The Heterogeneous Multi-Scale Method

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Abstract

The heterogeneous multi-scale method (HMM) is a general strategy for dealing with problems involving multi-scales, with multi-physics, using multi-grids. It not only unifies several existing multi-scale methods, but also provide a methodology for designing new algorithms for new applications. In this paper, we review the history of multi-scale modeling and simulation that led to the development of HMM, the methodology itself together with some applications, and the mathematical theory of stability and accuracy.

1 Introduction

In the past several years, there has been an explosive growth of interest on numerical computations for problems involving multi-scales, often with multiple levels of physical models and use multi-grids. Applications of these ideas are found in many different areas, including coupling quantum mechanics with molecular dynamics [12, 73, 75], coupling atomistics with continuum theory [8, 1, 55, 53, 11, 24, 45, 37], coupling kinetic theory with continuum theory [8, 30, 42, 72], coupling kinetic Monte Carlo methods with continuum theory [58], homogenization theory [8, 25, 41, 50, 11], and coarse-grained bifurcation analysis [67, 57].

From the point of view of numerical analysis, it is natural to ask whether these seemingly different applications can be put into a common framework, and whether a general theory of stability and accuracy can be provided. Such a theory should help us to improve existing methods, design new ones, and extend their applicability to other problems.

Finite element method provided an example of a success story of this kind. The practice of finite element methods was started by structural engineers on very specific applications.

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However, the work of mathematicians at the end of the 60’s and early 70’s put finite element method on a much more solid and general framework. This framework provided a thorough understanding of existing methods, suggested improvements and as well as extension to other areas such as fluid mechanics, electromagnetism, etc.

In this article, we will review the work in [21] that aimed at providing a general framework as well as a stability and accuracy theory for numerical methods involving multiscales, multi-grids and multi-physics. For convenience and to emphasize the multi-physics nature of these methods, we will call them Heterogeneous multiscale methods. In contrast, typical multi-grid methods are homogeneous in the sense that they use the same model at different levels of grids and are aimed at efficiently resolving the details at the finest grids.

To begin with, let us make some remarks about problems with multiple scales. Such problems are found everywhere around us. A classical example that has been extensively studied in the mathematics literature is the problem of homogenization.

\[-\nabla \cdot \left( a \left( x, \frac{x}{\varepsilon} \right) \nabla u(x) \right) = f(x), \quad x \in \Omega \quad (1)\]

with Dirichlet boundary condition \( u^\varepsilon \mid_{\partial \Omega} = 0 \), for example [6]. Here the multiscale nature is reflected in the coefficients \( a \left( x, \frac{x}{\varepsilon} \right), \varepsilon \ll 1 \). In the simplest models \( a(x, y) \) is assumed to be periodic in \( y \), say with period \( I = [0, 1]^d \), \( d \) is the dimension of the physical space. (1) can be used for modelling transport properties in a medium with microstructure, and the oscillatory nature of \( a \) is used to model the microstructures in the medium.

Traditionally problems of this type are dealt with either analytically or empirically by finding effective models that eliminate the small scales. For the homogenization problem (1), this means replacing (1) by a homogenized equation [6, 69] or effective equation

\[-\nabla \cdot (A(x) \nabla U(x)) = f(x) \quad x \in \Omega. \quad (2)\]

The solution \( U \) of this equation approximates the behavior of \( u^\varepsilon \) averaged over length scales that are much larger than \( \varepsilon \) but smaller than the slow variations of \( a \) and \( f \). In the special case when \( d = 1 \), \( A(x) \) is given simply by

\[A(x) = \left( \int_0^1 \frac{1}{a(x, y)}dy \right)^{-1} \quad (3)\]

An alternative to such analytical methods is the empirical modelling. As an example, let us consider simple incompressible fluids. Let \( u \) be the velocity field. Mass and momentum conservation gives,

\[u_t + (u \cdot \nabla)u + \frac{1}{\rho} \nabla p = \nabla \cdot \tau_d, \quad \nabla \cdot u = 0 \quad (4)\]

where \( \rho \) is the (constant) density, \( \tau_d \) is the viscous stress, which is a macroscopic idealization of the internal friction forces due to the short-ranged molecular interactions. \( \tau_d \) must be
modeled in order to close the equation (4). The simplest empirical model is to assume that \( \tau_d \) is linearly related to \( D = \frac{\nabla u + (\nabla u)^T}{2} \), the rate of strain tensor. Using homogeneity, isotropy and incompressibility gives the constitutive relation

\[
\tau_d = \nu D
\]  

(5)

where \( \nu \) is the viscosity of the fluid. In this model, all molecular details are lumped into a single number \( \nu \). It is quite amazing that such a simple ansatz describes very well the behavior of simple liquids in almost all regimes.

Despite all these successes, such traditional approaches also have their limitations. Although a nice set of equations can be derived rigorously for the effective coefficients \( A(x) \) in (2), they are not explicit and evaluating them involves a considerable amount of work. Finding empirical constitutive relations for complex fluids such as polymeric fluids or liquid crystals has also proven to be a difficult task. In general the constitutive relations tend to contain many empirical parameters and their accuracy is also often in serious doubt.

Such problems are not limited to hydrodynamics where constitutive relations are needed, but is common to most modeling process. In molecular dynamics, one needs to model, often empirically, the atomic potentials. In kinetic Monte Carlo methods, one needs to model the transition rates. In kinetic equations, one needs to model the collision cross-section. In nonlinear elasticity, one needs to model the stored-energy functional. In typical mean field theories, one needs to model the effective local fields and the free energy functional. In general, the empirical models work well for relatively simple systems, but lose their accuracy for complex systems.

In the last decade, a new approach, the “first principle-based” approach, has been vehemently pursued in various areas of applications. The basic idea is to replace empirical models by coupling with direct numerical simulations at a more microscopic level. Some of the best known examples of this approach include:

1. \textit{Ab initio} molecular dynamics \cite{12}. Here one replaces the empirical atomic potential in molecular dynamics by explicit calculations of the electronic structures. The Car-Parrinello method is a practical way of implementing this idea \cite{12}.

2. Quasi-continuum method \cite{66, 62}. This is a method for doing nonlinear elasticity calculations without the need of a stored-energy functional. Instead, the stored energy is computed directly from atomic potentials using the Cauchy-Born rule. We will return to this later.

3. The Gas-kinetic scheme \cite{71}. This is a method for doing gas dynamics calculations using directly the kinetic equations instead of the hydrodynamic equations. Since it played an important role in the framework developed in \cite{24}, we briefly review the important steps here.

Given \( \{\rho^n, u^n, T^n\} \), the density, velocity and temperature at time step \( n \) at each cell, the corresponding values at the next time step, \( \{\rho^{n+1}, u^{n+1}, T^{n+1}\} \) are computed by:
Step 1. Reconstruction. From \( \{\rho^n, u^n, T^n\} \), reconstruct \( f^n \), the one particle phase space distribution function near the cell boundaries.

Step 2. Solve the kinetic equation with initial data \( f^n \) near the cell boundaries. In [71], the kinetic equation is chosen as the BGK equation

\[
 f_t + (u \cdot \nabla) f = \frac{1}{\varepsilon} (\mathcal{X}_{(\rho, u, T)} - f)
\]

where \( \mathcal{X}_{(\rho, u, T)} \) is the local Maxwellian associated with \((\rho, u, T)\).

Step 3. Compute the average density, momentum and energy fluxes at the cell boundaries, from which one computes \( \{\rho^{n+1}, u^{n+1}, T^{n+1}\} \).

This procedure is an illustration of several of the key ingredients that we use in the general framework that we will discuss below: the selection of an overall macroscale scheme which in the present example is the finite volume method; the estimation of the macroscale data, here the flux, using the Godunov procedure which consists of the steps of reconstruction, microscale evolution and averaging; the cost reduction at the microscale evolution step by restricting to a small subset of the computational domain.

The examples we discussed so far belong to the class of problems referred to as type B problems in [21] where microscopic models are used to supply a closure to the macroscopic models. Another wide class of problems, called type A problems in [21] consist of problems with defects, interfaces or singularities, for which conventional macroscopic models are accurate enough away from the defects, and more detailed microscopic models are necessary near the defects. Type A problems are found in crack propagation, contact line dynamics, triple junctions, grain boundary motion, dislocation dynamics, etc.

This short review of existing work is by no means comprehensive. For the convenience of the reader, we include at the end an extensive list of references.

## 2 Relations between Macroscopic and Microscopic Models

Let us first fix the notations. We will denote the macroscopic and microscopic state variables as \( U \) and \( u \), defined on \( D \) and \( D \), respectively. Typically \( D \) is the physical space. As we will explain below using examples, it is convenient to view \( D \) loosely as a fiber bundle over \( D \), where the fiber \( D_x \) over \( x \in D \), is roughly the space of microstructures at \( x \). The macroscopic and microscopic state variables are connected by a compression operator \( Q \), and a reconstruction operator \( R \)

\[ Qu = U, \quad RU = u, \quad QR = I \]

where \( I \) is the identity operator. Typically there is a natural way to define \( Q \). But \( R \) is certainly not unique.
To illustrate these notions and notations, let us consider a few examples.

1. For the first example we will consider the case when the macroscopic variables are the hydrodynamic variables of density, velocity and temperature \((\rho, u, T)\), and the microscopic variable is the one particle phase space distribution function \(f\). In this case \(D\) is the physical space-time domain of interest, \(D = D \times R^3, D_x = R^3\), the momentum space which represents the microstructures in this problem. \(Q\) is defined by

\[
\rho(x, t) = \int_{R^3} f(v, x, t)dv, \quad u(x, t) = \int_{R^3} f(v, x, t)v dv, \quad T(x, t) = \frac{1}{3\rho} \int_{R^3} f(v, x, t)|v-u|^2dv
\]

2. For our second example, we will take the microscopic model to be the kinetic models of rod-like molecules in liquid crystals, where the microscopic variable is the orientation-position distribution function \(f(x, m, t)\), \((x, t) \in D, m \in S^2\), the unit sphere. Here \(D = D \times S^2, D_x = S^2\). The macroscopic model is the Landau-de Gennes type models with tensorial order parameter \(S\) which is our macroscopic variable. \(Q\) is defined as

\[
S(x, t) = \int_{S^2} \left(m \otimes m - \frac{1}{3} I\right) f(x, m, t)dm
\]

3. For the third example, we take the standard homogenization problem

\[
u^\varepsilon_t + a \left(x, \frac{x}{\varepsilon}\right) u^\varepsilon_x = 0
\]

where \(a(x, y)\) is smooth and periodic in \(y\) with period 1. In this case, the macroscopic variable will be the local space-time averages of \(u^\varepsilon\):

\[
U(x, t) = \frac{1}{|C|} \int_C u^\varepsilon(x + y, t + s)dyds
\]

where \(|C|\) denotes the area of \(c\) on which the averaging is taken. \(D_x = (x, t) + C\). The size of \(C\) should be larger than \(\varepsilon\).

4. Our last example is front propagation described by Ginzburg-Landau equations

\[
u^\varepsilon_t = \Delta u^\varepsilon + \frac{1}{\varepsilon^2} u^\varepsilon (1 - (u^\varepsilon)^2)
\]

To define the macroscopic variables, observe that \(u^\varepsilon\) is close to \(\pm 1\) in most of the physical domain \(D\), except in a thin region of thickness \(O(\varepsilon)\) where sharp transition between \(\pm 1\) takes place. Since the fast reaction term vanishes at three values \(-1, 0, +1\), it is natural to define \(U\) by:

\[
U(x, t) = Qu^\varepsilon(x, t) = \begin{cases} 
1 & \text{if } u^\varepsilon(x, t) > 0 \\
0 & \text{if } u^\varepsilon(x, t) = 0 \\
-1 & \text{if } u^\varepsilon(x, t) < 0
\end{cases}
\]
An equivalent definition of $U$ is via the $\theta$ level set of $u^\varepsilon$.

More examples are discussed in [21].

In the following we will concentrate on problems of type B, namely problems for which there exist a set of macroscopic variables that obey closed macroscopic models, but the macroscopic models are not explicitly available. We will describe general computational methodologies that enable us to do numerical computations efficiently based on the underlying microscopic models. We will comment on problems of type A at the end.

3 Abstract Formulations

A key component of HMM is the estimation of macroscale data using the microscale model. To see how this can be done, it is helpful to first give an abstract formulation of the macroscopic model in terms of the microscopic model. We start with variational problems.

Consider a microscopic variational problem

$$\min_{u \in \omega} e(u) \quad (6)$$

where $\omega$ is some function space over $\mathcal{D}$, the physical space. Let $Q$ be the compression operator. $Q$ maps $\omega$ to $\Omega$, a function space over $\mathcal{D}$. Since

$$\min_{u \in \omega} e(u) = \min_{U \in \Omega} \min_{Qu = U} e(u), \quad (7)$$

our macroscopic variational problem is given by

$$\min_{U \in \Omega} E(U) \quad (8)$$

where

$$E(U) = \min_{Qu = U} e(u) \quad (9)$$

For dynamic problems, let us denote by $s(t)$, the evolution operator for the microscopic process. In general $\{s(t), t > 0\}$ forms a semi-group of operators. This semi-group may be generated by a set of differential equations, a Markov process, or a discrete dynamical system. There are at two important time scales in our problem: $t_R$, the relaxation time scale of the microscopic process, and $t_M$, the macroscopic time scale of interest. Our basic assumption that there exists a well-defined macroscopic model over the macroscopic time scale of interest implies that $t_R \ll t_M$.

Denote by $R$ an appropriately chosen reconstruction operator. Given $U \in \Omega$, let

$$S(t)U = Qs(t)RU \quad (10)$$
Obviously $S(t)U$ depends on $R$ as it is defined. However, since $t_R \ll t_M$, we expect that the dependence on $R$ diminishes for $t \gg t_R$. Therefore we can define the macroscopic model approximately as

$$U_t = F(U)$$

where

$$F(U) = \frac{S(\Delta t)U - U}{\Delta t}$$

with appropriately chosen $\Delta t$, $t_R \ll \Delta t \ll t_M$.

4 The Structure of HMM

Our basic numerical strategy is now as follows. We will work with a macroscopic grid that adequately resolve the macroscopic problem, but do not necessarily resolve the microscopic problem, and we will attempt to solve directly the macroscopic model (11) and (8).

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.

4.1 The Overall Macroscopic Scheme

The right overall macroscopic scheme depends on the nature of the problem and typically there are more than one choice. For variational problems, we can use the standard finite element method. In fact our examples in the next section use the standard piecewise linear finite element method. For dynamic problems that are conservative, we may use the methods developed for nonlinear conservation laws (see, e.g. [44]). Examples include the Godunov scheme, Lax-Friedrichs scheme, and the discontinuous Galerkin method. For dynamic problems that are non-conservative, one could simply use a standard ODE solver, such as the forward Euler or the Runge-Kutta method, coupled with the force estimator that we discuss below.

4.2 Estimation of the Macroscopic Data

After selecting the overall macroscopic scheme, we face the difficulty that not all data for the macro scheme are available since the underlying macro model is not explicitly known. The next component of 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 the approximation to $Q$ and $U$ is the current macro state. For example, for the variational homogenization problem, the missing data is the stiffness matrix for the macro model. As we
explain in the next section, this data can be estimated by solving the original microscopic variational homogenization problem on a unit cell in each element of the triangulation, subject to the constraint that $\tilde{Q}u = U$. For dynamic problems, such data can be estimated from a Godunov procedure, namely, that we first reconstruct the micro state from $U$, and evolve the micro state subject to the constraint that $\tilde{Q}u = U$, and then estimate the missing data from $u$. The missing data can be either the forces or fluxes, or a part of the forces or fluxes such as the eddy viscosity term in a turbulence model. We also have the option of carrying out a number of such microscopic calculations (e.g. with different reconstruction or different realization of the randomness) and extract a more accurate estimate from the collection of microscopic calculations.

### 4.3 Examples

To illustrate the selection of the macroscale scheme and the estimation of missing macroscale data from microscale models, we will discuss some examples in more detail.

1. **Variational Problems**

Examples include

1. 

$$\min_{u \in H^1_0(D)} \int_D \left\{ \frac{1}{2} \sum_{i,j} a^{\varepsilon}_{i,j}(x,u) \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} - f(x)u(x) \right\} dx$$

where the multiscale nature of the problem is contained in the tensor $a^{\varepsilon}(x,u) = (a^{\varepsilon}_{i,j}(x,u))$ which can be of the form

(a) $a^{\varepsilon}(x,u) = a(x, \frac{y}{\varepsilon})$, where $a(x,y)$ is smooth and periodic in $y$ with period $[0,1]^d$. This is the classical homogenization problem we discussed earlier.

(b) $a^{\varepsilon}(x,u) = a(x, \frac{y}{\varepsilon})$, where $a(x,y)$ is random and stationary in $y$. This can be used to model random medium.

(c) $a^{\varepsilon}(x,u) = a(x, u, \frac{y}{\varepsilon})$, where $a(x,u,y)$ is smooth. The dependence on $u$ makes this problem nonlinear. The dependence on $y$ can be either periodic or random stationary.

The macroscale problem is of the type

$$\min_{U \in H^1_0(D)} \int_D \left\{ \frac{1}{2} A(x,U, \nabla U) - f(x)U(x) \right\} dx$$

2. Atomistic models of crystalline solids:

$$\min_{\{x_j\}} \sum_{y_i,y_j \in D} V(x_i - x_j)$$
subject to loading conditions, where $V$ is a pairwise atomistic potential, $x_i = y_i + u_i, y_i$ is the position of the $i$-th atom before deformation, $u_i$ is the displacement of the $i$-th atom. The macroscale problem is of the type considered in nonlinear elasticity

$$\min_U \int_D f(\nabla U)$$

where $U$ is the macroscale displacement field.

For these problems, we can choose the macroscale scheme to be the standard finite element method over a macroscale triangulation. The macroscale data that we need to estimate is either $\int_D A(x, U, \nabla U)dx$ or $\int_D f(\nabla U)dx$ for $U \in V_H$, the finite element space. These can be approximated via the following steps.

1. For each element $\Delta$, approximate $\int_{\Delta} A(x, U, \nabla U)dx$ or $\int_{\Delta} f(\nabla U)dx$ by a quadrature formula.

2. For each quadrature nodes $x_i \in \Delta$, approximate $A(x, U, \nabla U)(x_i)$ or $f(\nabla U)(x_i)$ by minimizing the original microscale problem over a micro-cell $\Delta_{x_i}$, subject to the constraint that $\int_{\Delta_{x_i}} u(x)dx = \int_{\Delta_{x_i}} U(x)dx, \int_{\Delta_{x_i}} \nabla u(x)dx = \int_{\Delta_{x_i}} \nabla U(x)dx$, with appropriate changes for the atomistic problem. For the periodic homogenization and crystalline solids problems, $\Delta_{x_i}$ can be chosen to be a unit cell around $x_i$, if we replace the constraint by a periodic boundary condition or the Cauchy-Born rule, as we explain in the next section. For the stochastic homogenization problem, $\Delta_{x_i}$ should be larger than the correlation length. In this case, it may also be of advantageous to perform ensemble averages over several realizations of $a(x, x_\xi)$.

2. **Dynamic Problems of Conservative Type**

Examples include

1.

$$\partial_t u^\varepsilon = \nabla \cdot (a^\varepsilon(x, u)\nabla u^\varepsilon)$$

where $\{a^\varepsilon(x, u)\}$ is as discussed above.

2.

$$\partial_t u^\varepsilon + \nabla \cdot (a^\varepsilon(x)u) = 0$$

where $a^\varepsilon(x) = a(x, x_\xi), a(x, y)$ can either be periodic or stochastic stationary in $y$.

3. Kinetic models such as the Boltzmann or BGK equations.

4. Molecular dynamics of the type discussed in Section 2.

5. Spin-exchange models via Kawasaki dynamics [64].
Other examples may include models of phase segregation, mixtures of binary fluids, elastic effects, etc. The macroscale models are of the type

\[ U_t + \nabla \cdot J = 0 \]  

(12)

where \( U \) is in general a vectorial macroscale variable, \( J \) may depend on \( x, U, \nabla U \), etc.

The macroscale scheme can be either a finite volume method, such as the Godunov scheme, or a finite element method, such as the discontinuous Galerkin method. We will discuss here the finite volume method. HMM based on the discontinuous Galerkin method is considered in \(^{23}\).

The missing macroscale data for a finite volume method for (12) is the macroscale flux \( J \) at the cell boundaries denoted by \( \{ J_{j+\frac{1}{2}} \} \). They can be estimated by the following “Godunov-like” procedure

1. Select a microcell \( \Delta_{j+\frac{1}{2}} \) around the cell boundary at \( x_{j+\frac{1}{2}} \).

2. From \( \{ U^n_j \} \), reconstruct the microstates \( \{ \tilde{u} \} \) on \( \{ \Delta_{j+\frac{1}{2}} \} \). \( \tilde{u} \) should be consistent with \( \{ U^n_j \} \) in the sense that \( \tilde{Q} u = U^n \), where \( \tilde{Q} \) is the approximation of \( Q \) restricted to \( \{ \Delta_{j+\frac{1}{2}} \} \).

3. Evolve the microstate \( u(t) \) using the microscale model inside \( \{ \Delta_{j+\frac{1}{2}} \} \), with initial state \( \{ \tilde{u} \} \), and subject to the constraint that

\[ \tilde{Q} u(t) = U \]

4. Evaluate the macroscale flux \( \{ J_{j+\frac{1}{2}} \} \) using \( \{ u(t) \} \).

The constraint \( \tilde{Q} u = U \) requires some additional comment. Take the example of molecular dynamics. If we would like to capture the macroscale behavior at the level of Euler’s equations, the constraint is simply that the average mass, momentum and energy should be given by the prescribed macroscale values given by \( \{ U^n \} \). If we would like to capture the viscous or higher order effects, we also need to constrain the system such that the average density, momentum and energy gradients be given by the macroscale values. This is less convenient to implement, particularly if higher order gradients are required. The discontinuous Galerkin formulation proposed in \(^{23}\) avoids this difficulty.

The rules for selecting \( \{ \Delta_{j+\frac{1}{2}} \} \) is the same as for the variational problems. As usual for periodic homogenization and crystalline solids problems, \( \Delta_{j+\frac{1}{2}} \) can be chosen to be the unit cell.

3. Dynamic Problems of Nonconservative Type

Examples include
1. 
\[ \partial_t u^\varepsilon = \sum_{i,j} a^\varepsilon_{i,j}(x,u) \frac{\partial^2 u}{\partial x_i \partial x_j} \]

where \( \{a^\varepsilon(x,u)\} \) is as discussed before.

2. Spin flip models \[33\] that leads to Ginzburg-Landau type of equations.

In this case, we write the macroscale model as
\[ U_t = F(U) \]

where \( F(U) \) can be a nonlinear operator acting on \( U \). For the macroscale scheme, we choose an ODE solver on a grid, such as forward Euler or Runge-Kutta, and we need to estimate \( F(U) \) on the macro grid.

For each macro grid point \( x_j \), we again select a microcell \( \Delta_j \) around \( x_j \). The principle for selecting \( \Delta_j \) is the same as before. From \( \{U^n_j\} \), we construct a piecewise polynomial of \( k \)-th order in \( \Delta_j \) denoted by \( U^n_j(x) \). The rest of the steps are the same as that for the conservative systems. We note that the constraint \( \tilde{Q} u = U \) can be interpreted as
\[ \int_{\Delta_j} (u(x) - U^n_j(x)) x^m dx = 0 \]

for \( 0 \leq m \leq k \).

4. Macroscale Markov Chains

When the macroscale process is a Markov chain, it is natural to use a kinetic Monte Carlo method as the macroscale scheme. The missing data might be the transition rates between macro states. Estimating such data is a rather non-trivial task. It is discussed in \[26\].

In the following, for dynamic problems we will concentrate on the simplest case when the macroscopic scheme itself is a Godunov scheme and the missing data is the macroscopic forces. Extension to more general situations will be studied in \[22\].

5. Compression Techniques

The key numerical problem now is how to construct approximations to \( E(U) \) and \( F(U) \). In this section, we review numerical techniques for efficiently approximating \( E(U) \) and \( F(U) \) by exploiting the separation of spatial/temporal scales.

5.1 Compression in the Spatial Domain

If the macroscopic and microscopic spatial scales are separated, we can effectively reduce the approximation of \( E(U) \) and \( F(U) \) to a unit of microscopic size on each macroscopic cell.
Such an idea is embodied in e.g. the quasi-continuum method. We will illustrate this with some examples.

Example 1. The Variational Homogenization Problem

Consider the variational problem

$$\min_{u \in H^1_0(D)} \frac{1}{2} \sum_{i,j} \int_D a_{ij} \left( x, \frac{x}{\varepsilon} \right) \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} dx - \int_D f(x)u(x)dx$$ (13)

where as usual we assume that $a(x,y)$ is smooth and periodic in $y$ with period $I = [0,1]^d$.

Let $T_H$ be a macroscopic triangulation of $D$ and $V_H \in H^1_0(D)$ be the standard piecewise linear finite element space over $T_H$. For $u \in H^1_0(D) = \omega$, define $Q u = U \in V_H = \Omega$, if

$$\int_K \nabla u dx = \int_K \nabla U dx$$ (14)

for all triangles $K \in T_H$. $E(U)$ as defined in (8) involves nonlocal coupling of all the triangles. However, we can approximate $E(U)$ efficiently if $\varepsilon \ll 1$. This is done as follows. Given $U \in V_H$ and $K \in T_H$, denote by $x_K$ the center of mass of $K$, and $u_K$ the solution of the problem

$$\min \frac{1}{2} \int_{x_K+\varepsilon I} \sum_{i,j} a_{ij} \left( x, \frac{x}{\varepsilon} \right) \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} dx$$ (15)

subject to the condition

$$u(x) - U(x) \text{ is periodic with period } \varepsilon I.$$ (16)

Let

$$A_K(U,U) = \frac{|K|}{\varepsilon^d} \int_{x_K+\varepsilon I} \sum_{i,j} a_{ij} \left( x, \frac{x}{\varepsilon} \right) \frac{\partial u_K}{\partial x_i} \frac{\partial u_K}{\partial x_j} dx$$ (17)

where $|K|$ is the volume of $K$, we then approximate $E(U)$ by

$$\tilde{E}(U) = \frac{1}{2} \sum_K A_K(U,U) - \int_D U(x)f(x)dx$$ (18)

In this example, the computation on the microscale model is reduced to a microscopic unit-cell problem on each macroscopic element.

The complexity of this method is comparable to solving directly the homogenized equation by evaluating the coefficients of the homogenized equations on each element. This is the minimal one can hope for. However, our method differs from solving the homogenized equation in one essential aspect: Our method is based on the finite $\varepsilon$-microscale model, not the homogenized equation which represents the $\varepsilon \to 0$ limit. Consequently our method can be readily extended to more complex problem such as the nonlinear homogenization problem at essentially the same cost.
Example 2. Quasi-Continuum Method [66, 62].

This is a way of doing nonlinear elasticity calculations using only atomic potentials. Denote by \(x_1, x_2, \ldots x_N\) the positions of all the individual atoms in a crystal. At zero temperature, the position of the atoms are determined by

\[
\min \left\{ V(x_1, x_2, \ldots x_N) - \sum_{i=1}^{N} f(x_i)u_i \right\} \tag{19}
\]

subject to appropriate boundary conditions. Here \(f\) is the external force, \(u_i\) is the displacement of the \(i\)-th atom, \(V\) is the interaction potential between the atoms.

Quasi-continuum method works with a macroscopic triangulation of the crystal and a standard piecewise linear finite element space for the displacement field. The compression operator is defined in a similar way as in (14):

\[
Q_u = U \in V_H \text{ if } <\nabla u>_{K} = \frac{1}{|K|} \int_K \nabla U dx \tag{20}
\]

for all \(K \in T_H\), where \(<\nabla u>_{K}\) denotes the average strain of the atoms on the element \(K\). Having defined \(Q, E(U)\) is defined as in Section 3.

To approximate \(E(U)\), Tadmor et.al. uses the Cauchy-Born rule. Given \(U \in V_H\), let \(e_K(U)\) be the potential energy of a unit cell of the crystal subject to the uniform strain \(\nabla U\) on \(K\). Let

\[
\tilde{E}(U) = \sum_K n_K e_K(U) - \int_D f(x)U(x)dx \tag{21}
\]

where \(n_K\) is the number of unit cells on \(K\). \(\tilde{E}(U)\) is the approximation of \(E(U)\).

Quasi-continuum method contains an additional element for dealing with defects and interfaces in crystals, i.e. type A problems, by replacing the Cauchy-Born rule with a full-atom calculation on elements near the defects and interfaces. We will return to this later.

### 5.2 Compression in the temporal domain

By resorting to the microscopic model in order to simulate the macroscopic dynamics, we are forced to resolve the microscopic times scales which are not of interest. This is particularly expensive if \(t_R \ll t_M\). However in this case we can explore this time scale separation to reduce the computational cost in the temporal domain.

It is helpful to distinguish two different scenarios by which relaxation to local equilibrium takes place. For some problems, such as the parabolic homogenization problem (22) and the Boltzmann equation, we have strong convergence to equilibrium. No temporal or ensemble averaging is necessary for the convergence of the physical observables. For other problems, such as the advection homogenization problem and molecular dynamics, convergence to
equilibrium is in the sense of distributions, i.e. physical observables converge to their local equilibrium values after time or ensemble averaging. Let us express the approximate $F(U)$, called a $F$-estimator, in the form

$$\tilde{F}(U) = Q \sum_{j=1}^{k} \psi_j f(u_j)$$

where the weights $\{\psi_j\}$ should satisfy

$$\sum_{j=1}^{k} \psi_j = 1$$

$u_j$ is the computed microscopic state at microscopic time step $j$, and $u_0 = RU$ where $R$ is some reconstruction operator. The selection of the weights in the $F$-estimator crucially depends on the nature of this convergence. In particular we note two special choices. The first is: $\psi_k = 1$ and $\psi_j = 0$ for $j < k$. This is suitable when we have strong convergence to equilibrium. The second choice is: $\psi_j = \frac{1}{k}$, for $1 \leq j \leq k$. This is more suited for the case when we have weak convergence to local equilibrium. More accurate choices of the weights are discussed in [22]. The time interval on which the microscopic model has to be solved depends on how fast the transient introduced by the reconstruction step dies out.

Consider the parabolic homogenization problem

$$u_t^\varepsilon = \nabla \cdot \left( a \left( x, \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right)$$  \hspace{1cm} (22)

on $D$, with Dirichlet boundary condition $u^\varepsilon|_{\partial D} = 0$. To approximate the macroscopic behavior of $u^\varepsilon$, we will work with a macroscopic grid of size $(\Delta x, \Delta t)$. Let $U = Qu^\varepsilon$ be the moving cell averages of $u^\varepsilon$ over a cell of size $\Delta x$. Let $R$ be the piecewise linear reconstruction. In one-dimension, this is $RU(x) = U_j + \frac{U_{j+1} - U_j}{\Delta x}(x - x_j)$, for $x \in [j\Delta x, (j+1)\Delta x]$. With this reconstruction, we proceed with the microscopic solver. Asymptotic analysis suggests that the relaxation time for this problem is $O(\varepsilon^2)$ [3]. We plot in Figure 1 a typical behavior of the microscopic flux $j^\varepsilon(x,t) = a \left( x, \frac{x}{\varepsilon} \right) \nabla u^\varepsilon(x,t)$ at a cell boundary over the time interval $[t^n, t^n + \Delta t]$ as a function of the micro time steps. It is quite clear that $j^\varepsilon(x,t)$ quickly settles down (after about 35 micro time steps) to a quasi-stationary value after a rapid transient. We obtain an efficient numerical scheme if we select this value as the macroscopic flux and use that to evolve $U$ over a much larger time step $\Delta t$.  

14
Figure 1. Computed flux $\tau^\varepsilon(x,t) = a(x, x^\varepsilon) \nabla u^\varepsilon(x,t)$ as a function of the micro time step over one typical macro time step, for the parabolic homogenization $a(x, x^\varepsilon) = 2 + \sin 2\pi x^\varepsilon$. The bottom figure is a detailed view of the top figure for small time steps. Notice that $j^\varepsilon(x,t)$ quickly settles down (after about 35 micro time steps) to a quasi-stationary value after a rapid transient.

Our next example is the advection homogenization problem

$$u_t^\varepsilon + \nabla \cdot (a(x, x^\varepsilon) u^\varepsilon) = 0$$

(23)

in one-dimension. We assume $a(x,y) > a_0 > 0$. We proceed as before, except that we take a piecewise constant reconstruction. In contrast to the previous example, the temporal oscillations in the solutions of (23) do not die out. This is reflected in Figure 2 where we plot the microscopic flux $j^\varepsilon(x,t) = a(x, x^\varepsilon) u^\varepsilon(x,t)$ over the time interval $[t^n, t^n + \Delta t]$ as a function of the microscale time steps. $j^\varepsilon$ remains oscillatory throughout the time interval. Nevertheless, if we plot the time average

$$\bar{j}(x,t) = \frac{1}{t} \int_{t^n}^{t^n+t} K \left(1 - \frac{\tau}{t}\right) j^\varepsilon(x, \tau) d\tau, \quad K(\tau) = 1 - \cos 2\pi \tau$$

(24)

as shown in Figure 3, we see that it settles down to a quasi-stationary value on a time scale of $O(\varepsilon)$. 

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15
Figure 2. Top figure: Computed flux $j^\varepsilon(x, t) = a(x, \frac{t}{\varepsilon}) u^\varepsilon$ as a fraction of the micro time step over one macro time step for the convection homogenization problem (23). Bottom figure: Time averaged flux $\bar{j}(x, t)$ as a function of the micro time step.

The fact that the microscopic process only has to be evolved on time scales comparable to $t_R$ leads to other possibilities of state space compression by neglecting the part of the state space which does not contribute significantly to the $F$-estimator.

In summary, we can express the $F$-estimator at time $t$ as

$$F^\varepsilon(U, t) = \tilde{Q}_{\Delta t}\{f(\tilde{u}(\tau)), t \leq \tau \leq t + \Delta t, \tilde{u}(t) = RU\}$$

where $\tilde{u}(t)$ is the solution of the compressed microscopic model (possibly over a truncated computational domain) with initial data $\tilde{u}(t) = RU, \tilde{Q}_{\Delta t}$ is the numerical approximation of the compression operator. Typically $\tilde{Q}_{\Delta t}$ has the form

$$\tilde{Q}_{\Delta t} = Q_e Q_x Q_t$$

where $Q_e, Q_x, Q_t$ denote the compression operators over the probability, spatial and temporal spaces respectively. Having $F^\varepsilon(U, t)$, the macroscopic state variables can be updated using standard ODE solvers. The simplest example of forward Euler scheme gives

$$U^{n+1} = U^n + \Delta t F^\varepsilon(U^n, t^n).$$

6 Stability and Accuracy of HMM

6.1 Variational Problems

The analysis of HMM proceeds in the same way as the analysis of traditional numerical methods, except we have to deal with in addition the effect of compression. For variational
problems, compression gives rise to additional error in the evaluation of the macroscale energy functional, or for linear problems, the stiffness matrix.

Take the example of the variational homogenization problem. The main error in the evaluation of the stiffness matrix comes from the inconsistency at the surface of the element where it meets another element. This error is of the order $\frac{\varepsilon}{\Delta x} \| \nabla U \|_{L^2}^2$. Consequently, one has

**Theorem 1.** Assume that the finite element triangulation is quasi-regular, then

$$\| U - Qu^\varepsilon \|_{H^1(D)} \leq C \left( H + \frac{\varepsilon}{H} \right)$$

where $U$ is the numerical solution of HMM, $H$ is the size of the macroscale element.

### 6.2 Dynamical Problems

For dynamical problems, it is helpful to define an auxiliary macroscale scheme, called the Generalized Godunov Scheme (GGS) in [21]. Roughly speaking, GGS is obtained if in HMM we replace the microscale solver in the data estimation step by the macroscale solver. Since the macroscale model is not explicitly known, the GGS is not a practical tool but only an analytical tool that is helpful for analyzing HMM.

For example, for the parabolic and advection homogenization problems discussed earlier, GGS is simply the Godunov scheme on the macroscale problem with appropriate reconstruction and approximate Riemann solvers.

Assuming that the macroscale model is in the form of a differential equation $U_t = F(U)$, we can write a one-step HMM in the form

$$U_{j}^{n+1} = U_{j}^{n} + \Delta t F_j(U^n)$$

and GGS in the form

$$\bar{U}_{j}^{n+1} = \bar{U}_{j}^{n} + \Delta t F_j(\bar{U}^n)$$

The basic stability result proved in [21] is that if GGS is stable, then the HMM is stable and

$$\| U^n - \bar{U}^n \| \leq C \left( \| U^0 - \bar{U}^{-\Delta t} \| + \max_{0 \leq k \leq \frac{T}{\Delta t}} \| \bar{F}(U^k) - F(U^k) \| \right)$$

for $n \Delta t \leq T$.

The notion of stability for the GGS has to be quantified appropriately for nonlinear problems. See [21] for details.

Noting that

$$\| U^n - Qu^\varepsilon \| \leq \| U^n - \bar{U}^n \| + \| \bar{U}^n - Qu^\varepsilon \|$$

we now conclude that the stability and accuracy of HMM depends on
1. Consistency of GGS with the macroscale model.

2. Stability of GGS.

3. The compression error $\|\bar{F}(U) - F(U)\|$

We discuss each of these in some more detail.

1. Consistency of GGS and the macroscale model might be lost if the overall macroscale scheme does not probe the macroscale properties to the right level of accuracy. For example, if the macroscale model is hydrodynamics including viscous effect, and in HMM we have only probed the flux in the convective terms by using a piecewise constant reconstruction near the cell boundaries, neglecting the dissipative terms. This results in inconsistency with the macroscale model. Other such examples are discussed in [21].

2. Stability of GGS usually results in the standard constraint on macro time step size. It may also impose constraints on the reconstruction operator.

3. The compression error has also several sources, e.g. compressions in the temporal or spatial domains. The nature of the temporal compression error depends on the nature of the relaxation to local equilibrium of the microscale process. In the case of strong relaxation, no temporal averaging is necessary for macroscale data estimation. In the case of weak relaxation, the temporal compression error depends strongly on the temporal and/or ensemble averaging operator used.

[21] also pointed out the importance of averaging out spatial small scales for HMM based on the flux-formulation.

7 Conclusion

There are two important questions that have to addressed in order to design efficient numerical methods that couple the macro and microscale models:

1. What is the best way to set up the individual microscale problems?

2. How do we couple the microscale problems together in order to simulate the macroscale behavior?
The second question is now fairly adequately addressed by HMM. The first question is tied more with specific applications. We have discussed a few examples. But much more work needs to be done in order to understand the issue in the general case.

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