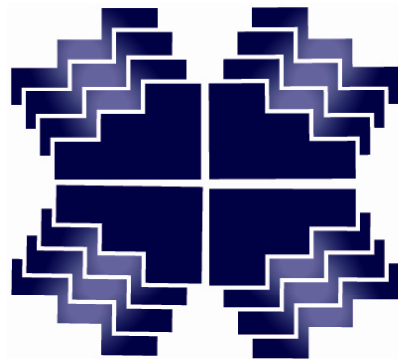# Multiscale Materials Modeling

Lecture 11

Multiscale Simulation involving the Continuum Level

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These notes created by David Keffer,
University of Tennessee, Knoxville, 2012.

Outline

In this lecture module, we present two review articles.

The first article discusses techniques to integrate atomistic and continuum level simulations with emphasis on the consistency in the spatial domain.

The second article discusses techniques to integrate atomistic and continuum level simulations with emphasis on the consistency in the temporal domain.

Atomistic/Continuum Coupling

There are many different ways being investigated to manage multiscale modeling techniques.

TOPICAL REVIEW

A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods

Ronald E Miller[1] and E B Tadmor[2]

Miller, R.E. Tadmor, E.B., Modelling Simul. Mater. Sci. Eng. 2009.

Atomistic/Continuum Coupling

Abstract

A partitioned-domain multiscale method is a computational framework in which certain key regions are modeled atomistically while most of the domain is treated with an approximate continuum model (such as finite elements). The goal of such methods is to be able to reproduce the results of a fully atomistic simulation at a reduced computational cost. In recent years, a large number of partitioned-domain methods have been proposed. Theoretically, these methods appear very different to each other making comparison difficult. Surprisingly, it turns out that at the implementation level these methods are in fact very similar. In this paper, we present a unified framework in which fourteen leading multiscale methods can be represented as special cases.

We use this common framework as a platform to test the accuracy and efficiency of the fourteen methods on a test problem; the structure and motion of a Lomer dislocation dipole in face-centered cubic aluminum. This problem was carefully selected to be sufficiently simple to be quick to simulate and straightforward to analyze, but not so simple to unwittingly hide differences between methods. The analysis enables us to identify generic features in multiscale methods that correlate with either high or low accuracy and either fast or slow performance.

All tests were performed using a single unified computer code in which all fourteen methods are implemented. This code is being made available to the public along with this paper.

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Atomistic/Continuum Coupling

This technique models some regions (the interesting regions) of the material with atomistic detail and other regions with a continuum. There is a hand-shaking region between them that attempts to properly transfer information important to such physical constraints as energy conservation between the two regions.

Miller, R.E. Tadmor, E.B., Modelling Simul. Mater. Sci. Eng. 2009.

Atomistic/Continuum Coupling
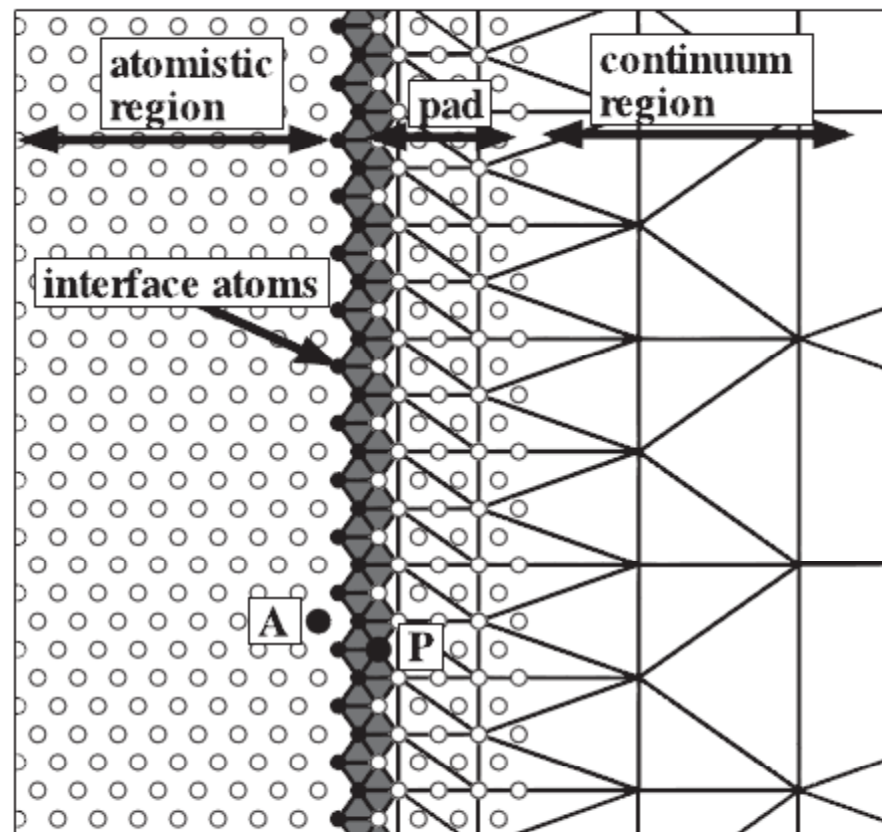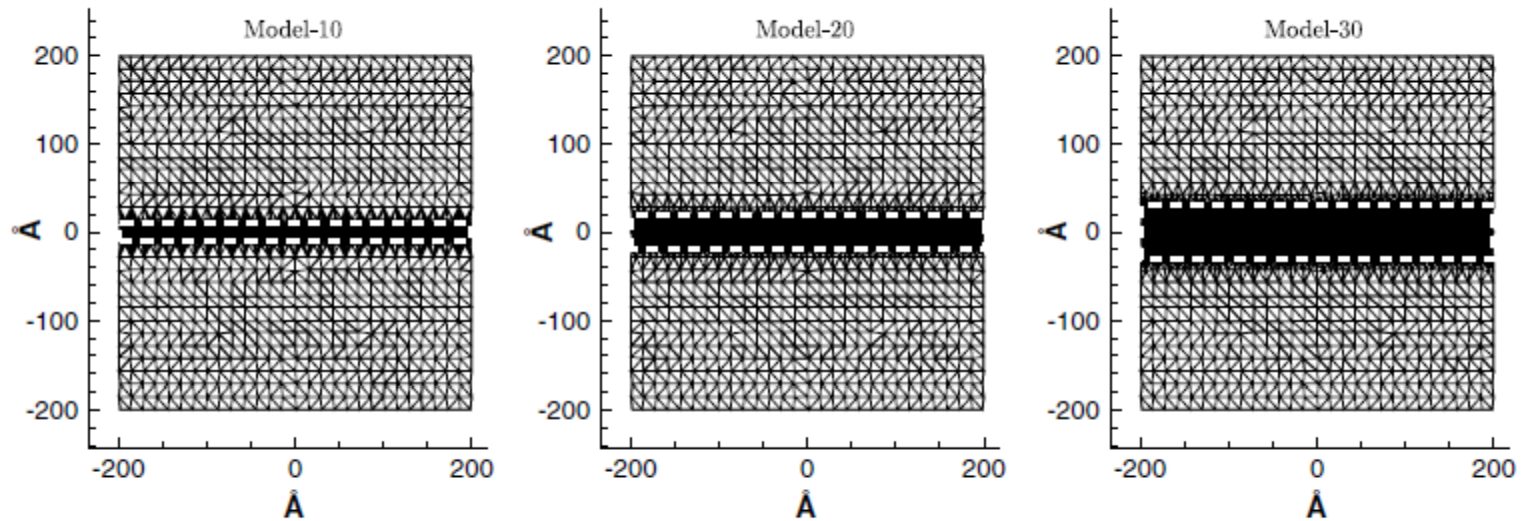
Figure 9. Meshes used in the test problem, whereby the width of the atomistic region (indicated by the dashed lines) is systematically increased.

7.2. The test problem

The test problem is a block of single crystal aluminum[21] containing a dipole of Lomer dislocations [21], as schematically illustrated in figure 8. The crystal is roughly 400 Å × 400 Å in the $X_1 X_2$ plane and periodic in X_3 (with a periodic length of 2.85 Å). Since the lattice constant for this model of aluminum is 4.032 Å, this region contains 27 760 atoms.

Miller, R.E. Tadmor, E.B., Modelling Simul. Mater. Sci. Eng. 2009.

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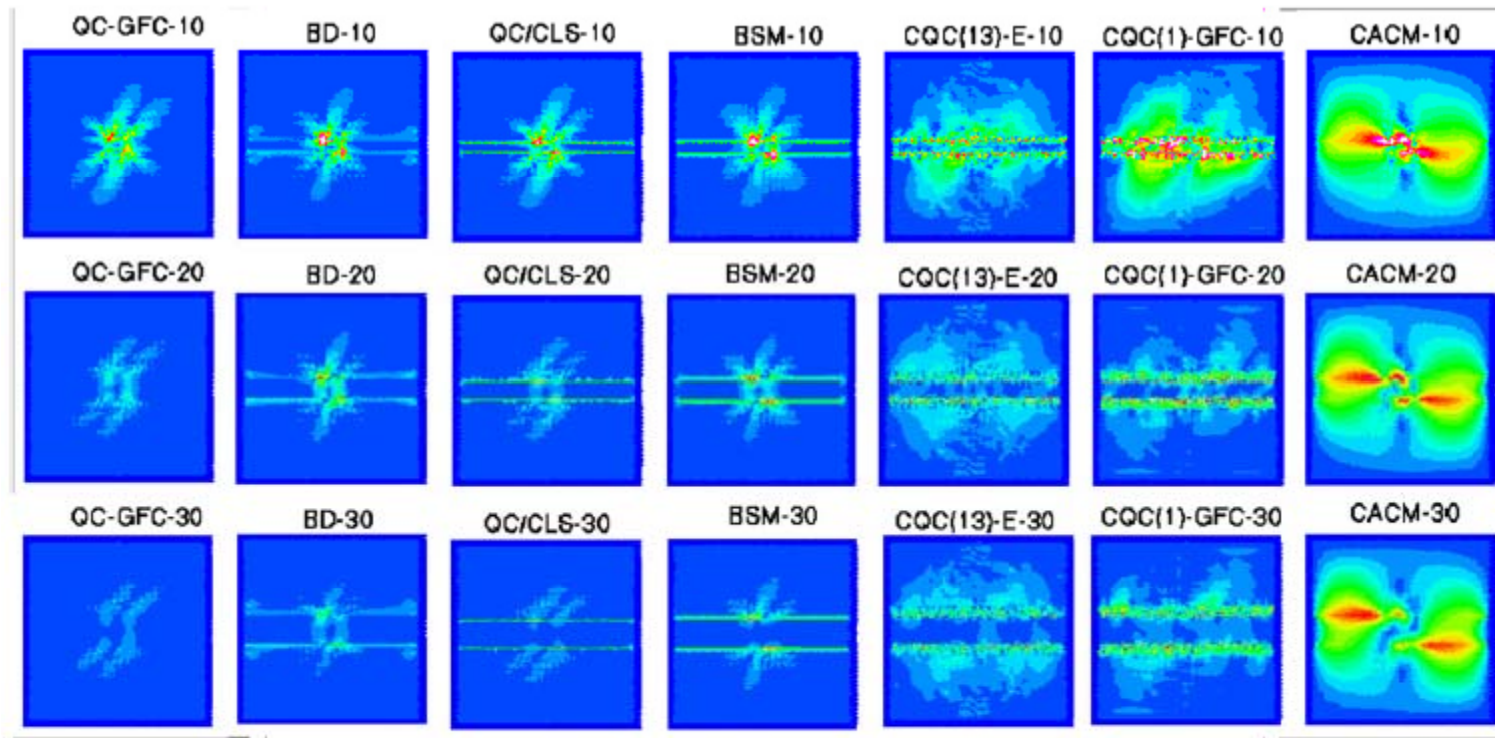
Atomistic/Continuum Coupling

Figure 14. Plots of the atomic displacement error, e^α (Å), for the energy-based multiscale models. The contour legend from figure 13 applies to this figure as well. Each image is of the entire model, which can be seen in figure 9.

Miller, R.E. Tadmor, E.B., Modelling Simul. Mater. Sci. Eng. 2009.

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Equation-Free Multiscale Computation: Algorithms and Applications

Ioannis G. Kevrekidis[1] and Giovanni Samaey[2]

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[2] Department of Computer Science, Katholieke Universiteit Leuven, 3001 Leuven, Belgium, email: giovanni.samaey@cs.kuleuven.be

Kevrekidis & Samaey, *Annu. Rev. Phys. Chem.* **60** 2009.

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Atomistic/Continuum Coupling

This article reviews a multiscale approach (16) to performing coarse-level computational tasks for systems that are modeled at a (much) finer scale (for an earlier review, see 17). In many cases, the explicit derivation of macroscopic equations can be circumvented by using short bursts of appropriately initialized microscopic simulation. A key tool is the coarse time-stepper, discussed in Section 2, which implements a time step of an unavailable macroscopic model as a three-step procedure: (*a*) lifting (i.e., the creation of initial conditions for the fine-scale model, conditioned upon the coarse state at t^*), (*b*) simulation (using the fine-scale model, over a time interval $[t^*, t^* + \delta t]$), and (*c*) restriction [i.e., the observation (estimation) of the coarse state at $t^* + \delta t$].

Kevrekidis & Samaey, *Annu. Rev. Phys. Chem.* **60** 2009.

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$$\frac{du_1}{dt} = -u_1 - u_2 + 2,$$

$$\frac{du_2}{dt} = \frac{1}{\varepsilon}\left(u_1^3 - u_2\right).$$

This sample problem illustrates the technique.
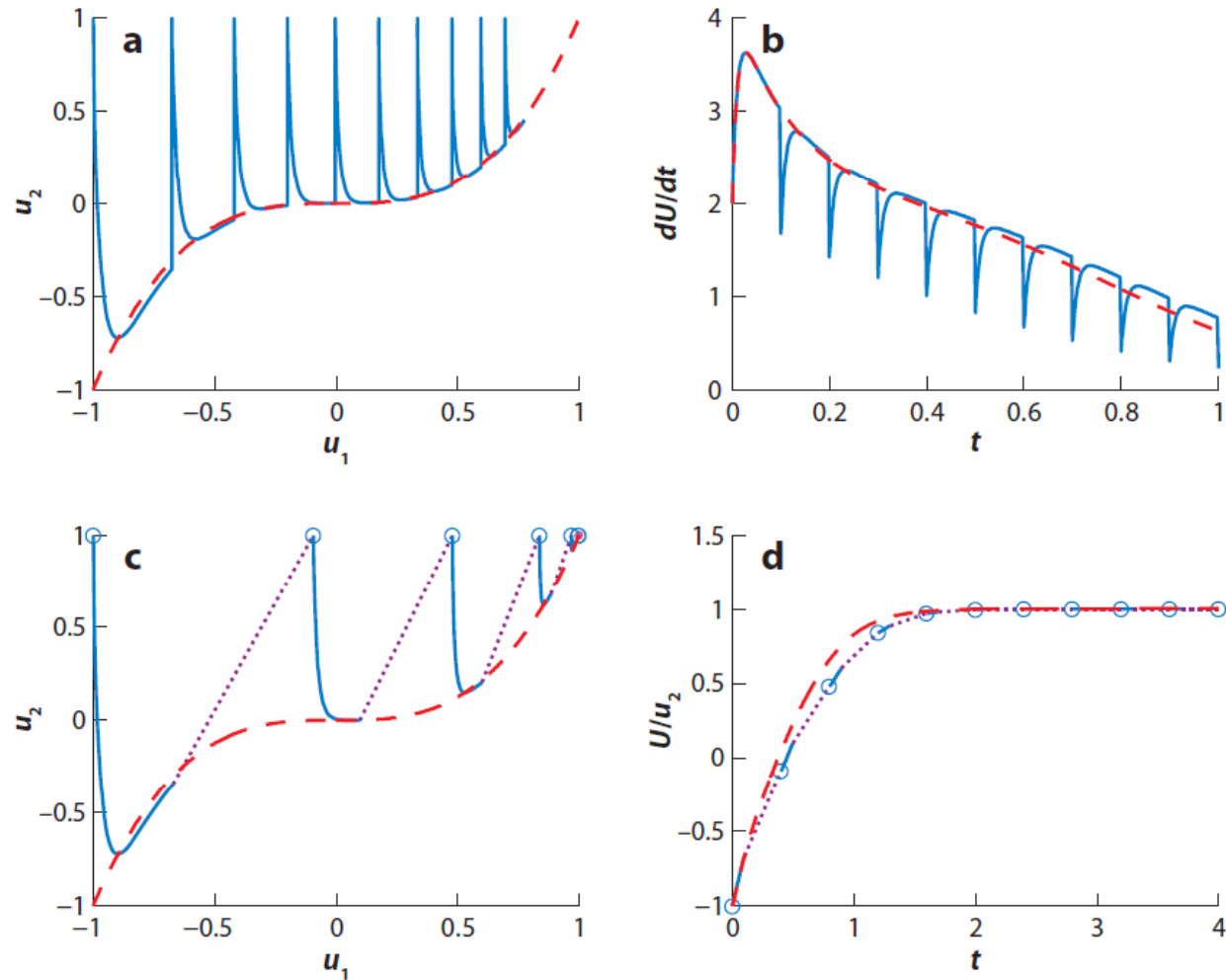
Figure 1

(a, b) Coarse time-stepper applied to Equation 7 using $\delta t = 10\varepsilon = 0.1$ and $U(0) = -1$. (a) The lifted solution (*blue solid line*) $u(t)$ plotted in the (u_1, u_2) phase space. At times $t = n\delta t$, the solution is restricted and then lifted again, which here amounts to setting $u_2(n\delta t) = 1$. The slow manifold is shown as a dashed red line. (b) The time derivative of the restricted solution $\mathcal{M}[u(n\delta t + s)]$ as a function of time $t = t$ (*blue solid line*), as well as the time derivative of the exact coarse solution $U(t) = u_1(t)$ (*red dashed line*). (c, d) Coarse projective integration. Intervals of full simulation are in blue, purple dotted lines represent projections in time, and the red dashed line is the full fine-scale simulation. (c) A phase space view. Whereas u_1 is projected in time corresponding to the estimated time derivative, u_2 is reset during the lifting so that the new initial condition is off the slow manifold. (d) The results of coarse projective integration with $\Delta t = 4\delta t$.

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Atomistic/Cont

Example: Water moving into carbon nanotubes through rapid jumps.

Figure 5

(a) Schematic of the carbon nanotube (CNT)-water system as a cylinder surrounded by water molecules, showing vestibules at the cylinder ends, introduced to allow smooth variation in the occupancy. (b) Coarse bifurcation diagram. Solid filled squares correspond to (stable) fully filled ($N > 5$) or empty ($N < 1$) states. Open circles correspond to (unstable) partially filled states. The turning points are indicated with filled diamonds. A number of representative structures are shown along the dashed vertical lines. (Inset) The effective bifurcation diagram obtained through histogram reweighting. (c) The effective free energy surfaces corresponding to the dashed vertical lines in panel b.
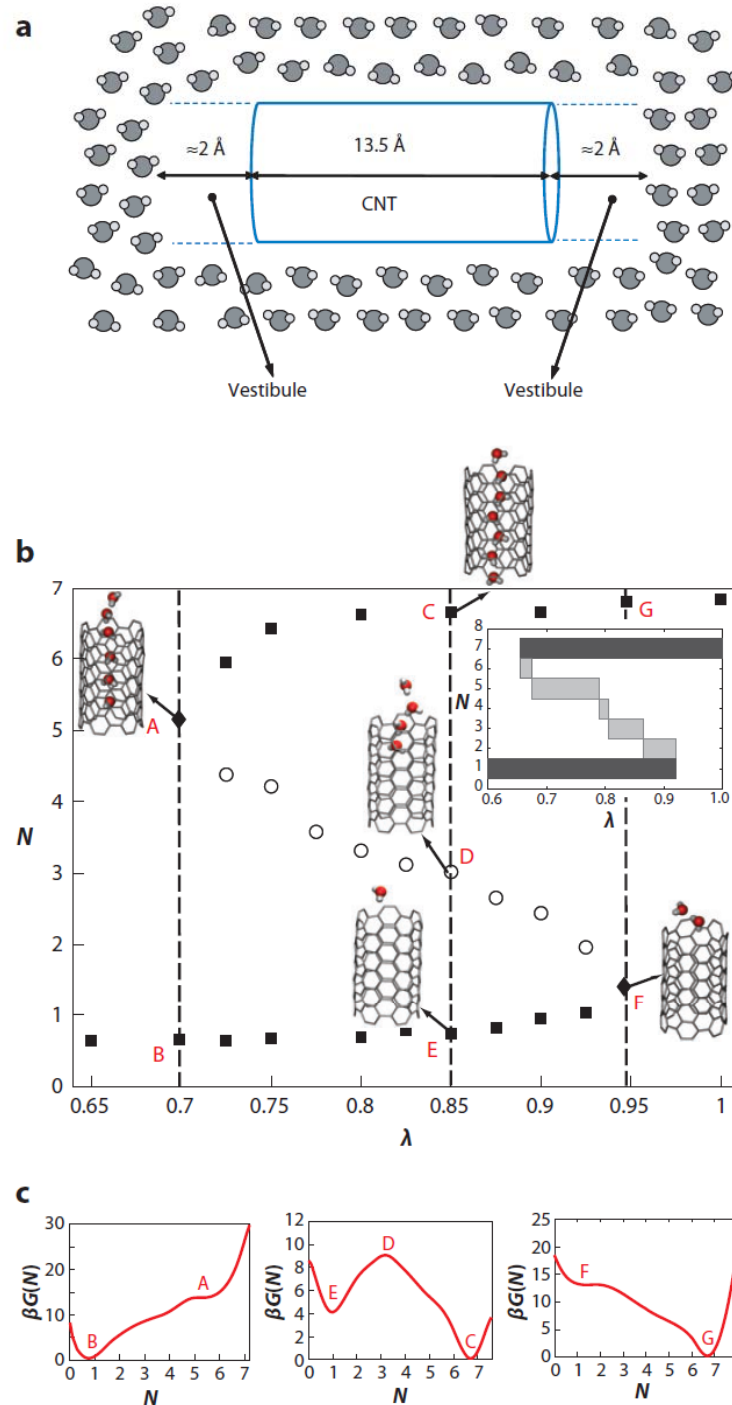
SUMMARY POINTS

1. Many complex physical/engineering problems are modeled at space and time scales drastically finer than the (macroscopic, coarse) level at which experimental observations are typically made and at which practical tasks such as prediction, design, and optimization need to be performed. Full simulation with these fine-scale models cannot hope to address such practical tasks. Traditionally, closures are obtained (through experiment and observation or through rigorous mathematics) to formulate useful models at the coarse level directly.

2. We present an approach that circumvents the explicit derivation of such closures and macroscopic models. The closure is obtained on demand through brief simulation of the fine-scale model over relatively short space and time scales. The approach is a design of (computational) experiments, using the fine-scale model as an experiment that can be initialized, executed, and observed at will.

3. In this framework, traditional numerical algorithms, from initial value solvers and spatial discretization techniques to contraction mappings and (especially) iterative matrix-free linear algebra, dictate the construction of computational wrappers: outer algorithms that perform coarse modeling tasks by designing, executing, and processing the results of computational experiments with an inner fine-scale solver.

4. Lifting operators that create fine-scale states consistent with coarse observations (a one-to-many procedure) and restriction operators that (conversely) coarsely observe fine-scale states are crucial elements of the framework. They correspond to initializing an experiment and observing/taking measurements from it. As our selected applications show, systematic lifting can be a computationally intensive process, for which problem-specific insight is often invaluable.

5. The scope of the framework (in terms of the type of outer solvers developed, the nature of the inner solvers, and the possible applications) is broad, as illustrated in our selected applications. It naturally brings together and functionally integrates elements of fine-scale/atomistic simulation, continuum numerical analysis, identification and control, statistics, and hypothesis testing.

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FUTURE ISSUES

1. Before the unavailable equation is solved, we need to be able to answer certain qualitative questions that crucially affect the algorithms and that are much easier to answer with closed-form models: What is the correct level at which a model can usefully close? Is the unavailable equation a PDE (of what order?), a stochastic PDE, or an integral equation? Is it Hamiltonian or a conservation law? Does it exhibit space or scale symmetry? Tools for answering these questions based on fine-scale simulation results should be systematically developed.

2. What are the right variables in terms of which the macroscopic model can be written? For many problems, they are known by experience and long experimentation, physical intuition, or rigorous mathematical derivation. Yet there is an increasing need to automatically extract such variables from available observations and to even design experimentation (possibly computational) for data acquisition with this purpose in mind. The link to modern data-mining/manifold learning techniques is a crucial one, and lifting/restriction based on such variables should be systematically studied.

3. Error analysis for the type of algorithms we describe (including a posteriori estimates) is at its infancy, especially for atomistic inner solvers. Issues of automatic adaptive refinement in space and time, adaptively controlled variance reduction of noise (linking to modern data-estimation techniques), and on-the-fly verification of the level of closure all are important research subjects. Numerical analysts are already studying several aspects (e.g., see the work of W.E, B. Engquist, and coworkers).

4. We believe this type of work may have a transformative impact on the individual-based modeling of social/economic phenomena, enabling a higher level of quantitative study.

5. We envision that, for physical systems in which enough spatiotemporally resolved sensing and actuation authority exists to initialize at will, the wrapper algorithms (computational experiment design protocols) we discuss may become laboratory experimental design protocols. One day, one might be able to perform computer-assisted mathematical tasks directly on nature through the same algorithms used today to perform these tasks on models.

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