multiscale phenomena.

Scaling in the Internet

Events on networks like the Internet take place on a variety of time scales. For example, packet transit times are often in microseconds, file transfers take seconds, routing table updates take minutes, and significant network topological changes may take days. The metaphor of mice and elephant coexisting in a common habitat is often used to describe Internet traffic: while most packets are small (mice), most bits reside in large packets (elephants).

Since the seminal paper of Leland, Taqqu, Willinger, and Wilson [LeT94], Internet researchers have come to accept that dealing with Internet traffic involves reckoning with features that transcend multiple time scales. 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 (HOT). These approaches stem from embracing a premise best articulated in a paper by Abry et al. [AbB02]: "Although created by man and machine, the complexity of teletraffic is such that in many ways it requires treatment as a natural phenomenon."

It turns out that not only in the time scale are scaling features observed: the topology of the internet also has scaling features. In a well-known recent study by Faloutsos et al. [FaF99], it was shown that the distribution of the number of neighboring nodes in the Internet topology follows a power law.

Interest in scaling features like the ones described above boil down to a concern that such features have impact on the design and performance of networks. For example, some have demonstrated

that self-similar traffic leads to poor behavior of queues. On the other hand, some have also been able to exploit such scaling features in the Internet, for example in prediction-based congestion control and in filtering for dealing with distributed denial of service attacks.

Scaling in Wireless Networks

Large wireless networks have received significant recent interest owing to the maturing of technologies enabling large numbers of devices to communicate over a common wireless channel. Interest in such networks are varied, ranging from the possibility of quickly deploying computer networks in battlefield environments, to the use of a large number of simple and inexpensive sensors in a collective way to perform demanding tasks.

The modeling and analysis of such networks is difficult because of the confluence of two factors: the nature of the interference-limited wireless channel and the large number of communicating devices. Fundamental issues like the capacity of such a network is not easily addressed by standard analytical techniques (e.g., calculating the Shannon capacity). Successful recent efforts have resorted to asking simpler questions. In particular, a promising line of work has focused on characterizing the scaling law of such networks as the number of devices (nodes) grows asymptotically. In the asymptotic regime, we find relief in analytical tractability and simplification.

Within the framework of scaling laws, it possible to answer questions like: 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 are questions that only recently have begun to be addressed.

Mathematical Models and Frameworks

The need for appropriate mathematical models and frameworks has become clear as network researchers struggle to make sense of the complexity of these man-made systems. While the traditional approaches common in networking research have focused on discrete mathematics, the techniques that have come to fore in dealing with issues like scaling phenomena and large networks have been of the continuous flavor. Differential equations (whether ordinary, stochastic, or partial), widespread in models of natural systems, now occupy firm ground in the modeling of man-made networks. This is a promising development, because it opens up vast possibilities for many more researchers to contribute to solving pressing problems in networks. In particular, the topics in multiscale mathematics traditionally funded by DoE is now of relevance in tackling problems in networking research. The successful marrying of these two areas will involve strategic collaborations and multidisciplinary efforts.

Continuum Models and Multiscale Methods in Simulating Large Networks

We describe here what we believe to be a promising current effort along the lines of bringing multiscale mathematics to bear on the problem of simulating large networks. The approach involves constructing partial differential equation models for large networks, and using multiscale methods in the solution of such models as a surrogate for detailed simulation, which becomes increasingly impossible as the size of networks grow. Below, we describe several examples to illustrate the critical need and rationale for this effort.

1. Internet

Simulation modeling has become the primary tool in the performance analysis of the Internet, with large research efforts directed toward enabling simulation of increasingly larger networks (e.g., DARPA's Network Modeling and Simulation program [NMS]). Such simulation tools are used in a

variety of ways, including in the evaluation of protocol designs and for network resource provisioning. High-performance computing techniques and technologies, such as parallel computing [WuF01], have been exploited to advance the frontier of network simulator performance. Yet, the current state-of-the-art in simulation tools does not support the simulation of networks with a hundred million nodes, roughly the current size of the Internet (see, e.g., [RiA02] for an assessment of the state-of-the-art in large-scale simulation tools). Indeed, a recent news release from Georgia Tech reports the creation of "the world's fastest detailed computer simulations of the internet," capable of simulating "networks from over 1 million web browsers in near real time" [GT03]. At numbers exceeding millions of nodes, we should expect continuous approximations in the topological domain to provide appropriate models of the network, at least at some levels of abstraction.

2. Wireless ad hoc networks

Interest in wireless ad hoc networks has flourished in recent years. At the same time, the analysis of such networks has proven to be challenging. A seminal paper by Gupta and Kumar [GuK00] show that under certain modeling assumptions, it is possible to characterize the scaling law of the transport capacity in the asymptotic regime where the number of nodes grows to infinity. Roughly, they show that the throughput grows as $O(n^{1/2})$. This result has spawned numerous papers that characterize asymptotic scaling laws for wireless networks in different settings (e.g., [GrT02], [XiK04]. Despite the ground-breaking nature of these scaling-law results, they do not provide any means to calculate the actual throughput of a network with, say, a million nodes. Simulation remains the only method of answering such questions. However, as is the case in Internet simulation, simulation tools do not currently support network sizes of millions of nodes.

3. Sensor networks

The possibility of networking not only computers and communication devices but also sensors has led to significant current interest in sensor networks (see, e.g., NSF's SENSORS AND SENSOR NETWORKS Program [NSF-SSN]). Like wireless ad hoc networks, sensor networks consist of sensors connected together via wireless links. However, sensor networks exhibit some unique features, including limitations in energy, bandwidth, and processing power. Analysis of such networks has closely followed that of wireless ad hoc networks, characterizing asymptotic scaling laws as the number of sensors grows (e.g., [GaV03], [El03]). The performance of large-scale sensor networks is still not possible with state-of-the-art simulators.

4. Dense traffic networks

Although our main motivators stem from problems in communication networks, we believe that other problems areas have similar needs, and would benefit from our work. One example is the simulation of dense traffic networks. This problem has become important in recent years because of the development of intelligent highway systems. Most recently, traffic simulation has become an important tool in the assessment of the impact of terrorist attacks in dense metropolitan areas [Sh03].

The state-of-the-art in traffic network simulation appears to be consistent with that of communication networks [HeK03]. The techniques that are brought to bear in advancing the state-of-the-art also appear to be similar: e.g., parallel processing [Sc00] and fluid traffic models [CONTRAM]. We believe that our work on continuous models for network simulation will be relevant to the development of simulation tools for traffic networks in dense metropolitan areas.

Factors to be considered in modeling.

In building network models, several factors have to be taken into account, depending on the type of network at hand. Here, we describe some salient factors to be considered and their bearing on our exploration of PDE-based models.

1. Simulation output

Network simulation models and tools are used for a variety of tasks:

- performance evaluation
- prototyping and benchmarking
- resource provisioning

In addition to conventional uses of network simulation, there is also interest in gathering qualitative system-wide information about the network, such as stability and propagation of local effects to the global network.

For some time there has been an interest in Internet traffic modeling, particularly to characterize the time-varying properties of traffic (e.g., long-range dependence and self similarity [PaW00]). In such models, time aggregation and continuous-time models have played key roles in the development of tractable models. There has been recent interest also in spatial traffic analysis [CrK03]. A PDE model of the network provides a natural means to explore both time as well as spatial variations.

2. Nature of network topologies

Network topologies vary depending on the type of network being considered. A well-known recent study shows that the Internet has an interesting topological characteristic: the distribution of the number of neighboring nodes follows a power law [FaF99]. This finding influences the way in which random graphs are used to model the Internet [ReN02], [NoR02]. Wireless ad hoc networks, on the other hand, are likely to me mesh-like [CoB96]. Sensor networks also exhibit unique topological features, usually tied to the particular application of the network (e.g., target tracking). Moreover, both wireless ad hoc and sensor networks often involve mobility of the nodes; this means that the network topology is evolving with time. The burden of modeling this evolving topology in graph-based simulators is a challenging issue. A PDE-based model has the potential to ameliorate such modeling challenges.

3. Physical characteristics

Wireline networks (e.g., the Internet) are often modeled without regard to detailed physical features (e.g., signal waveforms). The most detailed feature in the model is usually a “packet.” In contrast, wireless network models often incorporate some physical characteristics of the wireless medium (e.g., signal propagation, fading, and multiuser interference), because such characteristics bear heavily on the behavior and performance of the network. In a later section, we describe how we propose to take into account such modeling features in constructing a PDE model.

4. Traffic characteristics

In network modeling and simulation, we have to be concerned with the nature of the communication traffic. Internet traffic modeling has led to a myriad of models that capture important features of internet traffic, such as self similarity [PaW00]. A variety of continuous-time stochastic processes have come to be useful in network traffic models. More recently, interest in models for controlled traffic (e.g., TCP traffic) has led to the development of fluid models for such traffic (e.g., [LiP03]). Continuous-time processes and fluid models fit naturally into our PDE framework for network modeling.

5. Levels of model abstraction

In building network models, we invariably focus on some level of model abstraction, ignoring details that are irrelevant to the level of interest (e.g., [HuE98]). In the construction of PDE models for networks, we plan to take into consideration different levels of model abstraction, to provide answers to different types of modeling questions.

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