Heterogeneous multiscale method: A general methodology for multiscale modeling

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The heterogeneous multiscale method, is presented as a general methodology for an efficient numerical computation of problems with multiple scales. The method relies on an efficient coupling between the macroscopic and microscopic models. In case the macroscopic model is not explicitly available or is invalid in part of the domain, the microscopic model is used to supply the necessary data for the macroscopic model. Scale separation is exploited so that coarse-grained variables can be evolved on macroscopic spatial/temporal scales using data that are predicted based on the simulation of the microscopic process on *microscale* spatial/temporal domains. Applications to homogenization, dislocation dynamics and crack propagation are discussed.

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Many problems in nature involve multiple active scales. For example, chemical reactions may take seconds or hours, while the vibration of chemical bonds occurs at the time scale of femtoseconds (10^{-15}s). Vortical structures in the atmosphere may range from meters to thousands of kilometers. With few exceptions, the traditional approach for such problems is to obtain either analytically or empirically explicit equations for the scale of interest, eliminating other scales. This approach has been very successful for large classes of problems. However, for more complex systems this approach also forces us to introduce empirical closures that are often not justified or understood. Typical examples of such a situation are found in complex fluids, plasticity, and turbulent flows.

Recently there has been an explosive growth of interest in coupling different models with levels of detail in order to achieve a balance between accuracy and efficiency. Such a coupled multi-scale/multi-physics approach is discussed in many papers,[1–7] and is a central theme of the present paper.

In this paper, we present a general framework for designing and analyzing numerical methods that deal with problems of these types. Our basic setup is as follows. We are interested in a macroscale process with a state variable U. However, we do not have an explicit macroscale model which is valid everywhere. Instead we have at our disposal a microscopic model, such as molecular dynamics or quantum mechanics, that describes the microscopic state variable u. The two processes and state variables are related to each other by compression and reconstruction operators, denoted by Q and R, respectively: $Qu=U$ and $RU=u$, with the property $QR=I$, where I is the identity operator. The compression operators are in general local/ensemble averages, projection to low order moments, or slow manifolds. The reconstruction operator does the opposite. It is not unique in general.

Our aim is to accurately numerically approximate the macroscopic state of the system; therefore, we will work with a macroscopic grid that resolves the large scale of the system. There are two main components in the heterogeneous multiscale method: *An overall macroscopic scheme for* U and *estimating the missing macroscopic data from the microscopic model*. The right overall macroscopic scheme depends on the nature of the problem and typically there is more than one choice. For variational problems, we can use the standard finite element method with a piecewise polynomial finite element space. For dynamic problems that are conservative, we may use the methods developed for nonlinear conservation laws (see, e.g., Ref. 8). Examples include the Godunov scheme, and the discontinuous Galerkin method. For dynamic problems that are non-conservative, one could simply use a standard ordinary differential equation (ODE) solver, such as the Runge-Kutta method, coupled with the force estimator that we discuss below.

After selecting the overall macroscopic scheme, we face the difficulty that not all data needed for the macro scheme are available since the underlying macro model is not explicitly known everywhere. The next component of the heterogenous multiscale method (HMM) is to estimate such missing data from the microscopic model. This is done by solving the micro model locally subject to the constraint that $\tilde{Q}u=U$, where $\tilde{Q}$ is an approximation of Q and U is the current macro state. Depending on the problem, the missing data can be the stiffness matrix, or the flux or forces of the macro model, or the transition rates if the macro model is a Markov chain. It can also be only part of the macro model such as the eddy viscosity term in a turbulence model. For variational problems, such data can be estimated by solving the original microscopic variational problem on a unit cell in each element of the triangulation, subject to the constraint that $\tilde{Q}u=U$. The unit cell can be a unit cell in the crystal lattice, as in quasicontinuum method, or the unit periodic cell in a periodic homogenization problem.[9] For dynamic problems, such data can be estimated from a Godunov procedure, namely, that we first reconstruct the micro state from U, and then we evolve the micro state using the microscopic model subject to the constraint that $\tilde{Q}u=U$, and finally we estimate the missing data from u.

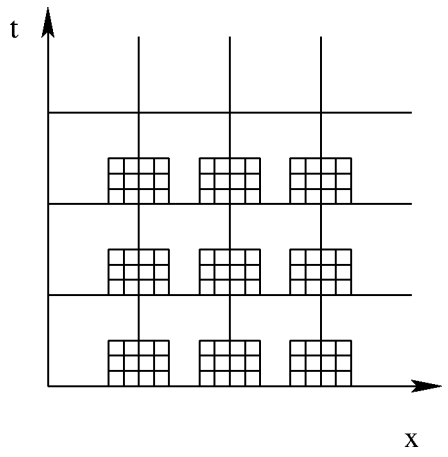

FIG. 1. Illustration of the computational domain for the HMM.

The key to the efficiency of such an approach is the possibility that the microscale model does not have to be solved over the whole computational domain, but rather over a small region near where data estimation is carried out; see Fig. 1. Traces of such ideas can already be found in the literature, for example for stiff ODEs in Refs. 10 and 11 for kinetic schemes in gas dynamics in Ref. 12. Our current work draws inspiration from the important work of Kevrekidis and co-workers.[10] Closely related ideas are also found in Refs. 13 and 14. We call this approach the heterogeneous multiscale method, abbreviated HMM, to emphasize the fact that different physical models are used at different scales. In contrast, standard multi-grid techniques employ the same physical model on different scales and are aimed at efficiently resolving the microscopic details.[15,16]

Most multiscale problems fit very well into this framework. For example the quasicontinuum method can be formulated as a special case of the HMM in which the macroscale scheme is the piecewise linear finite element method, and the estimation of the macroscale energy functional is done using the Cauchy-Born rule.[4] However, what is important is that the framework of the HMM allows us to design *new* numerical methods for a wide class of multiscale problems.

Consider first the example of a dynamic homogenization problem

$$\frac{\partial u^\varepsilon}{\partial t} = \nabla \cdot \left[a\left(x, \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right]. \tag{1}$$

Here the coefficient $a(x,x/\varepsilon)$ represents properties of a multiscaled medium, such as the conductivity of a composite material, or the permeability of a porous medium.[17] ε is assumed to be a small dimensionless number. For simplicity, we will assume that $a(x,y)$ is periodic in y with period P. We take the macroscale variable $U=Qu^\varepsilon$ to be the local averages of u^ε over macro cells of size $(\Delta t,\Delta x)$ which we also take as the size of the macro grid. Our aim is to compute accurately Qu^ε. Let $t^n=n\Delta t$ and $x_j=j\Delta x$. For the overall macroscale scheme, we choose the finite volume method

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x}(J_{j+(1/2)}^n - J_{j-(1/2)}^n),$$

where $J_{j+(1/2)}$ denotes the macroscale flux at time t^n and position $x_{j+(1/2)}$. To estimate this quantity, we proceed as follows:

(1) Reconstruction. From $\{U^n\}$, we reconstruct $\tilde{u}=RU^n$. The simplest way of doing this is the piecewise linear reconstruction

$$RU^n(x) = U_j^n + \frac{U_{j+1}^n - U_j^n}{\Delta x}(x - x_j)$$

for $j\Delta x \leqslant x < (j+1)\Delta x$.

(2) Microscopic evolution. We solve Eq. (1) with the initial data $\tilde{u}(x)=RU^n(x)$ on a much finer grid that resolves the small scales. The solution will be denoted by $u(x,t)$.

(3) Flux estimation. From u, we estimate the flux at cell boundaries $x_{j+(1/2)}=(j+\frac{1}{2})\Delta x$. For example, we may let

$$J_{j+(1/2)} = a\left(x_{j+(1/2)}, \frac{x_{j+(1/2)}}{\varepsilon} \right) \nabla u(x_{j+(1/2)}, \alpha\Delta t)$$

for some $\alpha < 1$.

If this is all we do, there is no significant savings in comparison with solving the microscopic model directly. The savings come from the reduction of size of the computational domain in space and time.

To begin with, we do not need to solve Eq. (1) over the whole physical domain. We only have to solve Eq. (1) on a unit cell of size ε around the points at the cell boundaries where flux evaluation is carried out. This reduces the spatial complexity of the problem by a factor of $(\Delta x/\varepsilon)^d$, where d is the spatial dimension. Specifically, if the macroscale flux is needed at point $x_{j+(1/2)}$ for the overall macroscale finite volume scheme, we place $x_{j+(1/2)}$ at the center of a cell of size ε, denoted by $C^\varepsilon_{j+(1/2)}=x_{j+(1/2)}+\varepsilon P$, and in step (2) above we evolve Eq. (1) on $C^\varepsilon_{j+(1/2)}$ subject to the boundary condition that $u^\varepsilon(x,t)-RU^n(x)$ is periodic with period εP.

Perhaps more significant is the possibility of reducing the temporal complexity. This is clearly suggested by the results in Fig. 2, where we plot the computed flux at one particular cell boundary over an interval $[t^n,t^n+\Delta t]$. It is clear that the flux quickly relaxes to a quasistationary value, in this example after about 40 microscopic time steps. This means that we can stop the microscale evolution after about 40 micro steps, and use the result on a macro time step which is more than 10^4 micro steps. This alone constitutes savings of more than 250 times.

This idea draws inspiration from the literature on numerical solutions of stiff ordinary differential equations[10,11]. It is an important ingredient that enables us to *perform simulations on microscopic models over a macroscopic time scale.*

We next discuss how the HMM can be applied to coupling atomistic (molecular dynamics) and continuum simulations. For clarity, we first discuss the relatively simple problem of dislocation dynamics in the Frenkel-Kontorova (FK)

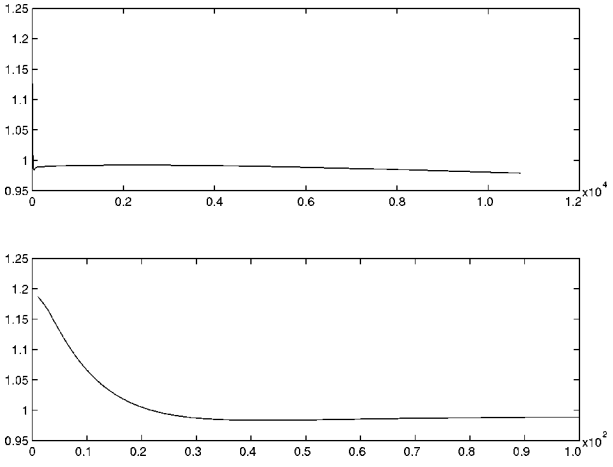

FIG. 2. Numerical flux as a function of the microscopic time steps over one macroscopic time step, for Eq. (1) with $a(x,x/\varepsilon)=2+\sin(2\pi x/0.01)$, and $\varepsilon=0.01$. The bottom figure is a detailed view of the transient period.

model.[18] This is a one-dimensional chain of atoms in a periodic potential, coupled by linear springs. We will take the potential to be

$$U(x)=\frac{1}{2}\mathcal{K}[x-a\,\mathrm{int}(x/a)]^2. \tag{2}$$

Here a is the equilibrium distance between neighboring atoms, $\mathrm{int}(x/a)$ is the nearest integer to x/a. Denoting the position of the nth atom by x_n, the dynamic equation for the atoms is given by

$$m\ddot{x}_n=k(x_{n+1}-2x_n+x_{n-1})-U'(x_n)+f, \tag{3}$$

where f is the applied force.

One interesting aspect of the Frenkel-Kontorova model is the possibility of having a dislocation in the system, which corresponds to vacant or doubly occupied potential wells. In the absence of dislocations, the equilibrium positions of the atoms are given by $x_j=ja$. In general, we let $x_j=a(j+u_j)$. u is then the displacement field. The displacement field is approximated by the Klein-Gordon equation

$$\partial_\tau^2 u=\partial_x^2 u-\overline{\mathcal{K}}u+\overline{f}, \tag{4}$$

where $\overline{\mathcal{K}}=\mathcal{K}/(ka^2)$ and $\overline{f}=f/(ka^3)$. Our numerical strategy is now as follows. We work with a macroscopic grid of sizes $(\triangle t,\triangle x)$. The macroscale scheme consists of two components: a finite difference scheme for Eq. (4) and an ODE solver for the position of the dislocation given its velocity. At each time step, we first perform an atomistic substep in order to estimate the velocity of the defects (here the dislocation) and the fluxes or forces in the atomistic region where continuum equations are not valid, and we then update the position of the defects and the displacement field over the macro grid using the estimated data in the atomistic region and the continuum equation (here the Klein-Gordon equation) elsewhere.

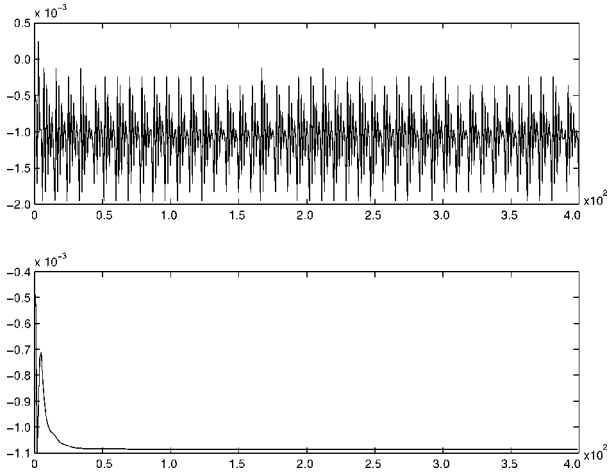

FIG. 3. Velocity of the dislocation in the FK model over a macroscopic time step. The upper figure is the result of the full FK model. The lower figure is the result after applying a third order filter.

At the atomistic substep, we first reconstruct the initial positions and velocities of the atoms using the displacement and velocity fields at the macro grid using interpolation, and we then evolve the atomistic model using boundary conditions constructed in Ref. 3, and we estimate the needed data by processing the data obtained from the atomistic model.

A remark about the data processing is in order. As before, the key to the feasibility of carrying out such simulations to macroscopic times (e.g., microseconds) lies in the fact that *the atomistic simulation only has to be done for a small number of steps in order to predict accurately the velocity of the dislocation*. To see this we plot in the upper panel of Fig. 3 the speed of the dislocation computed using Eq. (3) during a time interval of size $\triangle t$. If we process this data using suitable filters,

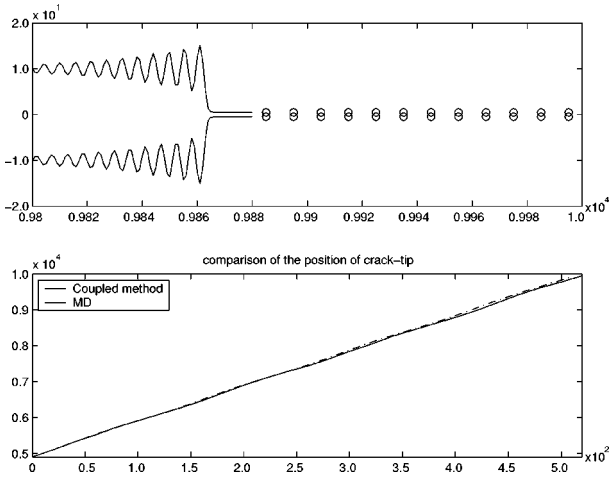

FIG. 4. Upper panel: displacement profile at the crack surface near the tip; circles denote the continuum region, lines denote the atomistic subdomain. Lower panel: comparison of the tip position as a function of time computed using the full atomistic model (solid line) and the HMM (dashed line).

$$\overline{g}(t)=\frac{1}{t}\int_{t^n}^{t^n+t}K\left(1-\frac{\tau}{t}\right)g^e(\tau)d\tau,\quad K(\tau)=1-\cos 2\pi\tau, \tag{5}$$

we obtain the lower panel of Fig. 3 and this resembles closely Fig. 2. Therefore to extract the dislocation velocity, we only have to simulate the microscale model for about 40 micro time steps. Yet we can use that value over one macro time step.

This strategy applies to more general situations when coupling atomistic and continuum models is necessary. As our last example, we discuss a two-dimensional model of mode-III crack propagation in an inhomogeneous medium. The details of the model was discussed in Ref. 19. Other examples can be found in Refs. 9 and 19. We follow the procedure outlined in the second example. The macroscale scheme consists of two components: A finite difference scheme for the linear elasticity equation away from the crack tip and an ODE solver for the position of the crack tip. At each macro time step, we predict the velocity of the crack tip by solving the atomistic model near the current position of the crack tip, using boundary conditions that minimize the reflection of the phonons.[3] We then update the position of the crack tip and the displacement fields away from the crack tip using standard finite difference schemes on the linear elasticity equation. In Fig. 4 we plot the displacement profile at the crack surface near the tip, together with a comparison of the tip position as a function of time computed using the full atomistic model as well as the HMM.

Again the key to the efficiency of this procedure is that we need only to simulate the atomistic model over few micro time steps, and by processing the velocity data for the crack tip, we can estimate its macroscale velocity and use it over the macro time step which is of several thousand micro time steps.

In summary, the HMM is a very general and very efficient methodology for dealing with multiscale/multiphysics problems. It provides a framework for bridging not only spatial scales, but also temporal scales. It also allows us to study macroscopic behavior of systems in the absence of explicit macroscopic models. A solid mathematical foundation for the HMM, including issues on numerical stability and accuracy, was presented in Ref. 9. Applications to a wide variety of problems, including complex interfaces, coupling molecular dynamics with hydrodynamics, are currently being actively pursued.

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