A Dynamic Atomistic-Continuum Method for the Simulation of Crystalline Materials

Weinan E*† and Zhongyi Huang*‡

* Department of Mathematics and PACM, Princeton University, Princeton, NJ 08544  † School of Mathematics, Peking University, Beijing, 100866, China  ‡ Department of Mathematical Sciences, Tsinghua University, Beijing, 100084, China

E-mail: weinan@princeton.edu, zhongyi@princeton.edu

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We present a coupled atomistic-continuum method for the modeling of defects and interface dynamics in crystalline materials. The method uses atomistic models such as molecular dynamics near defects and interfaces, and continuum models away from defects and interfaces. We propose a new class of matching conditions between the atomistic and continuum regions. These conditions 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 atomistic-continuum interface. They can be made adaptive by choosing appropriate weight functions. We present applications to dislocation dynamics, friction between two-dimensional crystal surfaces and fracture dynamics. We compare results of the coupled method and of the detailed atomistic model.

Key Words: Atomistic-Continuum Method, Molecular Dynamics, Dislocation, Phonons, Friction, Crack Propagation

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1. INTRODUCTION

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 nano- systems and devices. The second approach is atomistic, aiming at finding 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, 2, 3, 4, 5, 6, 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. The most successful and best-known implementation is the quasi-continuum method [1, 2] which combines the adaptive finite element procedure with an atomistic evaluation of the potential energy of the system. This method has been applied to a number of examples [8, 9, 10], and interesting details were learned about the structure of crystal defects.

Extension of the quasi-continuum method to dynamic problems has not been straightforward [5, 6, 7]. The main difficulty lies in the proper matching between the atomistic and continuum regions. Since the details of the 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 very small part of the computational domain, violation of this condition quickly leads to local heating of the atomistic region and destroys the simulation. In addition, the matching between the
atomistic-continuum interface has to guarantee that large scale information is accurately transmitted in both directions.

The main purpose of the present 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. As applications, we use our method to study the dynamics of dislocations in the Frenkel-Kontorova model, friction between crystal surfaces and crack propagation.

2. CONTINUUM APPROXIMATION OF ATOMIC MODELS

As a first step toward constructing a coupled atomistic-continuum method, we discuss briefly how continuum equations are obtained from atomistic models.

2.1. 1D Frenkel-Kontorova Model — the Klein-Gordon Equation

We first consider a simple problem, the Frenkel-Kontorova Model. This is a one-dimensional chain of particles in a periodic potential, coupled by springs. We will take the potential to be:

\[ U(x) = \frac{1}{2}k(x - a \text{int}(x/a))^2 \] (2.1)

Here \( a \) is the equilibrium distance between neighboring particles, \( \text{int}(x/a) \) denotes the integer closest to \( x/a \). Denote by \( x_n \) the position of the \( n \)-th particle, the dynamic equation for the particles is given by

\[ m \ddot{x}_n = k[x_{n+1} - x_n - a] - k[x_n - x_{n-1} - a] - U'(x_n) + f \] (2.2)

where \( f \) is the applied force.

In the absence of defects such as dislocations, the equilibrium positions of the particles are given
by \( x_j = ja \). In general, we let \( x_j = a(j + u_j) \) and \( \tilde{f} = f / a \). \( u \) is then the displacement field. We get

\[
 m \ddot{u}_j = k[u_{j+1} - 2u_j + u_{j-1}] - \kappa u_j + \tilde{f} \tag{2.3}
\]

Let \( \tau = t \sqrt{1/a^2} \), \( \kappa = \kappa / a^2 \), and \( \tilde{f} = f / a^2 \), we obtain:

\[
 m \frac{\partial^2 u_j}{\partial \tau^2} = k \frac{u_{j+1} - 2u_j + u_{j-1}}{a^2} - \kappa u_j + \tilde{f} \tag{2.4}
\]

Taking the limit as \( a \to 0 \), we obtain the continuum limit equation for the displacement field \( u \),

\[
 m \frac{\partial^2 u}{\partial \tau^2} = k \frac{\partial^2 u}{\partial x^2} - \kappa u + \tilde{f} \tag{2.5}
\]

This is simply the Klein-Gordon equation.

One can verify by direct simulation that (2.5) provides a good approximation to (2.2) for small displacements in the absence of defects. However, one interesting aspect of the Frenkel-Kontorova model is the possibility of having defects such as dislocations in the system, which corresponds to vacant or doubly occupied potential wells. A dislocation corresponds to a kink in \( u \). In this case the Klein-Gordon equation is no longer a good approximation near the dislocation, we need to couple it with the original Frenkel-Kontorova model in order to accurately model the overall dynamics of the defects as well the displacement field away from the defects.

### 2.2. 2D Triangular Lattice — Isotropic Elasticity

Next we consider a model for two-dimensional isotropic elasticity. We will assume that nearest neighbor atoms interact via central forces whose potential is given by \( \Phi(r^2) \) where \( r \) is the distance between the atoms (see Figure 1). From Newton's law, we have

\[
 m \ddot{r}_0 = - \sum_j \nabla_{r_0,j} \Phi(|r_{0,j}|^2), \tag{2.6}
\]

where \( m \) is the mass of the atoms, \( r_j \) is the position of the \( j \)-th atom \( (j = (j_1, j_2)) \), \( r_{0,j} = r_0 - r_j \). Let \( \{R_j\} \) be the equilibrium positions of the atoms. The lattice constant \( a \) satisfies the equilibrium condition \( \Phi'(a^2) = 0 \). Let \( \{u_j\} \) be the displacement vectors, \( u_j = r_j - R_j \). Taylor expanding and
omitting nonlinear terms in \( \mathbf{u} \), we get

\[
m \ddot{\mathbf{u}}_0 = - \sum_j \frac{\partial}{\partial |\mathbf{r}_{0,j}|^2} \Phi(|\mathbf{r}_{0,j}|^2) \frac{\partial |\mathbf{r}_{0,j}|^2}{\partial \mathbf{r}_{0,j}}
\]

\[
= -2 \sum_j \Phi(|\mathbf{r}_{0,j}|^2) \mathbf{r}_{0,j}
\]

\[
= -2 \sum_j [\Phi'(a^2) + 2 \Phi''(a^2) \mathbf{R}_j \cdot (\mathbf{u}_j - \mathbf{u}_0)] [-\mathbf{R}_j + \mathbf{u}_0 - \mathbf{u}_j]
\]

\[
= 4 \Phi''(a^2) \sum_j (\mathbf{R}_j \otimes \mathbf{R}_j)(\mathbf{u}_j - \mathbf{u}_0). \tag{2.7}
\]

Take the example of a Lennard-Jones potential:

\[
\Phi(r) = \epsilon_0 \left( \frac{1}{(r/a_0)^{12}} - \frac{1}{(r/a_0)^6} \right), \tag{2.8}
\]

then the lattice constant \( a \) is equal to \( 2^{1/6} a_0 \) under the assumption of nearest neighbor interaction.

In this case, equation (2.7) becomes

\[
m \ddot{\mathbf{u}}_0 = \frac{18}{a^2} \begin{bmatrix}
1 & 0 \\
0 & 0
\end{bmatrix} (\mathbf{u}_{1,0} - 2 \mathbf{u}_{0,0} + \mathbf{u}_{-1,0}) + \begin{bmatrix}
\frac{1}{4} & \frac{\sqrt{3}}{4} \\
\frac{\sqrt{3}}{4} & -\frac{1}{4}
\end{bmatrix} (\mathbf{u}_{0,1} - 2 \mathbf{u}_{0,0} + \mathbf{u}_{0,-1})
\]

\[
+ \begin{bmatrix}
\frac{1}{4} & -\frac{\sqrt{3}}{4} \\
-\frac{\sqrt{3}}{4} & \frac{1}{4}
\end{bmatrix} (\mathbf{u}_{-1,1} - 2 \mathbf{u}_{0,0} + \mathbf{u}_{1,-1}) \end{bmatrix}. \tag{2.9}
\]

The continuum limit (as \( a \to 0 \)) of the above equations is

\[
\frac{m}{\epsilon_0} \frac{\partial^2 \mathbf{u}}{\partial r^2} = \begin{pmatrix}
81/4 & 0 \\
0 & 27/4
\end{pmatrix} \frac{\partial^2 \mathbf{u}}{\partial x^2} + \begin{pmatrix}
27/4 & 0 \\
0 & 81/4
\end{pmatrix} \frac{\partial^2 \mathbf{u}}{\partial y^2} + \begin{pmatrix}
0 & 54/4 \\
54/4 & 0
\end{pmatrix} \frac{\partial^2 \mathbf{u}}{\partial x \partial y}
\]

\[
= (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) + \mu \Delta \mathbf{u}, \tag{2.10}
\]

where \( \lambda = \mu = \frac{27}{4} \). This is the equation for isotropic elasticity.

### 2.3. Slepyan Model of Fracture

Here we discuss the one- and two-dimensional Slepyan models of fracture [17]. In the 1D case, one can view it as a model for the atoms lying along a crack surface. Nearest neighbors are connected by elastic springs, with spring constant \( k \), and the atoms are tied to the atoms at the opposite side of the crack surface by similar springs, which however snap when extended past some breaking point. The
lines of atoms are being pulled apart by weak springs of spring constant \( k/N \). These weak springs are meant schematically to represent \( N \) vertical rows of atoms pulling in series. Let \( \{u_{j,+}, u_{j,-}\} \) be the displacement of atoms on the top and bottom crack surfaces respectively. The equation which describes the upper line of mass points in this model is

\[
m\ddot{u}_{j,+} = \begin{cases} 
  k(u_{j+1,+} - 2u_{j,+} + u_{j-1,+}) \\
  + \frac{k}{N}(U_N - u_{j,+}) \\
  + k(u_{j,-} - u_{j,+})\theta(2u_f - |u_{j,-} - u_{j,+}|) \\
  - b\dot{u}_{j,+}
\end{cases}
\]  

(2.11)

Here, the first term at the right hand side is elastic coupling to neighbors, the second term is the driving force by displacing edges of the strip, the third term is the bonding to atoms at the opposite side of the crack surface, the last term is the dissipation, \( \theta \) is a step function, and the term containing it describes bonds which snap when their total extension reaches the distance \( 2u_f \). Assume the lattice constant is \( a \). In the region far away from the fracture, we have

\[
m\ddot{u}_{j,+} = k(u_{j+1,+} - 2u_{j,+} + u_{j-1,+}) + \frac{k}{N}(U_N - u_{j,+}) + k(u_{j,-} - u_{j,+}) - b\dot{u}_{j,+}
\]  

(2.12)

Dividing by \( a^2 \) and taking the limit as \( a \to 0 \), we obtain

\[
m\frac{\partial^2 u}{\partial \tau^2} = k\frac{\partial^2 u}{\partial x^2} - \tilde{b} \frac{\partial u}{\partial \tau}
\]  

(2.13)

with \( \tau = t\sqrt{1/a^2}, \tilde{b} = b/(a) \).

Now we consider a simple 2D model (see Figure 2). A crack moves in a lattice strip composed of \( 2N \) rows of mass points. Assume that all the atoms are located at square lattice points if there is no exterior force on them. All of the bonds between lattice points behave as perfect linear springs until the instant they snap, from which point they exert no force. The displacement of each mass point is described by a single spatial coordinate \( u_{i,j} \), which can be interpreted as the height of mass point \((i,j)\) into or out of the page. The index \( i \) takes integer values, while \( j = 1/2 - N, \cdots, -1/2, 1/2, \cdots, N - 1/2 \).
The model is described by the equation

\[ m \ddot{u}_{i,j} = -b \dot{u}_{i,j} + \sum_{\text{nearest}} \mathcal{F}(u_{i',j'} - u_{i,j}), \quad (2.14) \]

with

\[ \mathcal{F}(r) = kr\theta(2u_f - |r|) \quad (2.15) \]

representing the brittle nature of the springs, \( \theta \) the step function, and \( b \) the coefficient of a small dissipative term. The boundary condition which drives the motion of the crack is

\[ u_{i,\pm(n-1/2)} = \pm U_N. \quad (2.16) \]

Similarly, we can get the continuum limit of (2.14):

\[ m \frac{\partial^2 u}{\partial t^2} = k \Delta u - b \frac{\partial u}{\partial t}, \quad (2.17) \]

where \( u \) is again the displacement field.

3. PHONONS

Among the most essential differences between the atomistic and continuum models is the presence of phonons, the lattice vibrations, at the atomistic scale. In this section we will briefly review the spectrum of the phonons. This will be useful later. Let us first consider the simplest model: 1D discrete wave equation (2.3) with \( k = 1 \), and \( f = 0 \). After discretization in time, we have

\[ \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\Delta t^2} = u_{j+1}^n - 2u_j^n + u_{j-1}^n - \mathcal{K}u_j^n \quad (3.1) \]

where \( u_j^n \) is the displacement of the \( j \)-th particle at time \( t = n\Delta t \).

First let \( \mathcal{K} = 0 \). The phonon spectrum for (3.1) is obtained by looking for solutions of the type

\[ u_j^n = e^{i(\omega \Delta t + j\xi)}. \]

This gives us the dispersion relation

\[ \frac{1}{\Delta t} \sin \frac{\omega \Delta t}{2} = \sin \frac{\xi}{2}. \quad (3.2) \]
For the case when $\Delta t = 0.01$, this dispersion relation is depicted in Figure 3. If $K \neq 0$, we have

$$\frac{1}{\Delta t} \sin \frac{\omega \Delta t}{2} = \sqrt{\sin^2 \frac{\xi}{2} + K/4}. \quad (3.3)$$

Consider now the 2D triangular lattice described by (2.7). Let us look for solutions of the type $u^n_j = e^{i(\xi_1 x_j - n \omega \Delta t)} U$ with $\xi = (\xi_1, \xi_2)^T$. Substituting this expression into (2.7), we obtain

$$\left( \frac{\sin \frac{\omega \Delta t}{2}}{\Delta t/2} \right)^2 U = \frac{18}{a^2} \left[ 4\sin^2 \frac{\xi_1 a}{2} \sin^2 \frac{\xi_1 + \sqrt{3} \xi_2}{4} a + \sin^2 \frac{\xi_1 - \sqrt{3} \xi_2}{4} a \right] U$$

$$\equiv \mathbf{A} \mathbf{U}. \quad (3.4)$$

The eigenvalues of the matrix $\mathbf{A}$ are given by,

$$\lambda_{\pm} = \frac{36}{a^2} \left\{ \alpha + \beta \pm \sqrt{\alpha^2 + \beta^2 + \gamma^2 - \alpha \beta - \alpha \gamma - \beta \gamma} \right\}, \quad (3.5)$$

where

$$\alpha = \sin^2 \frac{\xi_1}{2} a, \quad \beta = \sin^2 \frac{\xi_1 + \sqrt{3} \xi_2}{4} a, \quad \gamma = \sin^2 \frac{\xi_1 - \sqrt{3} \xi_2}{4} a.$$

The dispersion relation now has two branches

$$\omega_p(\xi_1, \xi_2) = \frac{2}{\Delta t} \arcsin \left( \frac{2}{\Delta t} \sqrt{\lambda_+} \right), \quad \omega_s(\xi_1, \xi_2) = \frac{2}{\Delta t} \arcsin \left( \frac{2}{\Delta t} \sqrt{\lambda_-} \right), \quad (3.6)$$

where “$p$” and “$s$” stands for “pressure” and “shear” waves respectively.

4. OPTIMAL LOCAL MATCHING CONDITIONS

We now come to the interface between the atomistic and continuum regions. As we mentioned earlier, designing proper matching conditions at this interface is a major challenge in such a coupled atomistic/continuum approach. The basic requirements for the matching conditions are the following:

(1). Reflection of phonons to the atomistic region should be minimal. This is particularly crucial since the atomistic regions are typically very small for the purpose of computational efficiency, reflection of phonon energy back to the atomistic region will trigger local heating and melt the crystalline structure.
(2). Accurate exchange of large scale information between the atomistic and continuum regions.

The first requirement is reminiscent of the absorbing boundary conditions required for the computation of waves [13, 14]. Indeed our work draws much inspiration from that literature. There are some crucial differences though between the phonon problem considered here and the ones studied in [13, 14]. The most obvious one is the fact that the electromagnetic or acoustic waves are continuum objects modeled by partial differential equations, and the associated absorbing boundary conditions often use small wavenumber and/or frequency approximations, whereas phonons are intrinsically discrete with substantial energy distributed at high wavenumbers.

In the following we will give an example of a simple discrete wave equation for which exact reflectionless boundary conditions can be found. Such exact boundary conditions are highly nonlocal and therefore not practical. But they give us guidelines on how approximate boundary conditions should be constructed. We then present a method that constructs optimal local matching conditions, given a predetermined stencil.

4.1. Exact Boundary Conditions for 1D Discrete Wave Equation

Consider equation (3.1). It is supposed to be solved for all integer values of \( j \). Now let us assume that we will truncate the computational domain and only compute \( u^n_j \) for \( j \geq 0 \). Assuming there are no sources of waves coming from \( j < 0 \), we still want to obtain the same solution as if the computation is done for all \( j \). 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 \( j = 0 \).

At \( j = 0 \), we replace (3.1) by

\[
u^n_0 = \sum_{k,j \geq 0} a_{k,j} u^{n-k}_j, \quad a_{0,0} = 0.
\]

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 (4.1) together with the solution of (3.1) for \( j > 0 \) reproduces exactly the solution of (3.1) if it was solved for all integer values of \( j \), i.e. an exact reflectionless boundary condition can be found. For a review on discrete transparent boundary
conditions, see [12].

First, let us consider the case of $\mathcal{K} = 0$. Let $\lambda = \Delta t$ and let us look for solutions of the form:

$$u_j^n = z^n \xi^j, \quad |\xi| \leq 1. \quad (4.2)$$

Substituting (4.2) into (3.1), we get

$$\frac{1}{\lambda^2}(z - 2 + \frac{1}{z}) = \xi - 2 + \frac{1}{\xi}. \quad (4.3)$$

This equation has two roots for $\xi$:

$$\xi_{1,2} = 1 + \frac{z^2 - 2z + 1}{2\lambda^2 z} \pm \frac{1}{2\lambda^2 z} \sqrt{(z - 1)^2[z^2 + (4\lambda^2 - 2)z + 1]} \quad (4.4)$$

Assume a boundary condition of the form

$$u_0^{n+1} = 2u_0^n - u_0^{n-1} + \lambda^2(u_1^n - 2u_0^n) + \sum_{k=1}^n s_k u_0^{n-k}. \quad (4.5)$$

Substituting (4.2) into (4.5), we get

$$z - 2 + \frac{1}{z} - \lambda^2(\frac{1}{\xi} - 2) = \sum_{k=1}^n s_k z^{-k}.$$

To find $s_k$, we have to find the Laurent expansion of the function on the left hand side. Let

$$H(z) = \sqrt{(z - 1)^2[z^2 + (4\lambda^2 - 2)z + 1]} \quad (4.6)$$

Observe that $H(z)$ satisfies

$$H'(z) = 2(z - 1)[z^2 + (3\lambda^2 - 2)z + 1 - \lambda^2]/H(z).$$

Hence

$$H'(z) \cdot [(z - 1)[z^2 + (4\lambda^2 - 2)z + 1]] = 2(z - 1)[z^2 + (3\lambda^2 - 2)z + 1 - \lambda^2]H(z). \quad (4.7)$$

Solving this equation by a Laurent series: $H(z) = \sum_{m \geq -2} \mu_m z^{-m}$, we obtain a recursion relation $\mu_m$ for $m \geq 1$,

$$(m + 2)\mu_m = [1 - 2\lambda^2 - m(4\lambda^2 - 3)]\mu_{m-1} + [4 - 6\lambda^2 - m(3 - 4\lambda^2)]\mu_{m-2} + (m - 3)\mu_{m-3}, \quad (4.8)$$

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and
\[ \mu_{-2} = 1, \quad \mu_{-1} = 2\lambda^2 - 2, \quad \mu_0 = 1 - 2\lambda^4. \]  
(4.9)

Then from (4.4) – (4.9), we have
\[ s_1 = \lambda^4, \quad s_k = -\frac{\mu_{k-1}}{2}, \text{ for } k \geq 2. \]  
(4.10)

(4.5) is nonlocal and has memory effects. In order to see how fast the memory decays, let us assume \( \mu_k \sim m^\alpha \) when \( m \gg 1 \), substituting into (4.8), and equating the coefficients of term order \( m^\alpha \), we get
\[ 2 = (4\lambda^2 - 3)(1 + \alpha) + (4 - 6\lambda^2) + 2(3 - 4\lambda^2)(1 + \alpha) + (2\lambda^2 - 2) - 3(1 + \alpha). \]

This gives \( \alpha = -2 \). The behavior of \( \mu_k \) is shown in Figure 4 when \( \lambda = 0.01 \).

If \( K \neq 0 \), we can proceed as before. But (4.4) changes to
\[ \xi_{1,2} = 1 + \frac{K}{2} + \frac{z^2 - 2z + 1}{2\lambda^2 z} \pm \frac{1}{2\lambda^2 z} \sqrt{[z^2 + (K\lambda^2 - 2)z + 1][z^2 + (K\lambda^2 + 4\lambda^2 - 2)z + 1]}, \]  
(4.11)

Assuming a boundary condition of the form
\[ u_0^{n+1} = 2u_0^n - u_0^{n-1} + \lambda^2[u_1^n - (2 + K)u_0^n] + \sum_{k=0}^n s_k u_0^{n-k}, \]  
(4.12)

Substituting (4.2) into (4.12), we get
\[ z - 2 + \frac{1}{z} - \lambda^2 \left( \frac{1}{z} - 2 - K \right) = \sum_{k=1}^n s_k z^{-k}. \]

To find the Laurent expansion of the function on the left hand side, let \( g(K, \lambda) = K\lambda^2 + 2\lambda^2 - 2 \) and
\[ H(z) = \sqrt{[z^2 + (K\lambda^2 - 2)z + 1][z^2 + (K\lambda^2 + 4\lambda^2 - 2)z + 1]}. \]  
(4.13)

Observe that \( H(z) \) satisfies
\[ H'(z) = \{2z^3 + 3g(K, \lambda)z^2 + [g^2(K, \lambda) + 2 - 4\lambda^4]z + g(K, \lambda)\}/H(z). \]

Hence
\[ H'(z) \cdot \{z^3 + 2g(K, \lambda)z^2 + [g^2(K, \lambda) + 2 - 4\lambda^4]z + 2g(K, \lambda)z + 1\} \]
\[ = H(z) \cdot \{2z^3 + 3g(K, \lambda)z^2 + [g^2(K, \lambda) + 2 - 4\lambda^4]z + g(K, \lambda)\}. \]  
(4.14)
Solving this equation by a Laurent series: $H(z) = \sum_{m \geq -2} \mu_m z^{-m}$, we obtain a recursion relation $\mu_m$ for $m \geq 2$,

$$(m + 2)\mu_m = (2m + 1)[2 - \lambda^2(\mathcal{K} + 2)]\mu_{m-1} + (1 - m)[2 - 4\lambda^4 + [2 - \lambda^2(\mathcal{K} + 2)]^2]\mu_{m-2}$$

$$+(2 - \mathcal{K}\lambda^2 - 2\lambda^2)(2m - 5)\mu_{m-3} + (4 - m)\mu_{m-4},$$

(4.15)

and

$$\mu_{-2} = 1, \quad \mu_{-1} = \mathcal{K}\lambda^2 + 2\lambda^2 - 2, \quad \mu_0 = 1 - 2\lambda^4, \quad \mu_1 = 2\lambda^4(\mathcal{K}\lambda^2 + 2\lambda^2 - 2).$$

(4.16)

Then from (4.11) - (4.16), we have

$$s_0 = -\lambda^2\mathcal{K}, \quad s_1 = \lambda^4, \quad s_k = -\frac{\mu_{k-1}}{2}, \text{ for } k \geq 2.$$  

(4.17)

In order to see how fast the memory decays, let us assume $\mu_k \sim m^{\alpha}$ when $m \gg 1$, substituting into (4.15), and equating the coefficients of the term $m^{\alpha-1}$, we get

$$0 = \alpha \{g(\mathcal{K}, \lambda)(2 - \alpha) - 2\alpha[g^2(\mathcal{K}, \lambda) + 2 - 4\lambda^2] - (6 + 9\alpha)g(\mathcal{K}, \lambda) - 8 - 8\alpha\}.$$ 

This gives $\alpha = 0$ or $\alpha = -2/\left\{1 + \frac{\mathcal{K}(\mathcal{K} + 4)}{\lambda + 2}\mathcal{K}^2\right\}$.  

These exact boundary conditions should be the same as the ones found numerically in [7]. It represents the exact Green’s function for (3.1) which is nonlocal. However, such boundary conditions appear to be impractical for realistic models since they are nonlocal and difficult to obtain, particularly when the atomistic region moves with time which is the case that interests us. But such calculations can at least give us guidelines on how to proceed to constructing approximately reflectionless boundary conditions.

### 4.2. Optimal Local Matching Conditions for 1D Discrete Wave Equation

A practical solution is to restrict (4.1) 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

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

(4.18)
where \( \omega \) is given by (3.2). \( R(\xi) \) is the reflection coefficient at wavenumber \( \xi \). Inserting (4.18) into (4.1), we obtain
\[
R(\xi) = -\frac{\sum a_{k,j} e^{i(\xi-k\omega\Delta t)} - 1}{\sum a_{k,j} e^{-(\xi+k\omega\Delta t)} - 1}
\] (4.19)

Our goal is to find \( \{a_{k,j}\} \) in order to:

(1). Minimize total reflection;

(2). Guarantee accuracy at large scales.

One way of achieving this is to require \( \{a_{k,j}\} \) to satisfy:
\[
\min \int_0^\pi W(\xi)|R(\xi)|^2 d\xi
\] (4.20)
subject to the constraint
\[
R(0) = 0, R'(0) = 0, \text{etc.}
\] (4.21)

Here \( W(\xi) \) is a weight function, which is chosen to be \( W(\xi) = 1 \) in the examples below. Condition (4.21) guarantees accuracy at large scales and (4.20) 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 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 \( \delta \), instead of \( \int_0^\pi |R(\xi)|^2 d\xi \), in order to minimize the influence of \( \xi = \pi \) which always satisfies \( R(\pi) = 1 \).

Let us look at a few examples. If in (4.1) we only keep the terms involving \( a_{1,0} \) and \( a_{1,1} \), then imposing the condition \( R(0) = 0 \) gives
\[
u_0^n = (1 - \Delta t)u_0^{n-1} + \Delta tu_1^{n-1}
\] (4.22)

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
\[
u_0^n = u_1^{n-1} + \frac{1 - \Delta t}{1 + \Delta t}(u_0^{n-1} - u_1^n)
\] (4.23)
Conditions of the type (4.22) and (4.23) are intimately related to the absorbing boundary conditions proposed and analyzed in [13, 14] for the computation of waves. These conditions perform well for low wavenumbers but are less satisfactory at high wavenumbers.

To improve the performance at high wavenumbers let us consider a case that include all terms with \( k \leq 2, j \leq 3 \) and minimize \( \int_0^\infty |R(\xi)|^2 d\xi \) (with \( \delta = 0.125\pi \)) subject to the condition \( R(0) = 0 \), the optimal coefficients can be easily found numerically and are given by

\[
(a_{k,j}) = \begin{pmatrix}
1.95264 & -7.4207 \times 10^{-2} & -1.4903 \times 10^{-2} \\
-0.95406 & 7.4904 \times 10^{-2} & 1.5621 \times 10^{-2}
\end{pmatrix}
\]  

(4.24)

If instead we only include all terms such that \( k \leq 3, j \leq 2 \), then

\[
(a_{k,j}) = \begin{pmatrix}
2.9524 & 1.5150 \times 10^{-2} \\
-2.9065 & -3.0741 \times 10^{-2} \\
0.95406 & 1.5624 \times 10^{-2}
\end{pmatrix}
\]  

(4.25)

The resulting reflection coefficients \( R \) are displayed in Figure 5.

### 4.3. Optimal Local Matching Conditions for Triangular Lattice

The above procedure can be easily generalized. Let us take the triangular lattice as an example, and the boundary to be along the \( x \)-axis. Given a boundary condition of the form:

\[
u_j^{n+1} = \sum_{i \leq 1} \sum J \ A_{ij} u_j^{n+i},
\]

(4.26)

where \( A_{ij} \) are some \( 2 \times 2 \) matrices \( (A_{ii} = 0) \), and the summation is done over a pre-selected stencil, we can find the reflection matrix associated with this boundary condition. For that purpose, we look for solutions of the form

\[
u_j^n = \sum_{\alpha = I, O} \sum_{\beta = s, p} C^\alpha_{\beta} e^{i(\xi^{\alpha,j} r_j - \omega t)} U^\alpha_{\beta},
\]

(4.27)

where \( \alpha = I, O \) correspond to “incoming” and “outgoing” waves respectively (see Figure 6), \( \beta = s, p \) correspond to “shear” and “pressure” waves respectively. Substituting into (3.4) we obtain a relation
between \((C^O_s, C^O_p)^T\) and \((C^I_s, C^I_p)^T\),

\[
M_O \begin{pmatrix} C^O_s \\ C^O_p \end{pmatrix} = M_I \begin{pmatrix} C^I_s \\ C^I_p \end{pmatrix},
\]

where

\[
M_O = e^{-i\omega \Delta t} [U^O_s, U^O_p] - \sum_{l \leq 1} \sum_{j} A_j \begin{bmatrix} e^{i(\xi^O_s - r_j - i\omega \Delta t)} U^O_s, e^{i(\xi^O_p - r_j - i\omega \Delta t)} U^O_p \end{bmatrix},
\]

\[
M_I = -e^{-i\omega \Delta t} [U^I_s, U^I_p] + \sum_{l \leq 1} \sum_{j} A_j \begin{bmatrix} e^{i(\xi^I_s - r_j - i\omega \Delta t)} U^I_s, e^{i(\xi^I_p - r_j - i\omega \Delta t)} U^I_p \end{bmatrix}.
\]

In principle, we can solve the minimization problem

\[
\min \int W(\xi) ||M_I^{-1} \cdot M_O(\xi)||^2 d\xi
\]

to find optimal \(\{A_j^I\}\), where the integration is over the Brillouin zone. But in practice, we find it much more convenient to restrict the integration over a few selected low symmetry atomic planes. In the present context, it amounts to choosing special incidences where the phonon energy dominates.

First, let us consider the case of normal incidence \(\theta = 90^\circ\). That means \(\xi_l = 0\). Then the matrix \(A\) in (3.4) becomes a diagonal matrix:

\[
A = \frac{18}{a^2} \begin{bmatrix} 2 \sin^2 \frac{\sqrt{3}a}{4} & 0 \\ 0 & 6 \sin^2 \frac{\sqrt{3}a}{4} \end{bmatrix}.
\]

with eigenvalues and eigenvectors:

\[
\lambda_1 = \frac{36 \sin^2 \frac{\sqrt{3}a}{4}}, \quad U_1 = (1, 0)^T,
\]

\[
\lambda_2 = \frac{108 \sin^2 \frac{\sqrt{3}a}{4}}, \quad U_2 = (0, 1)^T.
\]

The dispersion relations are

\[
\omega_s \Delta t = 2 \arcsin \left( \frac{3 \Delta t}{a} \sin \frac{\sqrt{3}a}{4} \right), \quad U_s = (1, 0)^T,
\]

\[
\omega_p \Delta t = 2 \arcsin \left( \frac{3 \sqrt{3} \Delta t}{a} \sin \frac{\sqrt{3}a}{4} \right), \quad U_p = (0, 1)^T.
\]

If we take the absorbing boundary condition as in (4.26), the matrices \(M_O\) and \(M_I\) are given by

\[
M_O = e^{-i\omega \Delta t} I - \sum_{l \leq 1} \sum_{j} A_j \begin{bmatrix} e^{i(\xi^O_s - r_j - i\omega \Delta t)} & 0 \\ 0 & e^{i(\xi^O_p - r_j - i\omega \Delta t)} \end{bmatrix},
\]
\[ M_I = -e^{-i\omega \Delta t} I + \sum_{l \leq 1} \sum_{j} A_j^{l} \begin{pmatrix} e^{i (\xi_j^l y_j - l \omega \Delta t)} & 0 \\ 0 & e^{i (\xi_j^l y_j - l \omega \Delta t)} \end{pmatrix}, \quad (4.35) \]

where \( I \) is the \( 2 \times 2 \) identity matrix. For consistency, we should require

\[ (M_I^{-1} M_O)(0) = 0 \]

Imposing this, we get

\[ I = \sum_{l \leq 1} \sum_{j} A_j^{l}, \quad (4.36) \]

\[ 0 = \Delta t I + \sum_{l \leq 1} \sum_{j} A_j^{l} \begin{pmatrix} \frac{2a}{\sqrt{3}} y_j - l \Delta t & 0 \\ 0 & \frac{2a}{\sqrt{3}} y_j - l \Delta t \end{pmatrix} \quad (4.37) \]

If we minimize (4.31) along normal incidence subject to the constraints (4.36) and (4.37), we obtain the desired matrices \( A_j^{l} \). For example, if we keep the terms with \( l = 0,1 \) and \( j = (0,0), (-1,0), (-1,1) \), the optimal coefficient matrices are

\[
\begin{align*}
A_{(0,0)}^{0} &= \begin{pmatrix} 0.947937634 & -0.423061769 E-09 \\ -0.411523005 E-09 & 0.911511476 \end{pmatrix} \\
A_{(-1,0)}^{0} &= A_{(-1,1)}^{0} = \begin{pmatrix} 0.500000011 & 0.604865049 E-08 \\ 0.105260341 E-07 & 0.499999996 \end{pmatrix} \\
A_{(-1,0)}^{1} &= A_{(-1,1)}^{1} = \begin{pmatrix} -0.473968784 & -0.603638049 E-08 \\ -0.102331855 E-07 & -0.455755718 \end{pmatrix}
\end{align*}
\]

Next we consider the cases when both \( \theta = 60^\circ \) and \( \theta = 120^\circ \) are taken into account. For \( \theta = 60^\circ \), we have \( \xi_2 = \sqrt{3} \xi_1 \), and

\[
A = \frac{18}{a^2} \sin^2 \frac{\xi_1 a}{2} \begin{pmatrix} 9 - 4 \sin^2 \frac{\xi_1 a}{2} & \sqrt{3}(3 - 4 \sin^2 \frac{\xi_1 a}{2}) \\ \sqrt{3}(3 - 4 \sin^2 \frac{\xi_1 a}{2}) & 15 - 12 \sin^2 \frac{\xi_1 a}{2} \end{pmatrix}
\]

with two eigenvalues and eigenvectors:

\[
\lambda_1 = \frac{108}{a^2} \sin^2 \frac{\xi_1 a}{2}, \quad U_1 = (\sqrt{3}, -1)^T, \\
\lambda_2 = \frac{36}{a^2} \sin^2 \frac{\xi_1 a}{2}(9 - 8 \sin^2 \frac{\xi_1 a}{2}), \quad U_2 = (1, \sqrt{3})^T.
\]

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The dispersion relations are

\[ \omega_0 \Delta t = 2 \arcsin \left( \frac{3 \sqrt{3} \Delta t}{a} \sin \frac{\xi p a}{2} \right), \quad U_s = (\sqrt{3}, -1)^T, \]  

(4.38)  

\[ \omega_p \Delta t = 2 \arcsin \left( \frac{3 \Delta t}{a} \sin \frac{\xi p a}{2} \sqrt{9 - 8 \sin^2 \frac{\xi p a}{2}} \right), \quad U_p = (1, \sqrt{3})^T. \]  

(4.39)  

The consistency constraints are

\[ I = \sum_{t \leq 1} \sum_j A_j^t, \]  

(4.40)  

\[ 0 = \Delta t \begin{pmatrix} \sqrt{3} & 1 \\ -1 & \sqrt{3} \end{pmatrix} + \sum_{t \leq 1} \sum_j A_j^t \begin{pmatrix} \sqrt{3}(\xi s \cdot r_j/\omega - l \Delta t) & \xi p \cdot r_j/\omega - l \Delta t \\ - (\xi s \cdot r_j/\omega - l \Delta t) & \sqrt{3}(\xi p \cdot r_j/\omega - l \Delta t) \end{pmatrix} \]  

(4.41)  

for \( \theta = 60^\circ \), and

\[ I = \sum_{t \leq 1} \sum_j A_j^t, \]  

(4.42)  

\[ 0 = \Delta t \begin{pmatrix} \sqrt{3} & -1 \\ 1 & \sqrt{3} \end{pmatrix} + \sum_{t \leq 1} \sum_j A_j^t \begin{pmatrix} \sqrt{3}(\xi s \cdot r_j/\omega - l \Delta t) & - (\xi p \cdot r_j/\omega - l \Delta t) \\ \xi s \cdot r_j/\omega - l \Delta t & \sqrt{3}(\xi p \cdot r_j/\omega - l \Delta t) \end{pmatrix} \]  

(4.43)  

for \( \theta = 120^\circ \). For example, if we keep the terms for \( t = 0, 1 \) and \( j = (0, 0), (-1, 0), (-1, 1) \), we have the optimal coefficient matrices

\[
A_{0,0}^0 = \begin{pmatrix}
0.929252841 & -0.861918368E - 09 \\
0.355336047E - 09 & 0.908823412
\end{pmatrix}, \\
A_{-1,0}^0 = \begin{pmatrix}
0.504255087 & 0.156041692E - 01 \\
0.161793547E - 01 & 0.499201553
\end{pmatrix}, \\
A_{-1,1}^0 = \begin{pmatrix}
0.504255087 & -0.156041692E - 01 \\
-0.161793547E - 01 & 0.499201553
\end{pmatrix}, \\
A_{-1,0}^1 = \begin{pmatrix}
-0.468881506 & 0.128308044E - 01 \\
0.118075167E - 01 & -0.453613259
\end{pmatrix}, \\
A_{-1,1}^1 = \begin{pmatrix}
-0.468881506 & -0.128308044E - 01 \\
-0.118075167E - 01 & -0.453613259
\end{pmatrix}. 
\]
If all three angles $\theta = 60^\circ, 90^\circ, 120^\circ$ are used with equal weight, then the optimal coefficient matrices are given by:

$$\mathbf{A}_{(0,0)}^{0} = \begin{pmatrix} 0.963685659E + 00 & 0.522045701E - 05 \\ 0.186532512E - 05 & 0.911580620E + 00 \end{pmatrix}$$

$$\mathbf{A}_{(-1,0)}^{0} = \begin{pmatrix} 0.190155146E + 00 & 0.439544149E - 02 \\ 0.132862553E - 01 & 0.497292487E + 00 \end{pmatrix}$$

$$\mathbf{A}_{(-1,1)}^{0} = \begin{pmatrix} 0.190158427E + 00 & -0.439289966E - 02 \\ -0.132859770E - 01 & 0.497292916E + 00 \end{pmatrix}$$

$$\mathbf{A}_{(-1,0)}^{1} = \begin{pmatrix} -0.171943945E + 00 & 0.439598834E - 02 \\ 0.132858254E - 01 & -0.459575584E + 00 \end{pmatrix}$$

$$\mathbf{A}_{(-1,1)}^{1} = \begin{pmatrix} -0.17194818E + 00 & -0.439293875E - 02 \\ -0.132856732E - 01 & -0.453075576E + 00 \end{pmatrix}$$

5. **THE OVERALL ALGORITHM**

Now we are ready to describe our overall coupled atomistic-continuum method. Our main objective is to accurately model the macroscopic behavior of the system, not the microscopic details. Therefore we will base our computation on a macroscopic grid, with grid sizes denoted by $\Delta t$ and $\Delta x$. The computational domain is divided into two non-overlapping continuum and atomistic regions. This division is done adaptively during the computation, as we explain below. In the continuum region, we solve the linear elasticity equation using conventional finite difference methods. In the atomistic region, we also evolve the macroscopic variables, but with elastic forces computed through averaging the result of the atomistic model.

Each macro time step contains solving a subproblem using the atomistic model in the atomistic region. This micro subproblem is solved via the following steps:

1. The initial data inside the atomistic region for the atomistic model is obtained from interpolating the macroscopic data.
(2). Evolve the atomistic model in the atomistic region using the boundary conditions discussed in the last section.

(3). Evaluate the macroscopic elastic forces in the atomistic region by averaging the result from the atomistic model.

In the current implementation for which no coarse graining in time is used, step (1) is only necessary when a macro cell is changed from a continuum cell to an atomistic cell.

At each macro step the overall scheme consists of:

(A). Select the atomistic and continuum regions. This is done adaptively by looking the stress at each cell. Cells of largest stress and their immediate neighbors are selected as atomistic cells.

(B). Solve the atomistic subproblem, as described above.

(C). Evolve the macroscopic variables using the continuum equation in the continuum region, and the empirically calculated elastic forces from the atomistic model in the atomistic region.

In this formulation, the passage of the macroscopic data to the atomistic region is done naturally at the initialization step for the atomistic subproblem, and the macro scale evolution step.

6. APPLICATIONS

6.1. Dislocation Dynamics in the Frenkel-Kontorova Model

As the simplest model that encompasses most of the issues in a coupled atomistic/continuum simulation, we consider the Frenkel-Kontorova model

\[ \ddot{x}_j = x_{j+1} - 2x_j + x_{j-1} - U'(x_j) + f \]  \hspace{1cm} (6.1)

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

\[ u_{tt} = u_{xx} - Ku + f \]  \hspace{1cm} (6.2)

where \( K = U''(0) \). We consider the case when there is a dislocation and study its dynamics under a constant applied forcing. In this example we take (6.1) as our atomistic model, and (6.2) as our
continuum model.

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 7 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 \( 10^3 \). 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. In Figure 9, we compare the positions of the dislocation as a function of time, computed using the coupled method and the detailed molecular dynamics. Extremely good agreement is observed.

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 Figure 8. The discrepancy seems to grow slowly in time (see Figure 10). Improving the matching conditions does not seem to lead to significant improvement.

The difference between this case and the case shown in Figure 7 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 Figure 8 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, unless we substantially increase the size of the atomistic region. 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. In this way, the continuum model in the transition region is able to capture the energy at the intermediate scales. The right column in Figure 8 shows the results of such a method that uses a gradual 1:2 transition. We see that the correct dislocation position is now recovered.
6.2. Friction between Flat and Rough Crystal Surfaces

Our second example is the friction between crystal surfaces. To model this process atomistically, we use standard molecular dynamics with the Lennard-Jones potential [15, 16]. First, we consider the case in which the two crystals are separated by a horizontal atomically flat interface. The atoms in the bottom crystal are assumed to be much heavier (by a factor of 10) than the atoms on top. To model the lack of chemical bonding between the atoms in the top and bottom crystals, the interaction forces are reduced by a factor of 5 between atoms in the top and bottom crystals. A constant shear stress is applied near the top surface. We use the periodic boundary condition in the $z$-direction.

From a physical viewpoint, one interesting issue here is how dissipation takes place. Physically the kinetic energy of the small scales appears as 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 [15, 16]. In contrast, we ensure the proper dissipation of phonons to the environment by imposing the reflectionless boundary conditions for the phonons. The results presented below are computed using the last set of coefficient matrices presented at the end of Section 4.

From Figure 11 we see that we indeed obtain a linear relation between the mean displacement of the atoms in the top crystal as a function of time. The temperature of the system also saturates. Also plotted in Figure 11 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 Lame coefficients computed from the Lennard-Jones potential. The agreement between the full atomistic and the atomistic/continuum simulation is quite satisfactory.

Next, we study the friction between two rough crystal surfaces. The setup is the same as before, except that the initial interface between the crystals takes the form $y = f(x)$. The numerical results obtained are displayed in Figure 12. In Figure 13, we plot the positions of the atoms in the top and bottom crystals. We see that gaps are created in the case of rough interfaces.

In Figure 14, we compare the force-velocity relations for both flat and rough interfaces. Again the
agreement between the coupled method and the full atomistic method is quite good.

In the present problem, we used atomistic model in a narrow strip near the interface, and continuum model away from the interface. An interesting question is how wide the atomistic strip has to be. Clearly for the purpose of computational efficiency, we want the atomistic strip to be as narrow as possible. On the other hand, it has to be wide enough to provide an accurate description inside the boundary layer where important atomistic processes can be relaxed. There are two important atomistic processes in the present problem. The first is the vibration of the atoms around their local equilibrium positions. The second is the process of moving from one local equilibrium to the next, i.e. sliding by one atomic distance. Clearly the second process works on longer time scale. This process has to be resolved by the atomistic layer. In Figure 15, we compare the atomic positions of a column of atoms which were initially vertical, i.e. they had the same x-coordinates. From this picture one can also estimate the strain rate. We can clearly see that if the atomistic layer does not resolve the phonons generated by the second process, we get inaccurate results.

6.3. Crack Propagation

Our third example is the Slepyan model of fracture dynamics (2.11). In our coupled atomistic/continuum method, we use full atomistic simulation (2.11) around the crack tip, and use (2.12) in the region away from the crack tip. For the continuum equation, we use the displacement boundary condition \( u_N = \pm U_N \) at the left boundary, and stress boundary condition \( \frac{\partial u}{\partial x} = 0 \) at the right boundary. Figure 16 is a comparison of the fracture surface computed using the full atomistic model and the coupled atomistic/continuum method.

Next we apply our method to the 2D Mode III fracture dynamics on a square lattice (2.14). Same boundary conditions as in the 1D case are used for the continuum model. For the matching conditions between the atomistic and continuum regions, we used a stencil that consists of seven points: the values of the three nearest grid points next to the boundary at the current and previous time steps, plus the value at the boundary grid point at the previous time step. The optimization is carried out using angles \( \theta = 45^\circ, 90^\circ, 135^\circ \). Figure 17 is a comparison of the fracture surface computed using the full
atomistic model and the coupled atomistic/continuum method. Comparisons of the positions of the fracture tip as a function of time is given in Figure 18. The results are quite satisfactory. Finally in Figure 19, we display the shear waves generated as a result of the crack propagation, No reflection is seen.

7. CONCLUSION

In conclusion, we presented a new strategy for the matching conditions at the atomistic/continuum interface in multiscale modeling of crystals. The main idea is to choose the boundary condition by minimizing the reflection of phonons along a few low symmetry atomic planes, subject to some accuracy constraints at low wavenumbers. These conditions are adaptive if we choose the weight functions in (4.20) and (4.31) 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. The coupled atomistic/continuum method presented here is quite robust and works well at low temperature. At finite temperature and when nonlinearity is important at large scales, a new method has to be worked out. This work is in progress. Also of interest is coarse-graining in time. This can be done naturally in the present framework by restricting the duration of the atomistic subproblem solved at each macro step to only a small portion of $\Delta t$ and estimate the need macroscale data from this restricted data set. This is carried out in [23].

Perhaps the most significant restriction of the present algorithm is that of low temperature. At finite temperature, phonons contribute to the dynamics of the system at both macro and micro scales. The matching condition at the atomistic/continuum interface should not just be the dissipation of phonons, but rather should model accurately the exchange of heat between the atomistic region and the environment. This again is work in progress.

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FIG. 1 Triangular Lattice

FIG. 2 2D Slepyan model of fracture. The white dots indicate the equilibrium locations, the black dots indicate the displaced points once stress is applied.

FIG. 3 Dispersion relation

FIG. 4 Decay tendency of $|\mu_k|$.

FIG. 5 Reflection coefficients for (4.24) and (4.25).

FIG. 6 The ‘Incoming’ and ‘Outgoing’ phonons near the boundary.

FIG. 7 Comparison of the displacement and velocity profiles computed using the full atomistic and the atomistic/continuum models, with $f = 0.04$. The top two graphs show the results in the whole computational domain. The bottom two graphs show the details near the dislocation. The solid line is the result of the atomistic/continuum method. The dash line is the result of the full atomistic method.

FIG. 8 Comparison of the displacement and velocity profiles computed using the full atomistic and the atomistic/continuum models, with $f = 0.02$. The top two graphs show the results when the transition from the atomistic to continuum regions is sharp. The bottom two graphs show the results when the transition is gradual. Solid line is the result of the atomistic/continuum method. The dash line is the result of the full atomistic method. Only the region near the dislocation is shown.

FIG. 9 Comparison of the positions of the dislocation as a function of time computed using the coupled method and the detailed molecular dynamics with $f = 0.04$. Dot line is the result of full MD simulation; solid line is the result with gradual transition between atomistic and continuum regions; dash line is the result with sharp transition.
**FIG. 10** Comparison of the positions of the dislocation as a function of time computed using the coupled method and the detailed molecular dynamics with $f = 0.02$. Dot line is the result of full MD simulation; solid line is the result with gradual transition between atomistic and continuum regions; dash line is the result with sharp transition.

**FIG. 11** Displacement and temperature as a function of time for the friction problem.

**FIG. 12** Displacement and temperature as a function of time for friction between rough surfaces.

**FIG. 13** The positions of the atoms near the interfaces. The white circles are light atoms, the black ones are heavy atoms. The top graph is the initial state, the bottom graph is the late state at $t = 1000$.

**FIG. 14** Comparison of the force-velocity relations for both flat and rough interfaces. The top two lines are the results for flat case, the bottom two lines are the results for rough case. The solid lines are the results for coupled atomistic/continuum method, the dash lines are the results for full MD simulation.

**FIG. 15** Comparison of the atomic positions of a column of atoms which had the same $x$-coordinates initially. Solid line is the result of full MD, the line with o is the result of coupled method with 96 layers in the atomistic region, the line with + is the result of coupled method with 16 layers in the atomistic region. In the coupled method, the ratio of atomistic and continuum grids is 1:8.

**FIG. 16** One-dimensional fracture problem. The left graph shows the fracture surface at time $t = 0$ and the right one shows the fracture surface at time $t = 600$ with $b = 0.01$, $N = U_N = 4$. The dash line is the result of the full molecular dynamics simulation. The solid line is the result of the coupled atomistic/continuum method. The ratio of atomistic and continuum grids is 1:8.

**FIG. 17** Two-dimensional fracture problem. The left graph shows the fracture surface at time $t = 0$ and the right one shows the fracture surface at time $t = 200$ with $b = 0.01$, $N = 512$, and $U_N = \sqrt{N}$. There are 800 atoms in each row. The dash line is the result of the full molecular dynamics simulation.
The solid line is the result of the coupled atomistic/continuum method. In coupled method, we divide the whole domain into three parts. The middle part including the crack surface with 800 × 64 atoms is the MD region. The top and bottom parts are continuum regions. The ratio of atomistic and continuum grids in each dimension is 1:8.

**FIG. 18** Comparisons of the positions of the crack-tip as a function of time. The dash line is the result of the full MD simulation, the solid line is the result of the coupled method.

**FIG. 19** The shear waves. We divide the whole domain with 2048 × 2048 atoms into three parts. The middle part including the crack surface with 2048 × 128 atoms is the MD region. The top and bottom parts are continuum regions with 128 × 62 finite difference grids in each region.

**FIG. 20** The enlarged picture of the MD region near the crack-tip.
FIG. 2
FIG. 3
FIG. 4
FIG. 5
FIG. 6
FIG. 8
FIG. 12
FIG. 17