Multiscale Modeling of Crystalline Solids

Introduction

Multiscale modeling and computation has recently become one of the most active research areas in applied science. With rapidly growing computing power, we are increasingly more capable of modeling the details of physical processes. Nevertheless we still face the challenge that the phenomena of interest are oftentimes the result of strong interaction between multiple spatial and temporal scales, and the physical processes are described by radically different models at different scales.

The mechanical behavior of solids is a typical example that exhibits such a multiscale characteristic. At the fundamental level, everything about the solid can be attributed to the electronic structures which obey the Schrödinger equation. Atomic interactions and crystal structures can be described at the atomistic scale using molecular dynamics. Mechanical properties at the scale of the material are often modeled using continuum mechanics for which one speaks of stresses and strains. In between there are various levels of mesoscales where one deals with defects such as grain boundaries, dislocation dynamics, and dislocation bundles. What makes the problem challenging is that these different scales are often strongly coupled with each other.

Continuum models usually offer an efficient way of studying material properties. But they suffer from inadequate accuracy and the lack of microstructural information that tells us the microscopic mechanisms for why the material responds in the way it does. Atomistic models, on the other hand, allow us to probe the detailed crystalline and defect structure. However the length and time scales of our interest are often far beyond what a full atomistic computation can reach. This is where multiscale modeling comes into play. The idea is that by coupling microscopic models such as molecular dynamics (MD) with macroscopic models such as continuum mechanics, one might be able to develop numerical tools that have the accuracy that is comparable with the microscopic model and the efficiency that is comparable to the macroscopic model. In this article we will review some of the strategies that have been proposed for this purpose. We will focus on the coupling between molecular dynamics and continuum mechanics, although some of the strategies can be formulated in a more general setting. In addition for simplicity we will concentrate on *concurrent* coupling methods that link different scales "on the fly".

Broadly speaking, concurrent coupling methods can be divided into two main categories, those based on energetic formulations and those based on dynamic formulations. We will discuss them separately.

Energy-based methods

At the atomistic scale, the deformation of a solid is described by the (displaced) positions of atoms that make up the solid. At zero temperature, the positions of the atoms are obtained by minimizing the total energy of the system which consists of the potential energy due to the interaction of the atoms and the energy due to applied forces:

$$E_{tot} = E(\mathbf{x}_1, \cdots \mathbf{x}_N) - \sum_j f(\mathbf{x}_j) \tag{1}$$

Here $\mathbf{x}_j$ denotes the displaced position of the j-th atom. We will use $\mathbf{x}_j^0$ to denote its reference position which is taken to be the equilibrium position. $\mathbf{u}_j = \mathbf{x}_j - \mathbf{x}_j^0$ is the displacement of the j-th atom.

At the continuum level, the deformation of the solid is described by the displacement field $\mathbf{u}(\mathbf{x}^0)$ which also minimizes the total energy of the system that consists of the elastic energy caused by the deformation and the energy due to external forces:

$$e[\mathbf{u}] = \int_\Omega \mathcal{E}(\nabla\mathbf{u}) - \mathbf{f}_{ex} \cdot \mathbf{u}\, d\mathbf{x}^0. \tag{2}$$

Here $\mathcal{E}$ is the strain energy density. Numerically this problem is solved by finite element methods on an appropriate triangulation $\{\Omega_\alpha\}$ of the domain that defines the solid.

In both cases, dynamics can be generated using Hamilton's equation for the corresponding energy functional.

Clearly the continuum approach is more efficient once we know the strain energy density. The conventional approach in continuum mechanics is to model this empirically using a combination of experimental data and analytical reasoning. Recently developed multiscale approach, on the other hand, aims at computing the strain energy directly based on the atomistic model. Next we will discuss several methods that have been developed for this purpose.

To begin with, let Q be an appropriately defined operator that maps the microscopic configuration $\{\mathbf{u}_j\}$ of the atoms to the macroscopic displacement field $\mathbf{u}$. Then consistency between (1) and (2) implies that the strain energy should be given in terms of the atomistic model by,

$$e[\mathbf{u}] = \min_{Q\{\mathbf{u}_j\}=\mathbf{u}} E_{tot}. \tag{3}$$

However this formula is quite impractical for numerical purpose since the number of atoms involved is often too large, and one has to come up with appropriate approximation procedures.

QC – Quasicontinuum method

One remarkably successful approach is the QC (quasicontinuum) method (Tadmor et al., 1996; Miller and Tadmor, 2003). QC is a way of simulating the macroscale nonlinear deformation of crystalline solids using molecular mechanics. It consists of three main components.

- A finite element method on an adaptively generated mesh, which is automatically refined to the atomistic level near defects. Away from the defects, the mesh is coarsened to reflect the slow variation of the displacement field.
- A kinematic constraint by which a subset of atoms, called representative atoms, are selected. The displacement of the other atoms are expressed in terms of the displacement of the representative atoms. This reduces the number of degrees of freedom in the problem.
- A summation rule that computes an approximation to the total energy of the system by visiting only a small subset of the atoms. A simple example of the summation rule is the Cauchy-Born rule which computes the local energy by assuming the deformation is locally uniform.

We now discuss these components in some detail.

Ideally, in order to calculate the total energy, one needs to visit all the atoms in the domain:

$$E_{tot} = \sum_{i=1}^{N} E_i(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N). \tag{4}$$

Here E_i is the energy contribution from site $\mathbf{x}_i$. The precise form of E_i depends on the potential one uses. In the region where the displacement field is smooth, keeping track of each individual atom is unnecessary. After selecting some representative atoms (repatoms), the displacement of the rest of the atoms can be approximated via linear interpolation,

$$\mathbf{u}_j = \sum_{\alpha=1}^{N_{rep}} S_\alpha(\mathbf{x}_j^0)\mathbf{u}_\alpha,$$

where the subscript α identifies the representative atoms, S_α is an appropriate weight function, N_{rep} is the number of repatoms involved.

This step reduces the number of degrees of freedom. But to compute the total energy, in principle we still need to visit every atom. To reduce the computational complexity involved in computing the total energy, several summation rules are introduced. The simplest of these is to assume that the deformation gradient $\mathbf{A} = \frac{\partial \mathbf{x}}{\partial \mathbf{x}^0}$ is uniform within each element: namely that the Cauchy-Born rule holds. The strain energy in the element Ω_k can be approximately written as $\mathcal{E}(\mathbf{A}_k)|\Omega_k|$ in terms of the strain energy density $\mathcal{E}(\mathbf{A})$. With these approximations, the evaluation of the total energy is reduced to a summation over the finite elements,

$$E_{tot} \approx \sum_{k=1}^{N_e} \mathcal{E}(\mathbf{A}_k)|\Omega_k| \tag{5}$$

where N_e is the number of elements. This formulation is called the *local* version of QC.

In the presence of defects, the deformation tends to be non-smooth. Therefore the approximation made in local QC will be inaccurate. A *nonlocal* version of QC has been developed in which the energy is computed using the following ansatz:

$$E_{tot} \sim \sum_{\alpha=1}^{N_{rep}} n_\alpha E_\alpha(\mathbf{u}_\alpha). \tag{6}$$

Here $\{n_\alpha\}$ is some suitably chosen weight. The energy from each repatom $\{E_\alpha\}$ is computed by visiting its neighboring atoms whose positions are generated using the local deformation. Near defects such as cracks or dislocations, the finite element mesh is also refined to atomic scale to reflect the local deformation more accurately. Practical implementations usually combine both local and nonlocal version of the method, and a criterion has been suggested to identify the local/nonlocal regions so that the whole procedure can be applied adaptively.

Another version of QC, which is based on force calculation, has been put forward in (Knap and Ortiz, 2001). The methods generate clusters around the repatoms and perform the force calculation using the atoms within the clusters, see Figure 1.

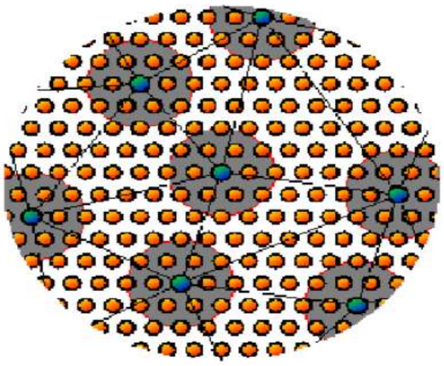

Figure 1: Schematic illustration of the cluster summation rule in QC (courtesy of M. Ortiz). Only atoms in the small cluster need to be visited during the computation.

QC has been successfully applied to a number of problems[1] including dislocation structure, nanoindentation, crack propagation, deformation twinning, etc. The use of local QC to control the far-field

[1]For recently development and source code, see `http://www.qcmethod.com`.

region and thus create a continuum environment for material defects is now more and more popular. In its simplest form, QC ignores atomic vibrations and thus the entropic effects. This restricts QC to static problems at zero temperature. Dynamics of defects can be studied in a quasi-static setting. Finite temperature can be incorporated perturbatively (Shenoy and Phillips, 1999; Miller and Tadmor, 2003).

MAAD – Macro Atomistic Ab initio Dynamics

MAAD (Macro Atomistic Ab initio Dynamics) was proposed in (Abraham et al., 1998; Broughton et al., 1999) to simulate crack propagation in Silicon. The computational domain is decomposed into three parts: the continuum region away from the crack tip where the linear elasticity model is solved using a finite element method, an atomistic region near the crack tip on which molecular dynamics

$$m_j \ddot{\mathbf{x}}_j = -\nabla_{\mathbf{x}_j} V, \quad j = 1, 2, \cdots, N_{atom}, \tag{7}$$

with the Stillinger-Weber potential is used, and a quantum mechanical region at the crack tip where the tight binding model (TB) is used to model bond breaking. This is done by writing the Hamiltonian in the form

$$H_{tot} = H_{FE} + H_{MD} + H_{FE/MD} + H_{TB} + H_{MD/TB}, \tag{8}$$

which represents the energy contribution from different regions and the interface between them. For brevity we will explain the calculation of the first three terms. In the FE (finite element) region, the variables are the displacement field $\mathbf{u}$, and the expression for the Hamiltonian is standard:

$$H_{FE} = \frac{1}{2} \sum_{k=1}^{N_e} \mathbf{u}_k^T \mathbf{K} \mathbf{u}_k + \dot{\mathbf{u}}_k^T \mathbf{M} \dot{\mathbf{u}}_k \tag{9}$$

Here $\mathbf{K}$ and $\mathbf{M}$ are the stiffness and mass matrices. The elastic coefficients can be obtained from the harmonic approximation of the interatomic potential. In the case of finite (but constant) temperature, these parameters are adjusted accordingly to be consistent with the atomistic system in the MD region. The Hamiltonian in the MD region is simply the total energy:

$$H_{MD} = \frac{1}{2} \sum_{i=1}^{N_{atom}} m_i \dot{\mathbf{u}}_i^2 + V \tag{10}$$

where $\mathbf{u}_i$ is the displacement of the i-th atom, V is the total potential energy in the MD region.

A key ingredient in this procedure is a *handshaking* scheme at the continuum/MD (and MD/TB) interface. Specifically, near the continuum/MD interface the finite elements are refined all the way to the atomistic level so that their vertices coincide with the reference atomic positions at the interface. The handshaking Hamiltonian $H_{FE/MD}$ accounts for the interaction across the interface. The energy is computed from the continuum side and the MD side using respectively the formulas

(9) and (10) with half and half weight for each. The continuum region and the atomistic region are then evolved simultaneously in time. Energy transport across the interface has been ignored.

An often discussed problem is the matching condition at the continuum/MD interface (see the discussion later). This is important since the MD region will generate phonons which are not represented in the continuum region and hence might be reflected at the continuum/MD interface. But by refining the finite element mesh to atomistic scale at the interface, MAAD avoids this issue.

CGMD – Coarse-Grained Molecular Dynamics

Coarse-grained molecular dynamics is a systematic procedure for deriving the effective Hamiltonian for a set of coarse-grained variables from the microscopic Hamiltonian (Rudd and Broughton, 1998). Starting from a microscopic Hamiltonian H_{MD} defined on the phase space and defining coarse-grained variables by

$$\mathbf{u}_\mu = \sum_j f_{j\mu}\mathbf{u}_j, \quad \mathbf{p}_\mu = \sum_j f_{j\mu}\mathbf{p}_j, \tag{11}$$

where $f_{j\mu}$ are appropriate weights, the effective Hamiltonian for the coarse-grained variables are obtained from

$$E(\mathbf{u}_\mu, \mathbf{p}_\mu) = \frac{1}{Z}\int H_{MD} e^{-H_{MD}/k_B T}\Delta d\mathbf{x}_j d\mathbf{p}_j, \tag{12}$$

where

$$\Delta = \Pi_\mu \delta(\mathbf{u}_\mu - \sum_k \mathbf{f}_{k\mu}\mathbf{u}_k)\delta(\mathbf{p}_\mu - \sum_k \mathbf{f}_{k\mu}\mathbf{p}_k),$$

and Z is a normalization constant, T is the temperature. Consistency with the coarse-grained variables is ensured through the presence of the delta functions, similar to the imposition of the kinematic constraint in QC. (12) plays the role of (3) at finite temperature, with Q defined via (11). The basic assumption in this formalism is that the small scale component is at equilibrium given the coarse-grained variables. Strictly speaking this is only true if the relaxation times associated with the small scales are much shorter than that of the coarse-grained variables.

In general the coarse-grained energy in (12) is still difficult to compute. It has been computed for the case of harmonic potential in (Rudd and Broughton, 1998) and more generally in (Rudd and Broughton, 2000).

Dynamics-based method

So far we have discussed energy based methods. In these methods, the key is to obtain a multiscale representation of the total energy of the system. In QC, this is done via the representative atoms and the summation rule. In MAAD, this is done by handshaking the atomistic and continuum regions through a gradual matching of the grids. In CGMD, this is done via thermodynamically integrating out the contribution of the small scales. Hamilton's equation is applied to the reduced

Hamiltonian in order to model dynamics.

An alternative approach is to model dynamics directly. Equilibrium states are obtained as steady states of the dynamics. This is essential if energy transport is coupled with the dynamics. At the present time, this approach is much less developed compared with energy-based approaches discussed earlier. So far the only general strategy seems to be that of Li and E (2003) which is based on the framework of the heterogeneous multiscale method (HMM) developed by E and Engquist (2002). This will be discussed next. We will also discuss a related topic, namely how to impose matching conditions at the atomistic-continuum interface in the setting when the computational domain in divided into a continuum region and an atomistic region.

Heterogeneous multiscale method

In order to develop a general multiscale methodology that can handle both dynamics and finite temperature effects, Li and E (2003) relied on the framework of the heterogeneous multiscale method (HMM) which has been used for designing multiscale methods for several different applications including fluids[2]. There are two major components in HMM. The selection of a macroscale solver and the estimation of the needed macroscale data using the microscale solver. In general the macroscale solver should be chosen to maximize the efficiency in resolving the macroscale behavior of the system and minimize the complexity of coupling with the microscale model.

In the context of solids, our starting point for both the macroscale and microscale models are the universal conservation laws of mass, momentum and energy in Lagrangian coordinates:

$$\left\{ \begin{array}{rcl} \partial_t \mathbf{A} - \nabla_{\mathbf{x}^0} \mathbf{v} & = & 0, \\ \rho_0 \partial_t \mathbf{v} + \nabla_{\mathbf{x}^0} \cdot \boldsymbol{\sigma} & = & 0, \\ \rho_0 \partial_t e + \nabla_{\mathbf{x}^0} \cdot \mathbf{j} & = & 0. \end{array} \right. \tag{13}$$

Here $\mathbf{A}, \mathbf{v}, e$ are the deformation gradient, velocity and total energy per particle respectively, ρ_0 is the density. At the macroscale level, i.e. continuum mechanics, $\boldsymbol{\sigma}$ is the first Piola-Kirchhoff stress tensor and $\mathbf{j}$ is the energy flux. The first equation in (13) is merely a compatibility statement. The second and third equations express conservation of momentum and energy respectively. After combining with proper constitutive relations these equations can be used to model nonlinear elasticity, thermoelasticity and even plasticity.

At the microscopic level, i.e. molecular dynamics, these conservation laws continue to hold with

[2]for other applications of HMM, visit `http://www.math.princeton.edu/multiscale`.

the stress and energy given in terms of the atomistic variables by,

$$
\left\{
\begin{array}{rcl}
\widetilde{\boldsymbol{\sigma}}(\mathbf{x}^0,t) & = & \displaystyle\frac{1}{2}\sum_{i\neq j}\mathbf{f}\big(\mathbf{x}_i(t)-\mathbf{x}_j(t)\big)\otimes(\mathbf{x}_i^0-\mathbf{x}_j^0) \\
& \times & \displaystyle\int_0^1 \delta\Big(\mathbf{x}^0-\big(\mathbf{x}_j^0+\lambda(\mathbf{x}_i^0-\mathbf{x}_j^0)\big)\Big)d\lambda, \\
\widetilde{\mathbf{j}}(\mathbf{x}^0,t) & = & \displaystyle\frac{1}{4}\sum_{i\neq j}\big(\mathbf{v}_i(t)+\mathbf{v}_j(t)\big)\cdot\mathbf{f}\big(\mathbf{x}_j-\mathbf{x}_i\big)(\mathbf{x}_i^0-\mathbf{x}_j^0) \\
& \times & \displaystyle\int_0^1 \delta\Big(\mathbf{x}^0-\big(\mathbf{x}_j^0+\lambda(\mathbf{x}_i^0-\mathbf{x}_j^0)\big)\Big)d\lambda.
\end{array}
\right. \tag{14}
$$

Here for simplicity we only provided these expressions for the case when the atomistic potential is simply a pair potential: $V=\frac{1}{2}\sum_{i\neq j}\phi\big(|\mathbf{x}_i(t)-\mathbf{x}_j(t)|\big)$ and $\mathbf{f}=-\nabla\phi$. It is well-known that pair potentials are quite inadequate for modeling solids, but one can find the formulas for more general potentials in (Li and E, 2003).

These conservation laws suggest a new coupling strategy in the HMM framework at the level of fluxes: the macroscopic variables can be used as constraints for the atomistic system, the needed constitutive data – the fluxes, can be obtained from results from the atomistic model via ensemble/time averaging after the microscale system equilibrates. This is the method proposed in Li and E (2003).

Compared with QC or CGMD, HMM is more of a top-down approach in that it starts with an incomplete macroscale model, and uses the microscale model as a supplement to provide the missing data, the fluxes. In QC or CGMD, one starts with a full atomistic description with all the physical details. A coarse graining procedure is then applied to remove the unnecessary degrees of freedom in order to arrive at a coarse-grained model.

We next describe the details of the HMM procedure.

Macroscale solver

Since the macroscale model is a conservation law, the macroscale solver is a method for conservation laws. Although there are plenty of methods available for conservation laws e.g. (Godlewski and Raviart, 1996), many of them involve the computation of the Jacobian for the flux functions, and this dramatically increases the computational complexity in a coupled multiscale method when the continuum equation is not explicitly known. An exception is the central scheme of Lax-Friedrichs type, such as (Nessyahu and Tadmor, 1990) which is formulated over a staggered-grid. As it turns out, this method can be easily coupled with molecular dynamic simulations.

To discuss such schemes, we first write the conservation laws in a generic form,

$$\mathbf{u}_t+\mathbf{f}_x=0, \tag{15}$$

We will confine our discussion to one dimensional continuum models since the extension to higher dimension is straightforward. A (macro) staggered grid is laid out as in Figure 2. First order central scheme represents the solutions by piece-wise constants, which are the average values over each cell:

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

Time integration over $[x_k,\ x_{k+1}] \times [t^n,\ t^{n+1})$ leads to the following scheme,

$$\mathbf{u}_{k+1/2}^{n+1} = \frac{\mathbf{u}_k^n + \mathbf{u}_{k+1}^n}{2} - \frac{\Delta t}{\Delta x}\left(\mathbf{f}_{k+1}^n - \mathbf{f}_k^n\right), \tag{16}$$

where

$$\mathbf{f}_k^n = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \mathbf{f}(x_k,t)dt$$

This is then approximated by numerical quadrature such as the mid-point formula. A simple choice is $\mathbf{f}_k^n \sim \mathbf{f}(x_k, t^n)$.

The stability of such a scheme, which usually manifests itself in the form of a constraint on the size of Δt, can be appreciated from considering the adiabatic case $\mathbf{f} = \mathbf{f}(\mathbf{u})$: if we choose the time step Δt small enough, the waves generated from the cell interface $\{x_{k+1/2}\}$ will not arrive at the grid points $\{x_k\}$, and therefore the solution as well as the fluxes at the grid points will not change until the next time step.

With this specific choice of the macro-solver, we can illustrate the HMM procedure schematically in Figure 2. At each macro time step, the scheme (16) requires as input the fluxes at grid point x_k to complete the time integration. These flux values are obtained by performing local MD simulations that are consistent with the local macroscopic state $(\mathbf{A},\ \mathbf{v},\ e)$. The equations (13) are then integrated to next time step using (16).

Reconstruction: Next we discuss how to set up the atomistic simulation to estimate the local fluxes. The first step is to reconstruct initial MD configurations that are consistent with the local macro state variables $(\mathbf{A}, \mathbf{v}, e)$.

The shape of the MD cell, and hence the new basis, is set up from the local deformation tensor. For example if the undeformed cell has basis $\mathbf{E}$, then the new basis is $\tilde{\mathbf{E}} = \mathbf{AE}$. Assuming that the deformation is uniform within the cell, the new basis then determines the displacement of each atom. From the atomic positions we can compute the potential energy. After subtracting the potential energy and the kinetic energy associated with the mean velocity from the total energy e, we obtain the temperature by assuming that the remaining energy is due to thermal fluctuation. Using the mean velocity and temperature we initialize the velocity of the atoms by Maxwell distribution.

Boundary conditions

Of central importance is the boundary condition imposed on the microscopic system in order to guarantee consistency with the local macroscale variables. In the case when the system is homogeneous, the most convenient boundary condition is the periodic boundary condition. The MD cell is first deformed according to the deformation gradient $\mathbf{A}$. Then the cell is periodically

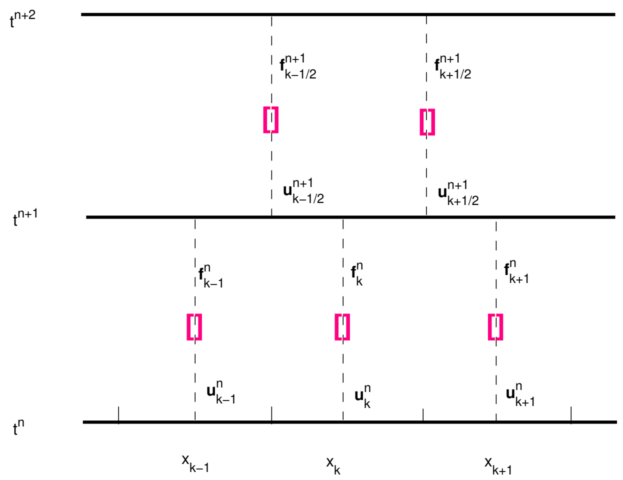

Figure 2: A schematic illustration of the numerical procedure for one macro time step: starting from piecewise constant solutions $\{\mathbf{u}_k^n\}$, one integrates (15) in time and in the cell $[x_k, x_{k+1}]$. The time step Δt is chosen in such a way that the waves coming from $x_{k+1/2}$ will not reach x_k, and thus for $t \in [t^n, t^{n+1})$, $\mathbf{u}(x_k, t) = \mathbf{u}_k^n$. To obtain the local flux, we perform a MD simulation using $\mathbf{u}_k^n$ as constraints. The needed flux is then extracted from the MD fluxes via time averaging.

extended to the whole space.

Estimating the data

The needed macroscale fluxes are estimated from the MD results by time averaging. To reduce the transient effects, we use a kernel that puts less weight on the transient period, e.g.

$$\langle A \rangle_K = \lim_{t \to +\infty} \frac{1}{t} \int_0^t K(1 - \frac{s}{t}) A(s) ds, \quad K(\theta) = 1 - \cos(2\pi\theta). \tag{17}$$

Experience suggests that using this kernel substantially improves the quality of the data than straightforward averaging.

Dealing with defects

In the presence of defects, QC and MAAD refine the grid to the atomic level to account for defect energy. This procedure is seamless but can become rather complicated in simulating dynamics.

HMM instead suggests keeping the macro-grid (which might be locally refined) in the entire computational domain but performing a model refinement locally near the defects. Away from the defects, the fluxes are computed using the procedure described before; or if an empirical model is accurate enough, one can simply compute the fluxes using the empirical model. Near the defects there are two cases to consider depending on whether there is scale separation between the local relaxation time around the defects and the time scale for the dynamics of the defects. In the absence of such a time scale separation, the molecular dynamics simulation around the defects will be kept for all times. This imposes a limitation on the time scales that can be accessed using such a procedure. But if the atomistic relaxation times can be very long, there is really little one can do other than following the history of the atomistic features near the defects. Macroscale fluxes can still be computed from the microscale fluxes via time averaging.

In this case, since the atomistic region near the defect is necessarily macroscopically inhomogeneous, the atomistic boundary conditions need to be modified. Li and E (2003) proposes using a biased Andersen thermostat at a border region that takes into account both the local mean velocity and local temperature. Finally the overall deformation is controlled by fixing the outmost atoms.

In the case when there is time scale separation, this procedure can be much simplified. In this case one can build the defect dynamics directly into the macro-solver and the atomistic simulations can be localized in space and time to predict the velocity of the defects and stress near the defects. Such a defect tracking procedure is implemented for twin boundary dynamics in (Li and E, 2003).

Atomistic-continuum interface condition

One issue that has received a great deal of attention is the matching condition at the atomistic-continuum interface. In a coupled MD-continuum calculation, the MD region is meant to be very small but inevitably at finite temperature. The phonons generated in the MD region need to be propagated out in order to keep the fluctuations in the MD region under control. This is achieved through imposing appropriate boundary conditions at the atomistic-continuum interface that limits phonon reflection.

The first attempt for deriving such boundary conditions is found in (Cai et al., 2000). Cai et al. suggested obtaining the exact linear response functions at the interface by precomputing. This strategy is in principle exact under the harmonic approximation. But it is often too expensive since the linear response functions (which are simply Green's functions) are quite nonlocal. When the MD region changes as a result of defect dynamics, these functions will have to be computed again. Further work along this line was done later by Wagner et al. (2003).

To achieve an optimal balance between efficiency and accuracy, a local method was formulated in E and Huang (2001, 2002) with the idea of minimizing phonon reflection, giving a pre-determined stencil for the boundary condition. To explain the optimal local matching conditions, we consider the one dimensional case where the continuum model is the simple wave equation,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$$

and its discrete form,

$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\Delta t^2} = u_{j+1}^n - 2u_j^n + u_{j-1}^n, \quad j \geq 1. \tag{18}$$

These equations can be obtained by linearizing (7). For simplicity we consider the case when the atomistic region is in the semi-infinite domain defined by $x > 0$ and $j = 0$ is the boundary. To prescribe the boundary condition we express u_0^n as

$$u_0^n = \sum_{k,j \geq 0} a_{k,j} u_j^{n-k}, \quad a_{0,0} = 0.$$

We start with a pre-determined set S of $\{k, j\}$'s outside of which we set $a_{k,j} = 0$. The set S is the stencil that we choose. Choosing the right S is a very crucial step in this procedure. Large S will lead to an increase in the complexity of the algorithm. But small S may not be enough for the purpose of suppressing phonon reflection.

Once S is selected, $\{a_{k,j}\}$ are chosen to minimize the total reflection in appropriate norm. The reflection coefficient, or more generally the reflection matrix can be obtained by looking for solutions in the form of

$$u_j^n = e^{i(n\omega\Delta t + j\xi)} + R(\xi) e^{i(n\omega\Delta t - j\xi)}.$$

Using (18), we obtain

$$R(\xi) = -\frac{\sum_{k,j} a_{k,j} e^{i(j\xi - k\omega\triangle t)} - 1}{\sum_{k,j} a_{k,j} e^{-i(j\xi + k\omega\triangle t)} - 1}, \tag{19}$$

where $\omega = \omega(\xi)$ is the dispersion coefficient satisfying

$$\frac{1}{\Delta t} \sin \frac{\omega \Delta t}{2} = \sin \frac{\xi}{2}.$$

Similar calculation can be done for general crystal structures in which case the phonon spectrum may consist of several branches.

Having $R(\xi)$, $a_{k,j}$ can be obtained by minimizing the total phonon reflection,

$$\min \int_0^\pi W(\xi) |R(\xi)|^2 d\xi,$$

with appropriately chosen weight function W. In addition constraints are needed at $\xi = 0$ in the form of $R(0) = 0, R'(0) = 0, \cdots$, to ensure accuracy at large scale.

As example, if one uses only the terms $a_{1,0}$ and $a_{1,1}$, and $W = 1$ with $R(0) = 0$ at the boundary, one has,

$$u_0^n = (1 - \Delta t) u_0^{n-1} + \Delta t u_1^{n-1}. \tag{20}$$

If instead one keeps the terms $\{a_{j,k}, j \leq 3, k \leq 2\}$, the minimization leads to the following coefficients:

$$(a_{j,k}) = \begin{pmatrix} 1.95264 & -0.074207 & -0.014903 \\ -0.95406 & 0.074904 & 0.015621 \end{pmatrix}.$$

In order to get better performance at high wave number, more coefficients (larger S) have to be included.

The method has been applied to dislocation dynamics in the Frenkel-Kontorova model and friction between rough crystal surfaces. It has shown great promise in suppressing phonon reflection.

Summary

We have based our presentation on dividing multiscale methods into energy-based and dynamics-based methods. From the viewpoint of coarse-graining, there are also two different set of ideas. The first set of ideas, used in QC, CGMD and HMM, is to pre-define a set of coarse-grained variables. By expressing the microscopic model in terms of the coarse-grained variables, one finds a relationship that express the macroscale data in terms of the microscopic quantities. In QC, this relationship is (3). In CGMD, this relationship is (12). In HMM, this relationship is (14). This relationship is the starting point of the micro-macro coupling. The second set of ideas, used in MAAD and E and Huang (2001), is to divide the computational domain into macro and micro regions. Separate models are used in different regions and an explicit matching condition is used to bridging the two regions.

Most existing work on multiscale modeling of solids deals with single crystal with isolated defects. Going beyond single crystals requires substantial work. Dealing with polycrystals with grain boundaries and plasticity with many interacting dislocations seem to require new ideas in coupling.

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