Some Recent Progress in Multiscale Modeling

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1 Introduction

In recent years we have seen an explosive growth of activities in multiscale modeling and computation, with applications in many areas including material science, fluid mechanics, chemistry, and biology. It is widely recognized that multiscale techniques will become an essential part of computational science and engineering. The main purpose of the present paper is to review some (not all) of these progresses, with a view toward building systematic, reliable and controlled multiscale techniques for a variety of applications.

The basic set-up will be the following. We are given a system whose microscopic behavior, with state variable u, is described by a given microscopic model. This microscopic model is too inefficient to be used in full detail. On the other hand, we are only interested in the macroscopic behavior of the system, described by the state variable U. U and u are linked together by a compression operator Q:

$$U = Qu.$$

The difficulty stems from the fact that the macroscopic model for U is either not explicitly available or it is invalid in some parts of the computational domain. Our basic strategy is to use the microscopic model as a supplement to provide the necessary information for extracting the macroscale behavior of the system. Our hope is that if this is done properly, the combined macro-micro modeling technique will be much more efficient than solving the full microscopic model in detail [18].

2 Examples of Multiscale Methods

For the purpose of a systematic study, it is useful to divide multiscale problems into several different types according to some common features. These features are used in designing efficient modeling strategies. Here we will concentrate on two types of problems [17]. Other types of problems can also be conceived, but currently they are less exploited.

2.1 Type A Problems – Dealing with Isolated Defects

Type A problems are problems that have isolated defects near which the macroscopic models are invalid. Elsewhere explicitly given macroscale models are sufficient. Such defects can be shocks and contact lines in fluids, cracks, dislocations and triple junctions in solids or enzymatic reaction regions in biopolymers. Numerous computational techniques have been developed for such problems. An incomplete list includes

1. The nonlocal quasi-continuum method (QC) [60] for simulating isolated defects such as dislocations and cracks in single crystals. In this case the microscale model is molecular mechanics. The macroscale model, which is not explicitly used in QC, is nonlinear elasticity. An adaptive mesh refinement procedure allows QC to identify where the defects are and refine locally to the atomistic scale in order to resolve the full details around the defects.

2. DSMC-gas dynamics [29]. This is a very elegant extension of the adaptive mesh refinement procedure developed through the years by Bell, Berger, Colella et al. that incorporates the kinetic model at the finest level near shocks or other regions of special interest. The kinetic model is solved using discrete simulation Monte Carlo (DSMC). The continuum model and DSMC are coupled together through exchanges of fluxes at the cell boundaries.

3. MAAD [1, 2]. This highly publicized calculation was responsible for inspiring numerous subsequent work on multiscale modeling. Crack propagation in silicon was simulated using a seamless coupling procedure between finite elements away from the crack tip, molecular dynamics around the crack tip and tight-binding at the crack tip. Tight-binding was chosen as the simplest model for describing bond breaking at the crack tip. Molecular dynamics (MD) around the crack tip is capable of modeling processes such as dislocation loop emission. Finally finite element calculation away from the crack tip serves as boundary conditions for MD and at the same time carries the macroscopic deformation.

4. Coupled continuum - MD models for fluids [43, 28, 50, 31, 51]. Numerous attempts have been made to couple continuum models with MD for the modeling of fluids, with potential applications to micro-fluidics. The basic idea is that of heterogeneous domain decomposition: The computational domain is divided into overlapping regions on which continuum and MD calculations are carried out. The results are matched in the overlapping region to ensure continuity of the overall calculation.

5. Coupled continuum - MD methods for solids [21, 10]. These are methods that couple continuum models with MD for the simulation of the dy-

namic behavior of solids. The main issue is the matching condition at the continuum-MD interface. Cai et al. proposed exact boundary condition for linear problems, which provides a conceptual starting point but is too expensive in practice. E and Huang [21] extended the absorbing boundary conditions, traditionally designed for continuum calculations of waves [25], to the discrete models of MD. This seems to be a good compromise between exact boundary conditions of Cai et al. and the straightforward extensions of the absorbing boundary conditions for continuum models. At low temperature when no thermal energy is supplied to the system, this method works quite well.

6. Coupled quantum mechanics - molecular dynamics (QM-MM) methods [65, 67]. This is a popular method that uses quantum mechanical models in regions of chemical reaction, and classical molecular mechanics models elsewhere.

2.2 Type B Problems – Constitutive Modeling Based on the Microscopic Models

Type B problems are those for which the macroscopic model is not explicitly available, instead it should be indirectly inferred from the underlying microscopic model. Such problems occur in molecular dynamics when the atomistic potential is not explicitly known (which is often the case), or in continuum simulations of solids and fluids when the constitutive relations are not explicitly given. This class of problems are referred to as "equation-free computation", or "solving equations without equations" in [37]. Examples include:

1. Artificial compressibility method for computing incompressible flows [12]. The motivation in this case is to simulate incompressible flows without using the equations for incompressible flows, but rather using the compressible flow equations. Even though the equations for incompressible flows, the Navier-Stokes equations, are explicitly known, solving them numerically is a non-trivial matter. The idea of Chorin's artificial compressibility method is to use instead the compressible flow equations with suitably chosen Mach number. The optimal choice of Mach number is a compromise between accuracy, which favors choosing small Mach number, and computational cost, which favors choosing a larger Mach number. Note that stability constraints the size of the time step in accordance with the Mach number.

2. The Car-Parrinello method [9]. One of the key questions in MD simulations is how to get accurate interaction potential between atoms. For many problems the right potential is the Born-Oppenheimer potential obtained by calculating the ground state energy of the electrons when the positions of the nuclei are fixed. However computing the Born-Oppenheimer potential for realistic systems is a rather daunting task.

In 1985, Car and Parrinello devised a strategy for probing the relevant part of the Born-Oppenheimer surface on the fly during MD simulations.

Their method is formulated in the framework of density functional theory. The Lagrangian for the system of nuclei is augmented with new degrees of freedom associated with the Kohn-Sham orbitals with fictitious mass. The new nuclei-orbital system evolves just as any classical system would do, but with energy computed from density functional theory. This method has become a popular tool and has found wide application in material science, chemistry and biology.

The time step size is controlled by the fictitious mass associated with the Kohn-Sham orbitals. On physical grounds, one might be tempted to use electron mass as the fictitious mass, but since we are only interested in the dynamics of the nuclei, it is more efficient to choose a larger fictitious mass so that larger time steps can be used, as long as the desired accuracy for the dynamics of the nuclei is retained. This is in the spirit of the artificial compressibility method [14].

3. Local QC [60, 58, 38]. QC can also be used as a way of simulating the macroscopic deformation of a material without using empirical stored energy functional, but using directly the atomic potential. Compared with full atom calculation, the savings come from the fact that the energy for a small cluster of atoms can be used to represent the average energy over a macroscopic cell (Figure 1). Therefore the atoms in the large voids do not have to be visited.

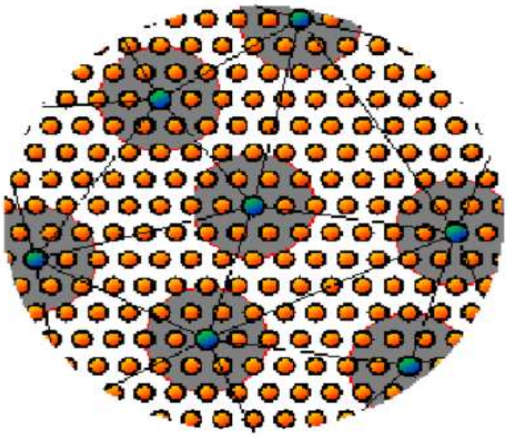

Fig. 1. Schematic illustration of QC (courtesy of M. Ortiz). Only atoms in the small cluster need to be visited during the computation.

4. Gas-kinetic scheme [66]. Even though originally it was not designed for the purpose of multiscale modeling, the gas-kinetic scheme provides one of the best examples of multiscale methods. Here the motivation is to compute

the macroscopic behavior of gases without using Euler's equation of gas dynamics but using directly the kinetic equations. Starting from a finite volume framework, hydrodynamic fluxes at cell boundaries are computed locally near the cell boundaries at each macro time step from the kinetic models, using a reconstruction-evolution-averaging procedure. This scheme served as the starting point for the heterogeneous multiscale method discussed later.

5. Stochastic ODEs [62]. This is discussed in Section 4 where we concentrate on time-scale issues.

6. Gap-Tooth scheme [37]. Gap-Tooth scheme [37] is an attempt to extend the philosophy illustrated in Figure 1 to a larger class of problems. Starting with a macroscopic initial data, the microscopic model is solved to the new macroscopic time step in small boxes (the tooth) centered around macroscale grid points, with suitable boundary conditions that are obtained from the macroscale data. The microscale solutions are then averaged in the boxes, and the macro state at the new time step is obtained by interpolating these averaged data. Gap-tooth scheme has been successfully applied to the one-dimensional heat equation, using the heat equation itself as the microscale model [37]. More recently it has been extended to solve the one-dimensional parabolic periodic homogenization problem [56]. However, it seems that this method is not suited for problems for which the macroscale dynamics is hyperbolic, e.g. convection equations, inviscid Burgers equations or equations of gas dynamics.

In connection with the quasi-continuum method, the clusters at the centers of the elements in Figure 1 would be the teeth, the voids would be the gaps.

2.3 Other Methods

We discuss briefly several other methods that are relevant to multiscale modeling.

1. Coarse-grained MD (CGMD) [55, 54]. This procedure works as follows. Starting with the microscopic Hamiltonian and after defining a set of coarse-grained degrees of freedom, one obtains a reduced Hamiltonian for the coarse-grained variables by averaging out the microscopic Hamiltonian with respect to the conditional equilibrium distribution. The coarse-grained MD is defined with respect to this reduced Hamiltonian.

2. Optimal prediction [13, 14]. In many complex systems we often have the problem that either the model or part of the data are not explicitly given. The idea of optimal prediction is to look for the best approximate solution with given information on the model and the data. A key technical aspect of this scheme is the norm used in defining the best approximation. In [13, 14] Chorin et al. use the L^2 norm with respect to the equilibrium distribution.

This requires knowing some information about the equilibrium distribution which can then be obtained perturbatively.

In general this procedure may result in an effective dynamics that is memory-dependent, as in the Zwanzig-Mori procedure. But the procedure simplifies if the problem has certain special features such as scale separation.

This philosophy is quite general. Indeed, coarse-grained MD, for example, is a special case of optimal prediction.

3. Projective dynamics for kinetic Monte Carlo models [39, 49] . This is a procedure for accelerating kinetic Monte Carlo simulations that involve disparate rates. The idea is to reduce the dynamics to a Markov chain that involves only the slow rates, by projecting out the fast processes.

4. Coarse-grained Monte Carlo [35, 36]. This is a semi-analytical and semi-numerical multiscale technique that systematically coarse grains Monte Carlo models with long range interaction [35]. Interaction parameters for the coarse-grained model were calculated analytically by suitably averaging the parameters in the microscopic model. Detailed balance is enforced at the coarse-grained level. Self-consistency is guaranteed by the fact that the microscopic model and the coarse-grained model share the same mesoscopic limit.

2.4 The Heterogeneous Multiscale Method

The heterogeneous multiscale method (HMM) [17] is an attempt to construct a unified framework for designing efficient simulation methods that couple the macro and microscale models. The framework should apply for both type A and type B problems. The basic principle of HMM is that one should start with a macroscale solver, taking into account as much as possible what is known about the macroscale process, and use the microscale model to provide the missing macroscale data that are necessary for implementing the macroscale solver. When measuring the macroscale data, the microscale model should be constrained by the (local) macro state of the system.

One distinct feature of HMM is its emphasis on selecting the right macroscale solver. This is especially important for problems whose macroscale behavior contains singularities. In general the principles for selecting the macroscale solver are the following: (1) It should be stable. (2) It should facilitate coupling with the microscale model.

3 Selecting the Macroscale Solvers

The emphasis on selecting the appropriate macro solver is motivated by the fact that for many problems of interest, the macroscale processes are also quite complicated and they may contain singularities, instabilities or phase transitions. The numerical problems can be very non-trivial even if a valid macroscale model is explicitly available.

To illustrate the selection of macro solvers, we will discuss two examples from gas dynamics. The first example is continuum gas dynamics locally corrected near shocks by the kinetic model. This is a type A problem. For this problem, the macroscopic process is gas dynamics, the microscopic process is kinetic model. Therefore we will choose the kinetic scheme for gas dynamics.

Recall the Euler equations for ideal gases,

$$\begin{cases} \rho_t + \nabla \cdot (\rho \boldsymbol{u}) = 0, \\ (\rho \boldsymbol{u})_t + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + \rho \theta I) = 0, \\ E_t + \nabla \cdot (\rho \boldsymbol{u}(|\boldsymbol{u}|^2 + \frac{5}{2}\theta)) = 0, \\ E = \rho(\frac{1}{2}|\boldsymbol{u}|^2 + \frac{3}{2}\theta), \end{cases} \tag{1}$$

where $\theta = RT$ with T being the temperature. A more detailed model is the Boltzmann equation,

$$f_t + \boldsymbol{\xi} \cdot \nabla f = \frac{1}{\varepsilon} C(f). \tag{2}$$

The function $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is the one particle phase-space distribution function. When the mean free path $\varepsilon \ll 1$, the system is close to local equilibrium states, or the local Maxwellians,

$$M(\boldsymbol{x}, \boldsymbol{\xi}, t) = \frac{\rho(\boldsymbol{x}, t)}{(2\pi\theta(\boldsymbol{x}, t))^{3/2}} \exp\Big(-\frac{(\boldsymbol{\xi} - \boldsymbol{u}(\boldsymbol{x}, t))^2}{2\theta(\boldsymbol{x}, t)}\Big). \tag{3}$$

In this regime, (1) can be derived using Chapman-Enskog expansion and moment closure with

$$\rho = \int f d\boldsymbol{\xi}, \quad \rho \mathbf{u} = \int f \boldsymbol{\xi} d\boldsymbol{\xi}, \quad E = \int f \frac{|\boldsymbol{\xi}|^2}{2} d\boldsymbol{\xi}. \tag{4}$$

Since we are interested in coupling the macroscale solver with the kinetic equation around the shock, we will choose a kinetic scheme as the macroscopic solver. Kinetic schemes take advantage of the fact that the solution of the Boltzmann equation is close to the local Maxwellian. We denote the grid points for the macro-mesh by x_j, the cell interface by $x_{j+1/2}$ and the time steps by t^n. For simplicity we only present the one dimensional version of the method. Extension to higher dimension is straightforward. For first order method, we represent the solution as piece-wise constant, i.e.

$$(\rho, \rho u, E) = (\rho_j, \rho_j u_j, E_j), \quad x \in (x_{j-1/2}, x_{j+1/2}],$$

and the grid values are the cell averages of the corresponding variables.

The derivation of the kinetic schemes consists of two steps. In the first step, we 'solve' the transport equation,

$$f_t + \xi f_x = 0.$$

Specifically we multiply the transport equation by $\xi, \xi^2, \xi^3/2$ and integrate within one grid cell and one time step, and also over the velocity space, to get

$$\begin{cases} \rho_j^{n+1} - \rho_j^n + \dfrac{\Delta t}{\Delta x}\big(F_{j+1/2}^{(1)} - F_{j-1/2}^{(1)}\big) = 0, \\ (\rho u)_j^{n+1} - (\rho u)_j^n + \dfrac{\Delta t}{\Delta x}\big(F_{j+1/2}^{(2)} - F_{j-1/2}^{(2)}\big) = 0, \\ E_j^{n+1} - E_j^n + \dfrac{\Delta t}{\Delta x}\big(F_{j+1/2}^{(3)} - F_{j-1/2}^{(3)}\big) = 0. \end{cases} \tag{5}$$

where

$$\rho_j^n = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} \rho(x, t^n)dx,$$

is the average of the solution within one cell, and

$$\boldsymbol{F}_{j+1/2} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}}\int_{\mathbb{R}} f(x_{j+1/2}, \xi, t)\begin{pmatrix} \xi \\ \xi^2 \\ \frac{1}{2}\xi^3 \end{pmatrix} d\xi dt$$

is the numerical fluxes across the cell interfaces.

The distribution function f can be decomposed into two parts: a left-moving part and a right-moving part. This gives rise to a natural splitting of the numerical fluxes:

$$\boldsymbol{F} = \boldsymbol{F}^+ + \boldsymbol{F}^-, \quad \text{with} \quad \boldsymbol{F}^\pm = \int_{\mathbb{R}^\pm} f(x_{j+1/2}^\mp, \xi, t)\begin{pmatrix} \xi \\ \xi^2 \\ \frac{1}{2}\xi^3 \end{pmatrix} d\xi. \tag{6}$$

Assume that $f(x, \xi, t)$ can be approximated by $M(x - \xi t, \xi, t^n)$. By direct computation we get,

$$\boldsymbol{F}^\pm = \begin{pmatrix} \rho u A^\pm(S) \pm \dfrac{\rho}{2\sqrt{\pi\beta}}B(S) \\ (p + \rho u^2)A^\pm(S) \pm \dfrac{\rho u}{2\sqrt{\pi\beta}}B(S) \\ (pu + \rho u e)A^\pm(S) \pm \dfrac{\rho}{2\sqrt{\pi\beta}}(\dfrac{p}{2\rho} + e)B(S) \end{pmatrix} \tag{7}$$

where

$$A^\pm = \frac{1 + \operatorname{erf}(S)}{2}, \quad B(S) = e^{-S^2}, \quad S = \frac{u}{\sqrt{2RT}}, \quad p = \rho RT.$$

In the second step, we include the collision term,

$$f_t = \frac{1}{\varepsilon}C(f).$$

Since the solution is close to the local Maxwellian, we include the effect of collision by simply setting $f(x, \xi, t^{n+1}) = M(x, \xi, t^{n+1})$. Also by doing this, one can continue to compute the numerical flux as in the previous time step. Despite the fact that the scheme is derived from kinetic models, the method only involves the computation of the numerical fluxes, and operates in the physical space. To achieve second order accuracy, one can use piecewise linear representation of the solutions. For other types of kinetic schemes see [52, 66].

In regions of large gradients where the local equilibrium approximation is inaccurate, we use directly the kinetic model. The transport part of the kinetic equation is solved using an upwind scheme. The collision part is added afterwards, which is usually done by particle method. The coupling of these two models in different regions is done as follows. Suppose that the interface between the kinetic region and the fluid domain is at $x_{j+1/2}$, with the fluid region on the left and the kinetic region on the right. Since we are using upwind scheme to solve the transport part of the Boltzmann equation, we only need the boundary condition for $\xi > 0$. For this we impose

$$f(x,\xi,t) = M(x^-_{j+1/2},\xi,t), \quad \xi > 0$$

where the right hand side is the local Maxwellian from the fluid side. On the other hand, in order to update the fluid equations to the next time step, we need to compute the fluxes at the interface. The splitting of the fluxes will automatically incorporate the contribution from the kinetic domain,

$$\begin{aligned}\boldsymbol{F}_{j+1/2} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} dt\Big\{ \int_{\mathbb{R}^+} M(x^-_{j+1/2},\xi,t)\begin{pmatrix}\xi\\ \xi^2\\ \frac{1}{2}\xi^3\end{pmatrix} d\xi \\ + \int_{\mathbb{R}^-} f(x^+_{j+1/2},\xi,t)\begin{pmatrix}\xi\\ \xi^2\\ \frac{1}{2}\xi^3\end{pmatrix} d\xi\Big\}.\end{aligned}$$

The coupling procedure will have to be more complicated if other macroscopic solver was used.

Our second example is again gas dynamics, but this time we assume that the equation of state is not given to us, instead we need to extract it from an underlying atomistic model of molecular dynamics. The macro solver in this case should be a conservative shock capturing scheme. Such schemes can be divided into two types, depending on whether a characteristic decomposition is used [42]. Since the nonlinear flux functions are not explicitly given to us, it is much easier to use a central type of scheme that does not use characteristic decomposition, the simplest of which is the Lax-Friedrichs scheme. Comparing with the Godunov scheme, central scheme uses the flux function at the cell center, which makes the coupling with MD simulation much easier.

The macroscopic equations are the usual conservation law of density, momentum and energy. We use the generic form of conservation laws in one dimension:

$$\boldsymbol{u}_t + \boldsymbol{f}(\boldsymbol{u})_x = 0. \tag{8}$$

The first order central scheme [48] constructs the solutions as piece-wise constants, which are the averaged values over each cell:

$$\boldsymbol{u}_k^n = \frac{1}{\Delta x}\int_{x_{k-1/2}}^{x_{k+1/2}} \boldsymbol{u}(x,t^n)dx.$$

Integration over $[x_j,\ x_{j+1}] \times [t^n,\ t^{n+1})$ leads to the following scheme:

$$\boldsymbol{u}_{k+1/2}^{n+1} = \frac{\boldsymbol{u}_k^n + \boldsymbol{u}_{k+1}^n}{2} - \frac{\Delta t}{\Delta x}\big(\boldsymbol{f}(\boldsymbol{u}_{k+1}^n) - \boldsymbol{f}(\boldsymbol{u}_k^n)\big). \tag{9}$$

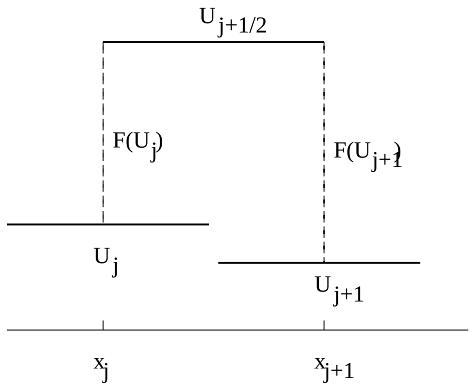

Fig. 2. Central scheme: starting with piecewise constant solution, one computes fluxes at x_j and x_{j+1}, and integrates the conservation laws to the next time step, where the grid points are shifted to the midpoints $x_{j+1/2}$.

At time t^{n+1} the numerical solutions are defined on a different set of grid points, as show in Figure 2. By applying the procedure again, one returns back to the original grid. The use of staggered grids has been shown to have less numerical viscosity than the usual Lax-Friedrichs scheme. Time steps have to be chosen to ensure stability. Let $A = \nabla \boldsymbol{f}$ and λ be the largest among the absolute values of the eigenvalues for A. Then it can be shown [48] that the central scheme is stable if

$$\lambda\frac{\Delta t}{\Delta x} \le \frac{1}{2}.$$

In our model, the fluxes are computed from local MD simulations: using the macroscale variables $\mathbf{u}$ we invoke the molecular system, evolve it to local equilibrium, and then estimate the fluxes via time and ensemble average. The accuracy of the overall scheme can also be analyzed. For more details and extensions see [44].

4 Time-Scale Problems in ODEs and Stochastic ODEs

We will distinguish four different types of multiple time-scale problems.

1. The first type, perhaps the simplest, is associated with the existence of a slow manifold, onto which the system is very rapidly attracted to. An example of this kind is the system

$$\begin{cases} \dot{x} = -\dfrac{1}{\varepsilon}(x - f(y)), \\ \dot{y} = g(x, y). \end{cases} \tag{10}$$

In this example the slow manifold is given by the graph $\{(x, y) : x = f(y)\}$. Starting from any initial condition, the system is attracted to this manifold in $O(\varepsilon)$ time-scale. x is the fast variable and y is the slow variable. On the slow manifold, y evolves according to an effective equation

$$\dot{y} = G(y) = g(f(y), y). \tag{11}$$

This class of problems are discussed in the context of stiff ODEs.
2. The second class of problems are often discussed in the context of averaging methods. In these problems, the slow variables feel the average effect of the fast variables. One simplest example is

$$\begin{cases} \dot{\varphi} = \dfrac{1}{\varepsilon}\omega(I) + f(\varphi, I) \\ \dot{I} = g(\varphi, I) \end{cases} \tag{12}$$

where f and g are periodic functions of φ, here the fast variable. The averaged system for the slow variable I is given by

$$\dot{I} = \frac{1}{2\pi} \int_0^{2\pi} g(\varphi, I) d\varphi = G(I). \tag{13}$$

Both (10) and (12) are special cases of

$$\begin{cases} \dot{x} = \dfrac{1}{\varepsilon} f(x, y), \\ \dot{y} = g(x, y). \end{cases} \tag{14}$$

Assume that for fixed y, the dynamics given by equation $\dot{x} = f(x, y)/\varepsilon$ is ergodic and denote by $\mu_y(dx)$ the unique invariant measure for x. The effective dynamics for the slow variable y is then given by

$$\dot{y} = G(y) \qquad \text{with} \;\; G(y) = \int g(x, y) \mu_y(dx) \tag{15}$$

(10) corresponds to the case when $\mu_y(dx) = \delta(x - f(y))$ and (11) corresponds to the case when $\mu_I(d\varphi) =$ Lebesgue measure on the circle. The first class of

problems are characterized by the fact that μ is dirac measure. (14) can be far more general. In particular, it can be a system of stochastic ODEs.

3. Effective stochastic dynamics. In these problems, the fast scale dynamics act effectively as noise on the slow dynamics. This is believed to be the case for example in molecular dynamics, which after coarse graining, may result in Brownian dynamics. Consider (14) in a special situation where the equation $\dot{x} = f(x, y)$ is ergodic but

$$\int g(x,y)\mu_y(dx) = 0. \tag{16}$$

In this case, the dynamics on the $O(1)$ time-scale is trivial, $\dot{y} = 0$, and the evolution of the slow variable arises on the longer, $O(\varepsilon^{-1})$ time-scale. On this time-scale, fluctuations becomes important, and the effective equation for the slow variable is an SDE:

$$\dot{y} = b(y) + \sigma(y)\dot{W}. \tag{17}$$

Here $\dot{W}$ is a white-noise process, and the coefficients $b(y)$ and $\sigma(y)$ satisfy

$$\begin{cases} b(y) = \displaystyle\int_0^\infty \int (g(x,y)\cdot\nabla_x) g(\varphi_t(x), y)\mu_y(dx)dt, \\ \sigma(y)\sigma^T(y) = \displaystyle\int_0^\infty \int g(x,y) g^T(\varphi_t(x), y)\mu_y(dx)dt, \end{cases} \tag{18}$$

where $\varphi_t(x)$ denotes the solution of $\dot{x} = f(x, y)$ at fixed y with initial condition $\varphi_0(x) = x$. Besides ergodicity, (17) requires enough mixing for the dynamics of the fast variable x in order that the time-integrals in (18) be finite. When the dynamics of the fast variables is governed by an SDE, this criterion is usually met, but explicit examples when y satisfies an ODE are rare, see for example [8].

It is also interesting to note that even if the expectation in (16) is non-zero, the effective equation (15) may only be valid on finite time intervals, and the small random perturbations that arise on the $O(\varepsilon^{-1})$ time scale are essential to describe the long-time behavior of the system. Here is an example. Consider

$$\begin{cases} \dot{x} = -\dfrac{1}{\epsilon}(y - x) + \dfrac{1}{\sqrt{\epsilon}}\dot{W} \\ \dot{y} = x - y^3. \end{cases} \tag{19}$$

For this system the effective equation (15) reads

$$\dot{y} = y - y^3, \tag{20}$$

according to which the motion of y converges to the stable fixed points $+1$ or -1 depending on the sign of the initial y. However, accounting for the next order correction in ε as in (17), the effective equation for y becomes

$$\dot{y} = y - y^3 + \sqrt{\epsilon}\,\dot{W}. \tag{21}$$

The additional noise term in this equation eventually drives the system back and forth between the two positions $y = \pm 1$. Note that this happens on the Arrhenius time-scale which is $O(\exp(1/\epsilon))$ because the switching from -1 to $+1$ involves a barrier crossing event. In this case, the effective equation (20) can be further reduced to that of a two-state Markov chain on $\{-1, +1\}$. This type of effective dynamics is discussed next.

4. Activated dynamics. In these examples the system spends most of its time in confined metastable sets, but occasionally hops from one metastable state to another. A simple example is (21) which can be rewritten as

$$\frac{dy}{dt} = -\frac{\partial V}{\partial y}(y) + \sqrt{\varepsilon}\,\dot{W}$$

where $V(y) = \frac{1}{4}(1 - y^2)^2$. Here the metastable states are around $y = \pm 1$. These examples are characterized by the exponentially long (in ε) time-scales that separate the individual hopping (transition) events between different metastable states.

Different techniques are required for these different problems. Stiff solvers are developed for problems of the first kind. These solvers are often implicit. But the work of Lebedev et al. makes an important exception. Lebedev et al. developed explicit Runge-Kutta methods, whose stage parameters are chosen to optimize their stability regions according to certain given distribution of the spectrum, which are assumed to be close to the real axis. For the special case of (10), the spectrum has a large gap. In this case, each step of the optimized Runge-Kutta method consists of many small stages followed by a few big stages, as shown in Figure 3.

In Lebedev's work only second order methods were discussed. Fourth order accurate Chebychev methods were constructed in [3].

The recent work of Gear et al. [30] can be considered as a simplified version of Chebychev methods that also uses a combination of small and large time steps but is otherwise unoptimized, in contrast to the Chebychev methods.

Chebyshev methods do not apply when the spectrum of the problem is far away from the real axis, as in the second kind of problems discussed above. However, these problems can be readily treated using HMM [16, 26]. The accuracy of HMM for these problems are greatly affected by the averaging procedure in the force estimator in HMM. These issues are discussed in [16, 22, 26] (see also [27]).

For stochastic ODEs, [62] proposed methods that use a combination of macro- and micro-solvers. The basic idea is to estimate the drift and diffusion coefficients in the macroscopic dynamics directly from solutions of the microscale model. Further analysis of these methods are presented in [22].

Even though Brownian dynamics has been used as a standard tool in the modeling of complex fluids, at the present time, there still lacks a systematic

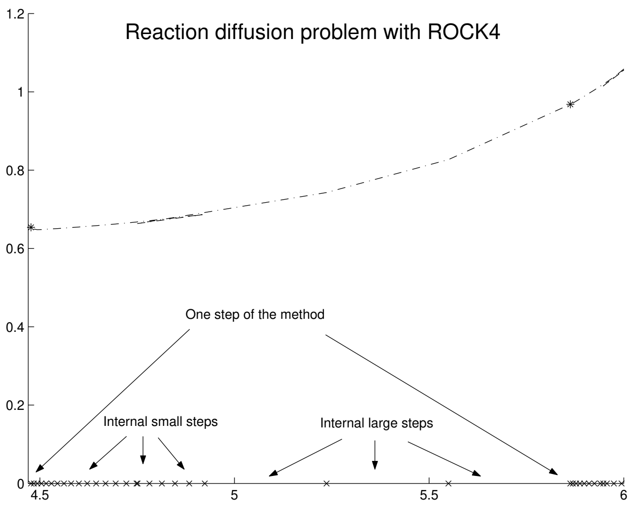

Fig. 3. Multistage Runge-Kutta: each step of the method consists of many small stages followed by a few big stages. (Courtesy of A. Abdulle)

coarse graining procedure for producing Brownian dynamics from more detailed models such as molecular dynamics. This is an area that deserves much more attention in the near future.

Activated dynamics can be considered as a sequence of transition events between metastable regions in the configuration space. Each event has an initial state and a final state. There has been two different approaches to activated dynamics, depending on whether the final state in the transition is assumed to be known. If the final state in a transition event is known, then the only remaining issue is to find the transition pathways and transition rates. Numerous numerical strategies have been proposed for this purpose. We refer to the papers [63, 34] in this volume for discussions on this class of methods. Several methods have been proposed to deal with the case when the final state is not assumed to be known. The best known among this class of methods are the hyperdynamics [64] and metadynamics [40, 33]. Hyperdynamics follows the dynamics in a modified potential energy surface and recovers information for the original dynamics using transition state theory. A related work is TAD (temperature accelerated dynamics) [59]. Metadynamics proceeds by first constructing the free energy surface associated with some judiciously chosen reaction coordinates, and then sample efficiently that free energy surface. Both the hyperdynamics and metadynamics are very promising ideas that should be exploited in the future.

5 Conclusions and Outlook

To conclude, let us ask the question: What is the current status of multiscale modeling? One thing that can be said about it is that it is now very popular. There are popular methods, such as the Car-Parrinello method and more recently the quasi-continuum method. There are popular ideas, such as hybrid atomistic-continuum methods, and macroscopic methods that use input obtained from pre-computed results using the microscopic models. There are also commonly realized issues, such as matching conditions between different levels of physical models.

As is the case for any fashionable subject, there is also the need for processing the rapidly generated information in this area with great care. With few exceptions, most of the recently proposed multiscale modeling techniques have not been tested on truly challenging problem. Most work remains at the level of testing concepts. Few have gone through the rigorous procedure of verifying the results. Instead, most seem to be content with producing reasonably looking pictures. Analytical results on error control are very rare. Moreover, some of the proposed multiscale methods are more expensive than solving directly the original microscale problem (see for example the discussions in [46]).

From a mathematical perspective, it is desirable to have a unified framework for studying multiscale methods. So far HMM seems to be a reasonable candidate. Several classes of problems are solved using this framework, including atomistic-continuum modeling for the dynamics of solids [44] and fluids [53], interface dynamics [11], and homogenization problems [4, 46]. In addition, several class of methods, including HMM for the homogenization problems [4, 24, 47], ODEs [16, 26], multiscale method for stochastic ODEs [62, 22], and the quasi-continuum methods [23], have been analyzed using this framework. But it should be emphasized that HMM provides only a starting point, for most problems of interest, highly non-trivial practical issues still remain. While HMM facilitates macro-micro coupling, it does not solve all the problems of macro-micro coupling. This is illustrated clearly in [53, 44]. Solutions to the remaining coupling issues are useful not only in the context of HMM, but also for other coupling strategies such as sequential coupling.

Finally it should be mentioned that most multiscale modeling work deals with almost homogeneous systems such as fluids. There is relatively little work for strongly heterogeneous systems such as macromolecules. The latter will undoubtedly be an area of great interest in the near future.

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References

1. F.F. Abraham, J.Q. Broughton, N. Bernstein and E. Kaxiras, “Spanning the continuum to quantum length scales in a dynamic simulation of brittle fracture, *Europhys. Lett.*, 44 (6), 783–787 (1998).
2. F.F. Abraham, J.Q. Broughton, N. Bernstein and E. Kaxiras, “Concurrent coupling of length scales: Methodology and application,” *Phys. Rev. B* **60** (4), 2391–2402 (1999).
3. A. Abdulle, “Fourth order Chebychev methods with recurrence relations”, *SIAM J. Sci. Comput.* **23**, 2041–2054 (2002).
4. A. Abdulle and W. E, “Finite difference HMM for homogenization problems”, *J. Comput. Phys.* **191**, 18–39 (2003).
5. J. Bourgat, P. Le Tallec and M. Tidriri, “Coupling Boltzmann and Navier-Stokes equations by friction”, *J. Comput. Phys.* **127**, 227 (1996).
6. A. Brandt, “Multigrid methods in lattice field computations”, *Nuclear Physics B Proc. Suppl.* **26** 137–180 (1992).
7. A. Brandt, “Multiscale scientific computation: Review 2001”. *Lecture Notes in Computational Science and Engineering*, T.J. Barth et.al eds., Springer, 2002.
8. L. A. Bunimovich, “Existence of transport coefficients”, in *Hard Ball Systems and the Lorentz Gas*, D. Szasz ed., Springer, 2000.
9. R. Car and M. Parrinello, “ Unified approach for molecular dynamics and density-functional theory”, *Physical Review Letters* **55**, 2471–2474 (1985).
10. W. Cai, M. de Koning, V.V. Bulatov and S. Yip, “Minimizing boundary reflections in coupled-domain simulations,” *Phys. Rev. Lett.* **85**, 3213–3216 (2000).
11. L. T. Cheng and W. E, “The heterogeneous multiscale method for interface dynamics”, *Contemporary Mathematics:* **330**, 43–53 (2003).
12. A. J. Chorin, “A numerical method for solving incompressible viscous flow problems”, *J. Comput. Phys.* **2**, 12–26, 1967.
13. A. J. Chorin, A. Kast and R. Kupferman, “Optimal prediction of underresolved dynamics”, *Proc. Nat. Acad. Sc. USA* **95**, 4094–4098 (1998).
14. A. J. Chorin, O. Hold and R. Kupferman, “Optimal prediction with memory”, *Physica D* **166**, 239–257 (2002).
15. S. M. Deshpande, Kinetic theory based new upwind methods for invisid compressible flows, *AIAA paper*, No. 86-0275.
16. W. E, “Analysis of the heterogeneous multiscale method for ordinary differential equations”, *Comm. Math. Sci.* **1**, 423–436 (2003).
17. W. E and B. Engquist,“The heterogeneous multi-scale methods”, *Comm. Math. Sci.* **1**, 87–132 (2003).
18. W. E and B. Engquist, “Multiscale modeling and computation”, *Notices of the American Mathematical Society* **50**, 1062–1070 (2003).
19. W. E, B. Engquist and Z. Huang, “Heterogeneous multi-scale method – a general methodology for multi-scale modeling”, *Phys. Rev. B* **67**, 092101 (2003)
20. W. E and Z. Huang, “Matching conditions in atomistic-continuum modeling of materials,” *Phys. Rev. Lett.* **87**, 135501 (2001).
21. W. E and Z. Huang, “A dynamic atomistic-continuum method for the simulation of crystalline materials”, *J. Comput. Phys.* **182**, 234–261 (2002).
22. W. E, D. Liu and E. Vanden-Eijnden, “Analysis of multiscale techniques for stochastic dynamical systems”, preprint, 2003.
23. W. E and P. B. Ming, “Analysis of the quasi-continuum method, I”, preprint, 2003.

24. W. E, P. B. Ming and P. W. Zhang, "Analysis of the heterogeneous multiscale method for elliptic homogenization problems", preprint. *Available at http://www.math.princeton.edu/multiscale.*
25. B. Engquist and A. Majda, "Radiation boundary conditions for acoustic and elastic wave calculations," *Comm. Pure Appl. Math.* **32**, 313–357 (1979).
26. B. Engquist and R. Tsai, "The Heterogeneous Multiscale Methods for a class of Stiff ODEs", submitted.
27. I. Fatkullin and E. Vanden-Eijnden, "Effective dynamics and efficient computations. Applications to Lorenz 95 system", submitted.
28. E. G. Flekkoy, G. Wagner and J. Feder, *Europhys. Lett.* **52**, 271 (2000).
29. A. L. Garcia, J. B. Bell, W. Y. Crutchfield and B. J. Alder, "Adaptive mesh adn algorithm refinement using direct simulation Monte Carlo" *J. Comput. Phys.* **154**, 134–155 (1999).
30. C.W. Gear and I.G. Kevrekidis, "Projective methods for stiff differential equations: problems with gaps in their eigenvalue spectrum," *SIAM J. Sci. Comp.* **24**, 1091-1106, 2003.
31. N. G. Hadjicontantinou, "Hybrid atomistic-continuum formulations and the moving contact line problem", *J. Comput. Phys.* **154**, 245–265 (1999).
32. E. Hairer and G. Wanner, *"Solving Ordinary Differential Equations II, Stiff and Differential-Algebraic Problems"*, Springer-Verlag, 1991
33. M. Iannuzzi, A. Laio, and M. Parrinello, "Efficient Exploration of Reactive Potential Energy Surfaces Using Car-Parrinello Molecular Dynamics,", *Phys. Rev. Lett.* **90**, 238302 (2003)
34. H. Jonsson, this volume.
35. M. Katsoulakis, A. J. Majda and D. G. Vlachos, "Coarse-grained stochastic processes for lattice systems", *Proc. Natl. Acad. Sci. USA* **100**, 782–787 (2003).
36. M. Katsoulakis, A. J. Majda and D. G. Vlachos, Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems, *J. Comp. Phys.* **186**, 250-278 (2003).
37. I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg and C. Theodoropoulos, "Equation-free multiscale computation: enabling microscopic simulations to perform system-level tasks", in preparation.
38. J. Knap and M. Ortiz, "An analysis of the quasi-continumm method", *J. Mech. Phys. Sol.*, **49**: 1899–1923 (2001).
39. M. Kolesik, M. A. Novotny and P. Rikvold, "Projection method for statics and dynamics of lattice spin systems", *Phys. Rev. Lett.* **80**, 3384–3387 (1998).
40. A. Laio and M. Parrinello, "Escaping free-energy minima," *Proc. Nat. Acad. Sc. USA* **99**, 12562–12566 (2002).
41. V. I. Lebedev and S. I. Finogenov, "Explicit methods of second order for the solution of stiff systems of ordinary differential equations", *Zh. Vychisl. Mat. Mat Fiziki*, **16**. 895–910 (1976).
42. R. LeVeque, *"Numerical Methods for Conservation Laws,"* Birkhäuser, 1990.
43. J. Li, D. Liao and S. Yip, "Nearly exact solution for coupled continuum/MD fluid simulation", *J. Computer-Aided Materials Design* **6**, 95–102 (1999).
44. X.T. Li and W. E, "Heterogeneous multiscale method for the modeling of solids", preprint, 2003.
45. R. E. Miller and E. B. Tadmor, "The quasicontinuum method: Overview, applications and current directions", preprint.
46. P. B. Ming and X. Yue, "Numerical methods for multiscale elliptic problems", preprint. *Available at http://www.math.princeton.edu/multiscale.*

47. P. B. Ming and P. W. Zhang, "Analysis of the heterogeneous multiscale method for dynamic homogenization problems", preprint.
48. H. Nessyahu and E. Tadmor, Nonoscillatory central differencing for hyperbolic conservation laws, *J. Comp. Phys.* **87**, 408–463 (1990).
49. M. A. Novotny, "A tutorial on advanced dynamic Monte Carlo methods for systems with discrete state spaces", *Ann. Rev. Comput. Phys.,* 153–210 (2001).
50. S. T. O'Connell and P. A. Thompson, *Phys. Rev. E* **52**, R5792 (1995).
51. X. Nie, S. Chen, W. E and M. O. Robbins, submitted to *Phys. Fluids.*
52. B. Perthame, Second-order Boltzmann schemes for compressible Euler equations in one and two space dimensions. *SIAM J. Numer. Anal.* **29**, 1–19 (1992).
53. W. Ren and W. E, "Heterogeneous multiscale method for the modeling of fluids", in preparation.
54. R.E. Rudd and J.Q. Broughton, "Coarse-grained molecular dynamics and the atomic limit of finite elements," *Phys. Rev. B* **58**, R5893–R5896 (1998).
55. R.E. Rudd and J.Q. Broughton, "Atomistic simulation of MEMS resonators through the coupling of length scales," *J. Modeling and Simulation of Microsystems* **1**, 29–38 (1999).
56. G. Samaey, private communication, 2003.
57. T. Schulze, P. Smereka and W. E, "Coupling kinetic Monte-Carlo with continuum models with applications to epitaxial growth", *J. Comput. Phys.* **189**, 197–211 (2003).
58. G.S. Smith, E.B. Tadmor, and E. Kaxiras, "Multiscale simulation of loading and electrical resistance in silicon nanoindentation", *Phys. Rev. Lett.* **84**, 1260–1263 (2000).
59. M. R. Sorensen and A. Voter, *J. Chem. Phys.* **112**, 9599–9606 (2000).
60. E. B. Tadmor, M. Ortiz and R. Phillips, "Quasicontinuum analysis of defects in crystals," *Phil. Mag. A* **73**, 1529–1563 (1996).
61. S. Tiwari and A. Klar, an adaptive domain decomposition procedure for Boltzmann and Euler equations, *J. Comput. Appl. Math.* **90**, 223–237 (1998).
62. E. Vanden-Eijnden, "Numerical techniques for multiscale dynamical systems with stochastic effects", *Comm. Math. Sci.*, **1**, 385–391 (2003).
63. W. E and E. Vanden-Eijnden, this volume.
64. A. Voter, "Hyperdynamics: Accelerated molecular dynamics of infrequent events", *Phys. Rev. Lett.* **78**, 3908–3911 (1997).
65. A. Warshel and M. Levitt, "Theoretical studies of enzymic reactions", *J. Mol. Biol.* **103**, 227–249 (1976).
66. K. Xu and K.H. Prendergast, "Numerical Navier-Stokes solutions from gas kinetic theory," *J. Comput. Phys.* **114**, 9–17 (1994).
67. Y. Zhang, T.-S. Lee and W. Yang, "A pseudobond approach to combining quantum mechanical and molecular mechanical methods", *J. Chemical Phys.* **110**, 46–54 (1999).