Matching Conditions in Atomistic-Continuum Modeling of Materials

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A new class of matching conditions between the atomistic and continuum regions is presented for the multiscale modeling of crystals. They ensure the accurate passage of large scale information between the atomistic and continuum regions and at the same time minimize the reflection of phonons at the interface. These matching conditions can be made adaptive if we choose appropriate weight functions. Applications to dislocation dynamics and friction between two-dimensional atomically flat crystal surfaces are described.

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Traditionally, two apparently separate approaches have been used to model a continuous medium. The first is the continuum theory, in the form of partial differential equations describing the conservation laws and constitutive relations. This approach has been impressively successful in a number of areas such as solid and fluid mechanics. It is very efficient, simple, and often involves very few material parameters; but it becomes inaccurate for problems in which the detailed atomistic processes affect the macroscopic behavior of the medium, or when the scale of the medium is small enough that the continuum approximation becomes questionable. Such situations are often found in studies of properties and defects of micro- or nanosystems and devices. The second approach is atomistic, aiming at knowing the detailed behavior of each individual atom using molecular dynamics or quantum mechanics. This approach can, in principle, accurately model the underlying physical processes; but it is often times prohibitively expensive.

Recently, an alternative approach has been explored that couples the atomistic and continuum approaches [1–7]. The main idea is to use atomistic modeling at places where the displacement field varies on an atomic scale, and the continuum approach elsewhere. Two representative examples of such a coupled approach are the quasicontinuum method [1,2] and the coarse-grained molecular dynamics (MD) [5,6]. Both methods have been successfully applied to quasistatic examples, but extension to dynamic problems has not been straightforward. The main difficulty lies in the proper matching between the atomistic and continuum regions. Since the details of lattice vibrations, the phonons, which are an intrinsic part of the atomistic model, cannot be represented at the continuum level, conditions must be met that the phonons are not reflected at the atomistic-continuum interface. Since the atomistic region is expected to be a small part of the computational domain, violation of this condition quickly leads to local heating of the atomistic region and destroys the simulation result. In addition, the matching between the atomistic-continuum interface has to be such that large scale information is accurately transmitted in both directions.

The main purpose of this paper is to introduce a new class of matching conditions between atomistic and continuum regions. These matching conditions have the property that they allow accurate passage of large scale (scales that are represented by the continuum model) information between the atomistic and continuum regions and no reflection of phonon energy to the atomistic region. These conditions can also be used in pure molecular dynamics simulations as the border conditions to ensure no reflection of phonons at the boundary of the simulation.

For the sake of clarity, we will first explain the main issues and ideas on a simple problem: a one-dimensional chain of particles coupled by springs:

$$\ddot{u}_j = u_{j+1} - 2u_j + u_{j-1}. \tag{1}$$

The spring constant is set to be 1. After discretization in time, we have

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

where u_j^n is the displacement of the jth particle at time $t = n\Delta t$.

Equation (2) is supposed to be solved for all integers j. Now let us assume that we will truncate the computational domain and compute only u_j^n for $j \geq 0$. At $j = 0$, we will impose a new boundary condition to make sure that the phonons arriving from $j > 0$ are not reflected back at $j = 0$.

The phonon spectrum for (2) is obtained by looking for solutions of the type $u_j^n = e^{i(n\omega\Delta t + j\xi)}$. This gives us the relation

$$\frac{1}{\Delta t}\sin\frac{\omega\Delta t}{2} = \sin\xi. \tag{3}$$

At $j = 0$, we replace (2) by

$$u_0^n = \sum_{k,j\geq 0} a_{k,j} u_j^{n-k} \qquad a_{0,0} = 0. \tag{4}$$

We would like to determine the coefficients $\{a_{k,j}\}$. For the simple problem at hand, it is possible to obtain analytical formulas of $\{a_{k,j}\}$ such that the imposition of (4) together with the solution of (2) for $j > 0$ reproduces exactly the solution of (2) if it was solved for all integer values of j; i.e., an exact reflectionless boundary condition can be found. The details of this are given in [8]. This exact boundary condition should be the same as the one found numerically in [7]. It represents the exact Green's function for (2) which is nonlocal. However, this procedure appears to be impractical for realistic models, particularly when the atomistic region moves with time, which is the case that interests us. Therefore we will not pursue this direction here.

A practical solution is to restrict (4) to a finite number of terms and look for the coefficients $\{a_{k,j}\}$ that minimize reflection. In order to do this, let us look for solutions of the type

$$u_j^n = e^{i(n\omega\Delta t + j\xi)} + R(\xi)e^{i(n\omega\Delta t - j\xi)}, \tag{5}$$

where ω is given by (3). $R(\xi)$ is the reflection coefficient at wave number ξ. Inserting (5) into (4), we obtain

$$R(\xi) = -\frac{\sum a_{k,j}e^{i(j\xi - k\omega\Delta t)} - 1}{\sum a_{k,j}e^{-i(j\xi + k\omega\Delta t)} - 1}. \tag{6}$$

The optimal coefficients $\{a_{k,j}\}$ are obtained by

$$\min \int_0^\pi W(\xi)\,|R(\xi)|^2\,d\xi, \tag{7}$$

subject to the constraint

$$R(0) = 0, R'(0) = 0, \text{ etc.} \tag{8}$$

Here $W(\xi)$ is a weight function, which is chosen to be $W(\xi) = 1$ in the examples below.

Condition (8) guarantees that large scale information is transmitted accurately, whereas (7) guarantees that the total amount of reflection is minimized. This procedure offers a lot of flexibility. For example, instead of $\int_0^\pi |R(\xi)|^2\,d\xi$, we can minimize the total reflection over a certain carefully selected interval. Another possibility is to choose the weight function to be the (empirically computed) energy spectrum. The coefficients $\{a_{k,j}\}$ may then change in time to reflect the change of the nature of the small scales. In practice, we found it preferable to use $\int_0^{\pi-\delta} |R(\xi)|^2\,d\xi$ with some small δ, instead of $\int_0^\pi |R(\xi)|^2\,d\xi$, in order to minimize the influence of $\xi = \pi$ for which we always have $R(\pi) = 1$.

Let us look at a few examples. If in (4) we keep only the terms involving $a_{1,0}$ and $a_{1,1}$, then imposing the condition $R(0) = 0$ gives

$$u_0^n = (1 - \Delta t)u_0^{n-1} + \Delta t u_1^{n-1}. \tag{9}$$

If instead we keep terms involving $a_{0,1}$, $a_{1,0}$, and $a_{1,1}$, we can then impose both $R(0) = 0$, and $R'(0) = 0$. This gives us

$$u_0^n = u_1^{n-1} + \frac{1 - \Delta t}{1 + \Delta t}(u_0^{n-1} - u_1^n). \tag{10}$$

Conditions of the type (9) and (10) are intimately related to the absorbing boundary conditions proposed and analyzed in [9,10] for the computation of waves. These conditions perform well for low wave numbers but are less satisfactory at high wave numbers.

To improve the performance at high wave numbers, let us consider a case that includes terms with $k \le 2, j \le 3$ and minimize $\int_0^{\pi-\delta} |R(\xi)|^2\,d\xi$ (with $\delta = 0.125\pi$) subject to the condition $R(0) = 0$; the optimal coefficients can be easily found numerically and are given by

$$(a_{k,j}) = \begin{pmatrix} 1.95264069 & -7.4207 \times 10^{-2} & -1.4903 \times 10^{-2} \\ -0.95405524 & 7.4904 \times 10^{-2} & 1.5621 \times 10^{-2} \end{pmatrix}. \tag{11}$$

If instead we include only terms such that $k \le 3, j \le 2$, then

$$(a_{k,j}) = \begin{pmatrix} 2.9524 & 1.5150 \times 10^{-2} \\ -2.9065 & -3.0741 \times 10^{-2} \\ 0.9541 & 1.5624 \times 10^{-2} \end{pmatrix}. \tag{12}$$

The resulting reflection coefficients R are displayed in Fig. 1.

We have applied this method to a number of problems. As the simplest model that encompasses most of the issues in a coupled atomistic/continuum simulation, we consider the Frenkel-Kontorova model,

$$\ddot{x}_j = x_{j+1} - 2x_j + x_{j-1} - U'(x_j) + f, \tag{13}$$

where U is a periodic function with period 1, and f is an external forcing. The continuum limit of this equation is simply the Klein-Gordon equation,

$$u_{tt} = u_{xx} - Ku + f, \tag{14}$$

where $K = U''(0)$. We consider the case when there is a dislocation and study its dynamics under a constant applied forcing. We take $U(x) = (x - [x])^2$, where $[x]$ is the integer part of x. In this example, we take (13) as our atomistic model, and (14) as our continuum model. For the coupled atomistic-continuum model, we use a standard second order finite difference method for (14) in the region away from the dislocation, and we use (13) in the region around the dislocation. However, we also place finite difference grid points in the atomistic region. At these points, the values are obtained through averaging the values from the atomistic model. At the interface between the atomistic and continuum regions, we decompose the displacement into a large scale and a small scale part. The large scale part is computed on the finite difference grid, using (12). The small scale part is computed using the reflectionless boundary conditions described earlier. The interfacial position between the MD and continuum regions is moved adaptively according to an analysis of the wavelet coefficients or the local stress. Both strategies lead to similar

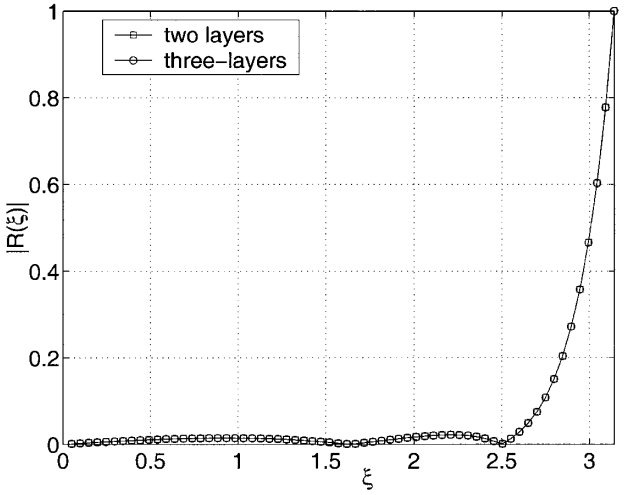

FIG. 1. Reflection coefficients for (11) and (12).

results. Care has to be exercised in order to restrict the size of the atomistic region. For example, when wavelet coefficients are used in the criteria to move the atomistic region, we found it more efficient to use the intermediate levels of the wavelet coefficients rather than the finest level.

We first consider the case when a sharp transition is made between the atomistic and continuum regions with a 1:16 ratio for the size of the grids. Figure 2 is a comparison of the displacement and velocity fields computed using the full atomistic model and the coupled atomistic/continuum model, with $f = 0.04$. The atomistic region has 32 atoms. The full atomistic simulation has 10^4. Dislocation appears as a kink in the displacement field. Notice that, at the atomistic/continuum interface, there is still substantial phonon energy which is then suppressed by the reflectionless boundary condition. No reflection of phonons back to the atomistic region is observed.

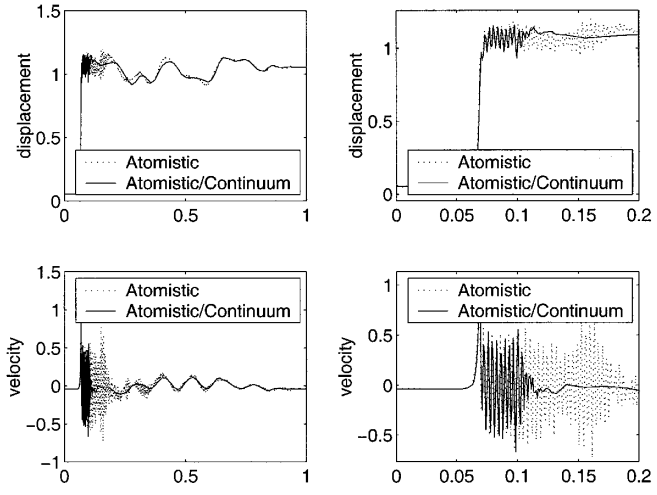

FIG. 2. Comparison of the displacement and velocity profiles computed using the full atomistic and the atomistic/continuum models, with $f = 0.04$. The left column shows the results in the whole computational domain. The right column shows the details near the dislocation.

We next consider a case with $f = 0.02$, which alone is too weak to move the dislocation, but, to the left of the dislocation, we add a sinusoidal wave to the initial data. The dislocation moves as a consequence of the combined effect of the force and the interaction with the wave. Yet, in this case the same atomistic/continuum method predicts an incorrect position for the dislocation, as shown in Fig. 3. The discrepancy seems to grow linearly in time. Improving the matching conditions does not seem to lead to significant improvement.

The difference between this case and the case shown in Fig. 2 is that there is substantially more energy at the intermediate scales. This is clearly shown in the energy spectrum that we computed for the two cases, but it can also be seen in Fig. 3 where an appreciable amount of small scale waves are present in front of the dislocation. Such intermediate scales are suppressed in a method that uses a sharp transition between the atomistic and continuum regions. We therefore consider the next alternative in which the atomistic/continuum transition is made gradually in a 1:2 or 1:4 ratio between neighboring grids. The right column in Fig. 3 shows the results of such a method that uses a gradual 1:2 transition. We see that the correct dislocation position is now recovered.

Our second example is the friction between atomically flat crystal surfaces. To model this process atomistically, we use standard molecular dynamics with the Lennard-Jones potential [11,12]. The two crystals are separated by a horizontal interface. The atoms in the bottom crystal are assumed to be much heavier than the atoms on top. A constant shear stress is applied at the top surface. The main issue here is how dissipation takes place. Physically, the

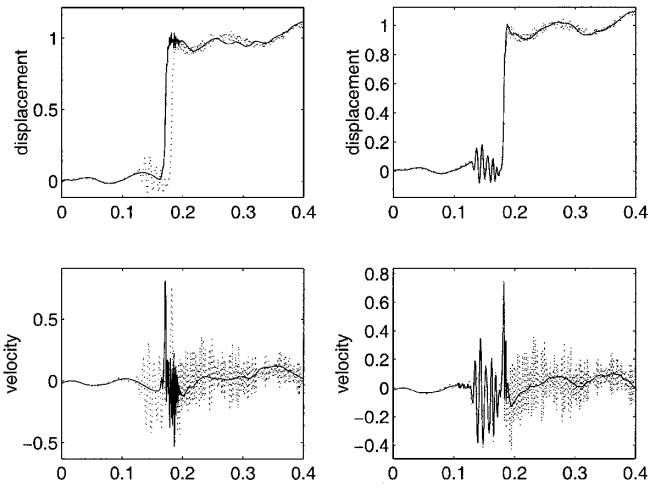

FIG. 3. Comparison of the displacement and velocity profiles computed using the full atomistic and the atomistic/continuum models, with $f = 0.02$. The left column shows the results when the transition from the atomistic to continuum regions is sharp. The right column shows the results when the transition is gradual. The solid line is the result of the atomistic/continuum method. The dashed line is the result of the full atomistic method. Only the region near the dislocation is shown.

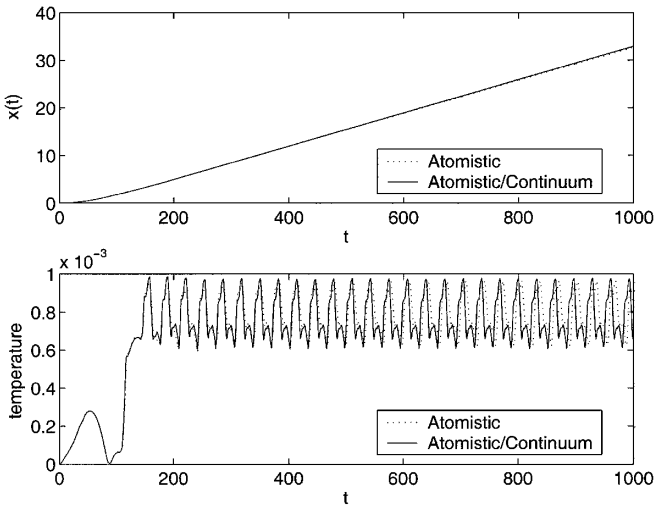

FIG. 4. Displacement and temperature as a function of time for the friction problem. The dashed line is the result of the full molecular dynamics simulation. The solid line is the result of the coupled atomistic/continuum method.

mean kinetic energy is dissipated through conversion into phonons which then convert into heat and exit the system. A standard practice in modeling such a process is to add a friction term to the molecular dynamics in order to control the temperature of the system [11,12]. In contrast, we ensure the proper dissipation of phonons to the environment by imposing the reflectionless boundary conditions for the phonons. As a result, we obtain a linear relationship between the mean displacement of the atoms in the top crystal as a function of time (see Fig. 4). The temperature of the system also saturates (Fig. 4). Also plotted in Fig. 4 is the result of the mean displacement computed using the combined atomistic/continuum method. Here, the continuum model is the linear elastic wave equation with Lamé coefficients computed from the Lennard-Jones potential. The agreement between the full atomistic and the atomistic/continuum simulation is quite satisfactory.

In conclusion, we presented a new strategy for the matching condition at the atomistic/continuum interface in multiscale modeling of crystals. These conditions are adaptive if we choose the weight functions in (7) to reflect the evolving nature of the small scales. They minimize the reflection of phonons and, at the same time, ensure accurate passage of large scale information.

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