Traction Boundary Conditions for Molecular Static Simulations

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Abstract

This paper presents a consistent approach to prescribe traction boundary conditions in atomistic models. Due to the typical multiple-neighbor interactions, finding an appropriate boundary condition that models a desired traction is a non-trivial task. We first present a one-dimensional example, which demonstrates how such boundary conditions can be formulated. We further analyze the stability, and derive its continuum limit. We also show how the boundary conditions can be extended to higher dimensions with an application to a dislocation dipole problem under shear stress.

Keywords: Atomistic models, boundary conditions.

1. Introduction

Atomistic models have established a critical role in material modeling and simulations. In order to study the mechanical responses, boundary conditions (BC) must be imposed. While specifying the displacement of the atoms at the boundary is straightforward, imposing a traction is much more challenging due to the fact that the range of the atomic interactions typically goes beyond nearest neighbors. In direct contrast to continuum mechanics, where the boundary is of lower dimension (curves or surfaces), the ‘boundary’ in an atomistic model often consists of a few layers of atoms. As a result, there are multiple ways to prescribe a BC. For Dirichlet type of BCs, this is typically treated by assigning the displacement for the atoms at the boundary. However, Neumann type of BCs, where the tractions have to be imposed, have not been investigated in the literature. For instance, forces can be applied directly to atoms at the boundary

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7 in such a way that they add up to the given traction. However, it is unclear how to dis-
8 tribute these forces among the atoms. In particular, boundary layers may develop and
9 create large modeling error.

10 Meanwhile, many mathematical problems associated with material defects have
11 been formulated as a system under traction. Examples include cracks under mode-
12 I loading [47], where uniform stress can be specified in the far field, and dislocations
13 under shear stress [22], which led to the important concepts of Peierls barrier. Prob-
14 lems of this type can not simply be treated with BCs that prescribe the displacement
15 of the atoms at the boundary. Another possible approach to introduce traction is the
16 Parrinello-Rahman method [41], where the stress is created by allowing the shape of
17 the simulation cell to change, which is particularly useful when phase transformation
18 processes occur. But the method is limited to periodic cells, and it can not treat material
19 defects without introducing artificial images.

20 The purpose of this paper is to formulate a proper BC that represents a traction
21 force along the boundary. We set up the problem by embedding the computational
22 domain within an infinite molecular system, where the traction in the far-field can be
23 introduced. This is motivated by the observation that molecular simulations are typi-
24 cally conducted within part of the entire sample, due to the heavy computational cost.
25 Mathematically, the extra degrees of freedom in the surrounding region can be elim-
26 inated by solving the finite difference equations associated with the molecular statics
27 model. This gives rise to a BC, which is expressed as an extrapolation of the displace-
28 ment to the atoms outside the boundary, along with a shift vector, which depends on
29 the traction in the far field. We further demonstrate that the typical approach in which
30 external forces are directly applied at the boundary might be incompatible with these
31 BCs, and that they can lead to ill-posed problems.

32 The present approach allows one to simulate a material system with local defects
33 under traction load, which mimics a surround elastic medium. Another potential appli-
34 cation is to the atomistic to continuum (AtC) coupling methods, in which the atomistic
35 model is interfaced with a continuum description, e.g., [4, 6, 8, 14, 24, 35, 38, 39, 42, 43]
36 [40, 45, 46, 49, 55]. We refer the readers to the review papers [9, 35, 38] and references
37 therein. We also remark that instead of using the traction boundary condition for the
38 atomistic simulation, an alternative way is to couple the atomistic simulation with a
39 macroscopic model and apply the boundary conditions at the continuum level. This
40 coupling raises issues at the interface between the atomistic and continuum coupling,
41 and leads to similar difficulties as we address in the current work.

42 The traction boundary condition can be also applied together with methods that
43 are based on domain decomposition (DD), such as [24, 29] where the problem is di-
44 vided into sub-problems, each of which is associated with a sub-domain. In particu-
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lar, the Dirichlet-Neumann and Neumann-Neumann coupling methods (e.g., see [53]) offer a coupling strategy without creating overlapping regions. These methods involve the application of Neumann boundary conditions to some of the domains. Our method can be implemented within the DD framework to facilitate consistent AtC coupling and parallelization.

The issues with correct BCs also arise in the dynamics setting, where the atomistic description is the molecular dynamics model, expressed in terms of Newton's equations of motion. Typically, the goal is to eliminate the reflection of phonons to minimize the interference with the dynamics in the interior [1, 2, 5, 5, 11, 12, 19, 23, 26, 28, 30, 31, 54], which is similar to the absorbing BCs in the simulation of wave propagations [17, 20, 21]. Such BCs can be derived using the Laplace transform, which reduces the system to a time-independent finite-difference equations [1, 2, 31, 54]. We also point out a very recent work for macroscale mechanical loads in molecular dynamics simulations [52]. The method that is presented in this paper can also be formulated for dynamics problems, in which case the traction BC would be given in the form of a convolutional integral as a result of the Laplace transform.

The paper is organized as follows: We first consider a one-dimensional system to demonstrate how the BC can be derived. We further analyze the stability of the resulting boundary value problem and the continuum limit. As an application, and a demonstration of such BCs in high dimensions, we consider a dislocation dipole problem in section 3. We close the paper by a summary and some discussions.

2. A one-dimensional example

To better illustrate the idea, let us first consider a one-dimensional semi-infinite chain of atoms with undeformed position $x_i = i$, where $i \in \mathbb{Z}_+ \cup \{0\}$. We will also use the undeformed position to label the atoms. The deformed position is denoted by y_i with displacement u_i . We assume that the atomistic potential has next-nearest-neighbor pairwise interactions. Namely, the total energy in the bulk can be written as,

$$E = \sum_{i \geq 0} (V(y_{i+2} - y_i) + V(y_{i+1} - y_i)).$$

This one-dimensional example, albeit simple, would serve the purpose of illustrating the necessity of having an appropriate traction boundary condition, particularly when the interactions are beyond the nearest neighbors. Another similar issue that arises from multiscale modeling of crystalline system is the ghost forces [49], for which one-dimensional models with multiple-neighbor interactions have served as important examples to identify the original of the problem and examine methods that attempt to

address the issue [13, 35]. The extension to more general potentials and higher dimensions will be discussed later.

Intuitively, there are at least two ways to impose a traction at the boundary. For instance, one may apply forces, denoted by T_0 and T_1 , to the first two atoms, located at y_0 and y_1 , respectively. Alternatively, one can introduce two additional atoms outside the boundary, which in the present case, have current positions y_{-2} and y_{-1} . These additional atoms will be referred to as *ghost atoms*, since they play different roles as the atoms in the interior. By specifying y_{-2} and y_{-1} (or u_{-2} and u_{-1}), one also creates a traction at the boundary. These two methods are illustrated in Fig. 1.

Figure 1: A one-dimensional chain with next nearest-neighbor interactions. Top: Traction, in the form of point forces, are applied to the two atoms at the left boundary; Bottom: two ghost atoms are introduced outside the boundary.

Remark 1. *At this point, both methods seem plausible, and it is not immediately clear how they are related to each other. Also notable is that there are two parameters available to specify one traction condition. This will be clarified in the next section.*

We illustrate possible BCs with the following numerical experiment: We consider the one-dimensional chain model with harmonic interactions. The force constants are $\kappa_1 = 1$ and $\kappa_2 = -0.2$ for the nearest neighbor and next nearest neighbor interactions. The negative value for κ_2 is motivated by the Lennard-Jones potential, which is concave around the distance of second neighbors. A traction force needs to be applied at the left boundary, while the atoms at x_N and x_{N+1} are fixed. We choose $N = 20$. Three traction BCs are tested. In the first case, we apply a unit force on the first atom, and in the second case, we apply the same force to the second atom. In the third test, we split the force among the first two atoms ($\frac{1}{2}$ and $\frac{1}{2}$). For such a simple setup, one would anticipate that the corresponding continuum model has a simple solution which is given by a uniform deformation gradient. These results are shown in Fig. 2. In all these cases, the solutions develop a boundary layer, and none of them is fully consistent with the

continuum solution. As comparison, we include the result from the traction BC that will be derived later, in which the position of the first two atoms is determined based on the given traction. It is clear that the boundary layer has been eliminated.

Figure 2: Testing several boundary conditions for the one-dimensional model. Left to right: A unit force applied to the first atom; A unit force applied to the second atoms; Forces applied to both atoms; Traction boundary condition that will be derived in the next section.

2.1. The derivation of the traction BC

To understand the traction BC, we start by embedding the semi-infinite atom chain into an infinite chain. We recall that $x_i = i$, $i \in \mathbb{Z}$ denotes the equilibrium positions. We take the view point that the BCs acting on the atom at x_0 should be determined by the interaction of the semi-infinite chain with the atoms on the left ($i < 0$), whose degrees of freedom will be implicitly incorporated. In other words, the atoms x_i , $i \in \mathbb{Z}_-$ serves as an environment for the system we consider. We will hence distinguish the two groups of atoms by referring them as system atoms and environment atoms, respectively. This is based on our observation that most atomistic simulations are focused on part of the entire sample due to the small spatial scale associated with molecular models.

The problem now is reduced to removing the atoms in the environment. To facilitate the reduction of degrees of freedom from the whole chain to the semi-infinite, we will take the harmonic approximation. This amounts to assuming that the interaction between the atoms x_i and x_j is harmonic if either $i < 0$ or $j < 0$. In this paper, we focus our attention to static problems, which can be formulated as an energy minimization problem. For the current problem, the potential energy will be divided into several

terms in accordance with the partition of the system,

$$E = E_{\text{sys}} + E_{\text{int}} + E_{\text{env}} \quad (1)$$

where E_{sys} is the interaction among the atoms in the semi-infinite chain on the right:

$$E_{\text{sys}} = \sum_{i \geq 0} (V(y_{i+2} - y_i) + V(y_{i+1} - y_i)). \quad (2)$$

Meanwhile E_{int} collects the interaction terms between a system atom and an environmental atom. In terms of the displacement $u_j = y_j - x_j$, we have,

$$E_{\text{int}} = \frac{\kappa_1}{2}(u_0 - u_{-1})^2 + \frac{\kappa_2}{2}(u_0 - u_{-2})^2 + \frac{\kappa_2}{2}(u_1 - u_{-1})^2, \quad (3)$$

where $\kappa_1 = V''(1)$ and $\kappa_2 = V''(2)$ are two stiffness constants for nearest-neighbor and next-nearest-neighbor interactions. Further, E_{env} denotes the energy for the environment, given by

$$E_{\text{env}} = \sum_{i < 0} \left[\frac{\kappa_1}{2}(u_i - u_{i-1})^2 + \frac{\kappa_2}{2}(u_i - u_{i-2})^2 \right]. \quad (4)$$

Since the interaction is assumed to be next-nearest-neighbor, the environment atoms only interact with atoms with reference positions x_0 and x_1 , but not other system atoms. Given the displacement u_0 and u_1 , the force balance equations for the environment atoms can be written as

$$\kappa_2(u_{j+2} - 2u_j + u_{j-2}) + \kappa_1(u_{j+1} - 2u_j + u_{j-1}) = 0, \quad j \in \mathbb{Z}_-. \quad (5)$$

The associated characteristic equation of this finite difference equation [25] is given by

$$\kappa_2(\lambda^2 - 2 + \lambda^{-2}) + \kappa_1(\lambda - 2 + \lambda^{-1}) = 0. \quad (6)$$

The roots are given by 1 with multiplicity 2, λ , and λ^{-1} with

$$\lambda = -1 - \frac{\kappa_1}{2\kappa_2} \left[1 - \sqrt{1 + \frac{4\kappa_2}{\kappa_1}} \right]. \quad (7)$$

Thus, the general solution of (5) is given by,

$$u_j = A + Bj + C\lambda^j + D\lambda^{-j}. \quad (8)$$

We collect some elementary properties of λ in the following lemma.

Lemma 1. Assume $\kappa_1 > 0$, $\kappa_2 \neq 0$, and $\kappa = \kappa_1 + 4\kappa_2 > 0$, we have $|\lambda| < 1$ and $-\kappa_2\lambda \geq 0$.

Proof. First notice that

$$1 + \frac{4\kappa_2}{\kappa_1} < 1 + \frac{4\kappa_2}{\kappa_1} + \frac{4\kappa_2^2}{\kappa_1^2} = \left(1 + \frac{2\kappa_2}{\kappa_1}\right)^2,$$

which yields

$$1 - \sqrt{1 + \frac{4\kappa_2}{\kappa_1}} > -\frac{2\kappa_2}{\kappa_1}.$$

For $\kappa_2 > 0$, we then get

$$0 < -\frac{\kappa_1}{2\kappa_2} \left(1 - \sqrt{1 + \frac{4\kappa_2}{\kappa_1}}\right) < 1.$$

Hence, by definition of λ in (7), we get $\lambda \in (-1, 0)$.

For $\kappa_2 < 0$, we have

$$-\frac{\kappa_1}{2\kappa_2} \left(1 - \sqrt{1 + \frac{4\kappa_2}{\kappa_1}}\right) > 1.$$

This yields $\lambda > 0$. Since $1 + 4\kappa_2/\kappa_1 < 1$, we also have

$$\sqrt{1 + \frac{4\kappa_2}{\kappa_1}} > 1 + \frac{4\kappa_2}{\kappa_1}$$

and hence

$$-\frac{\kappa_1}{2\kappa_2} \left(1 - \sqrt{1 + \frac{4\kappa_2}{\kappa_1}}\right) < -\frac{\kappa_1}{2\kappa_2} \left(1 - 1 - \frac{4\kappa_2}{\kappa_1}\right) = 2.$$

We conclude that $\lambda < 1$. □

Since $|\lambda| < 1$, λ^j grows exponentially as $j \rightarrow -\infty$ and hence is unphysical. This leads to the requirement that $C = 0$. The positions of the atoms at x_0 and x_1 further provide two BCs for (5). The remaining one degree of freedom is determined by the traction at the boundary,

$$-\kappa_1(u_0 - u_{-1}) - \kappa_2(u_0 - u_{-2}) - \kappa_2(u_1 - u_{-1}) = T, \quad (9)$$

where T is the prescribed traction at the boundary (scalar in 1D). Intuitively, the traction across a material interface is given by the sum of the forces between two atoms that are on different sides of the interface [3, 57]. This is indeed non-trivial, especially for multi-body interactions. But formulas are available for most empirical potentials [57].

Remark 2. We further remark that the traction is conserved since no external force acts on the fictitious atoms: For $j \in \mathbb{Z}_-$,

$$\begin{aligned} & \left(-\kappa_1(u_j - u_{j-1}) - \kappa_2(u_j - u_{j-2}) \right) - \kappa_2(u_{j+1} - u_{j-1}) \\ & \stackrel{(5)}{=} \left(-\kappa_1(u_{j+1} - u_j) - \kappa_2(u_{j+2} - u_j) \right) - \kappa_2(u_{j+1} - u_{j-1}) \\ & = -\kappa_1(u_{j+1} - u_j) - \kappa_2(u_{j+1} - u_{j-1}) - \kappa_2(u_{j+2} - u_j). \end{aligned}$$

The solution to (5) can now be found. In particular, the coefficients are

$$A = \frac{-\lambda^{-1}u_0 + u_1 + T/\kappa}{1 - \lambda^{-1}}, \quad B = -T/\kappa, \quad \text{and} \quad C = \frac{u_0 - u_1 - T/\kappa}{1 - \lambda^{-1}},$$

where $\kappa = \kappa_1 + 4\kappa_2$. As a result, the displacements u_{-1} and u_{-2} are given by

$$u_{-1} = (1 + \lambda)u_0 - \lambda u_1 + (1 - \lambda)T/\kappa; \quad (10a)$$

$$u_{-2} = (1 + \lambda)u_{-1} - \lambda u_0 + (1 - \lambda)T/\kappa. \quad (10b)$$

Notice that u_{-1} and u_{-2} depend linearly on the displacements u_0 , u_1 and the traction T . This is a result of the harmonic approximation in the environment. Now that the degrees of freedom associated with the atoms further on the left are removed, we can formulate the boundary value problem for the semi-infinite atom chain x_i , $i \in \mathbb{Z}_+ \cup \{0\}$ in terms of ghost atoms x_{-1} and x_{-2} at the boundary. In general, the number of needed layers of atoms is determined by the interaction range.

With the BCs, the molecular statics model is complete. We consider a slightly more general problem by allowing body forces f_i to be applied to the system atoms. In this case, the force balance equations read as follows,

$$-V'(y_{j+2} - y_j) - V'(y_{j+1} - y_j) + V'(y_j - y_{j-1}) + V'(y_j - y_{j-2}) = f_j, \quad j \geq 2 \quad (11a)$$

$$-V'(y_3 - y_1) - V'(y_2 - y_1) + V'(y_1 - y_0) + \kappa_2(u_1 - u_{-1}) = f_1, \quad (11b)$$

$$-V'(y_2 - y_0) - V'(y_1 - y_0) + \kappa_1(u_0 - u_{-1}) + \kappa_2(u_0 - u_{-2}) = f_0, \quad (11c)$$

together with the BCs given by (10).

Another observation is that due to the semi-infinite nature, (11)-(10) can only determine u up to a constant. To uniquely fix the arbitrary constant, we choose $u_0 = 0$. In addition, while the solution u can be a linear function that corresponds to a uniformly stretched (or compressed) state, it is natural to exclude those solutions that grow superlinearly at infinity [35]. Hence, the complete set of BCs for the semi-infinite chain

consists of the traction BC (10) and the conditions

$$u_0 = 0; \tag{12a}$$

$$\limsup_{j \rightarrow \infty} \frac{|u_j|}{j} < \infty. \tag{12b}$$

We emphasize that the above two BCs are associated with the *semi-infinite* chain under consideration, but not the traction at the left end of the chain. For finite system with a right boundary, appropriate BCs should be chosen to replace (12) according to the physical situation. Our emphasis, however, is on the traction condition at the left boundary.

Let us summarize the general framework for our BC construction in one-dimensional systems as follows

- Step 1. Supplement the system with a fictitious environment of atoms with linear approximation;
- Step 2. Solve the positions of the environmental atoms with the condition of fixed traction;
- Step 3. The BC of the atomistic system is then given in terms of the positions of the ghost atoms.

This procedure can be clearly generalized to one-dimensional atomistic systems with arbitrary short-range interactions. The number of BCs depends on the interaction range.

Next, we turn to several properties of the BCs. These will help us better understand the traction BC and also facilitate the extension to higher dimension.

2.2. The continuum limit

For continuum elasticity models, traction BCs are imposed as the normal component of the stress. In this subsection, we show that the continuum limit of the reduced system (11), together with the BCs (10), leads to the Cauchy-Born elasticity with continuum traction BC in elasticity. Hence, our BCs (10) can be viewed as the molecular statics analog of the traction boundary condition in continuum elasticity.

To this end, we adopt the natural rescaling of the system such that the distance between nearest-neighbor atoms in equilibrium becomes ε . We will use superscript to make explicit the dependence on the scaling parameter ε . Hence, the equilibrium positions scale to $x_j^\varepsilon = j\varepsilon$, $j \in \mathbb{Z}_+ \cup \{0\}$ and the deformed positions are $y_j^\varepsilon = x_j^\varepsilon + u^\varepsilon(x_j^\varepsilon)$. We

rewrite the force balance equation and the traction BC accordingly:

$$-V'\left(\frac{y_{j+2}^\varepsilon - y_j^\varepsilon}{\varepsilon}\right) - V'\left(\frac{y_{j+1}^\varepsilon - y_j^\varepsilon}{\varepsilon}\right) + V'\left(\frac{y_j^\varepsilon - y_{j-1}^\varepsilon}{\varepsilon}\right) + V'\left(\frac{y_j^\varepsilon - y_{j-2}^\varepsilon}{\varepsilon}\right) = \varepsilon f_j, \quad j \geq 2 \quad (13a)$$

$$-V'\left(\frac{y_3^\varepsilon - y_1^\varepsilon}{\varepsilon}\right) - V'\left(\frac{y_2^\varepsilon - y_1^\varepsilon}{\varepsilon}\right) + V'\left(\frac{y_1^\varepsilon - y_0^\varepsilon}{\varepsilon}\right) + \kappa_2\left(\frac{u_1^\varepsilon - u_{-1}^\varepsilon}{\varepsilon}\right) = \varepsilon f_1, \quad (13b)$$

$$-V'\left(\frac{y_2^\varepsilon - y_0^\varepsilon}{\varepsilon}\right) - V'\left(\frac{y_1^\varepsilon - y_0^\varepsilon}{\varepsilon}\right) + \kappa_1\left(\frac{u_0^\varepsilon - u_{-1}^\varepsilon}{\varepsilon}\right) + \kappa_2\left(\frac{u_0^\varepsilon - u_{-2}^\varepsilon}{\varepsilon}\right) = \varepsilon f_0 \quad (13c)$$

with

$$u_{-1}^\varepsilon = (1 + \lambda)u_0^\varepsilon - \lambda u_1^\varepsilon + \varepsilon(1 - \lambda)T/\kappa; \quad (14a)$$

$$u_{-2}^\varepsilon = (1 + \lambda)u_{-1}^\varepsilon - \lambda u_0^\varepsilon + \varepsilon(1 - \lambda)T/\kappa. \quad (14b)$$

We now take the continuum limit $\varepsilon \rightarrow 0$. To the leading order, the equation (13a) becomes

$$-\operatorname{div}[V'(y'(x)) + 2V'(2y'(x))] = f(x). \quad (15)$$

Note that for the current atomistic interaction potential, the Cauchy-Born stored energy density is given by [15]:

$$W_{\text{CB}}(A) = V(I + A) + V(2(I + A)). \quad (16)$$

Hence, (15) is exactly the force balance equation for the Cauchy-Born elasticity since

$$\partial_A W_{\text{CB}}(u') = V'(1 + u'(x)) + 2V'(2 + 2u'(x)). \quad (17)$$

Combining (13b), (13c) and the BCs (14), we get

$$-V'\left(\frac{y_3^\varepsilon - y_1^\varepsilon}{\varepsilon}\right) - V'\left(\frac{y_2^\varepsilon - y_1^\varepsilon}{\varepsilon}\right) - V'\left(\frac{y_2^\varepsilon - y_0^\varepsilon}{\varepsilon}\right) = \varepsilon f_1 + \varepsilon f_0 + T. \quad (18)$$

To the leading order, this yields

$$-V'(1 + u'(0)) - 2V'(2 + 2u'(0)) = T. \quad (19)$$

As the left hand side is equal to $n \cdot \partial_A W_{\text{CB}}(u')|_{x=0}$, where n is the unit exterior normal, the BC (19) is exactly the traction BC for the elastic energy density W_{CB} .

2.3. Linear stability at the equilibrium

We also make the observation that the force balance equations (13) with the traction BC (14) can be viewed as a finite difference system with BCs. It is then natural to analyze the stability of such a finite difference system, similar in spirit to the analysis in the context of atomistic-to-continuum methods [33, 34]. We also note that the stability is the crucial ingredient for the rigorous proof of the continuum limit in §2.2. The stability of molecular statics models under periodic and Dirichlet BCs have been analyzed in [15, 16].

To understand the stability, we linearize the force balance equations (11) at the equilibrium (undeformed) state, yielding,

$$-\kappa_2(u_{j+2} - 2u_j + u_{j-2}) - \kappa_1(u_{j+1} - 2u_j + u_{j-1}) = f_j, \quad j \geq 0, \quad (20)$$

supplemented by the BC (10) and (12). Given T , we define the map $H_T : l^2(\mathbb{N}) \rightarrow l^2(\mathbb{N})$ as

$$(H_T u)_j = -\kappa_2(u_{j+2} - 2u_j + u_{j-2}) - \kappa_1(u_{j+1} - 2u_j + u_{j-1}), \quad j \geq 0 \quad (21)$$

with u_{-1} and u_{-2} determined by (14) (and hence the dependence on T). Thus we have

$$H_T(u)_j - H_0(u)_j = \begin{cases} -(\kappa_2(2 + \lambda) + \kappa_1)(1 - \lambda)T/\kappa, & j = 0; \\ -\kappa_2(1 - \lambda)T/\kappa, & j = 1; \\ 0, & \text{otherwise.} \end{cases} \quad (22)$$

Let us introduce a few short-hand notations. First we define the forward difference as

$$(Du)_j = u_{j+1} - u_j. \quad (23)$$

Moreover, the discrete Laplacian is given by

$$(\Delta_d u)_j = u_{j+1} - 2u_j + u_{j-1}. \quad (24)$$

Direct calculations yield,

$$\begin{aligned} (\Delta_d \Delta_d u)_j + 4(\Delta_d u)_j &= (u_{j+2} - 4u_{j+1} + 6u_j - 4u_{j-1} + u_{j-2}) + 4(u_{j+1} - 2u_j + u_{j-1}) \\ &= (u_{j+2} - 2u_j + u_{j-2}). \end{aligned} \quad (25)$$

With these preparations, we calculate the quadratic form $\langle u, H_0(u) \rangle$:

$$\begin{aligned} \langle u, H_0 u \rangle &= -\kappa_2 \sum_{j=0}^{\infty} u_j ((\Delta_d \Delta_d u)_j + 4(\Delta_d u)_j) - \kappa_1 \sum_{j=0}^{\infty} u_j (\Delta u)_j \\ &= -\kappa_2 \sum_{j=0}^{\infty} u_j (\Delta \Delta u)_j - \kappa \sum_{j=0}^{\infty} u_j (\Delta u)_j \end{aligned} \quad (26)$$

Summation by parts gives (recall that $u_0 = 0$)

$$\sum_{j=0}^{\infty} u_j (\Delta u)_j = - \sum_{j=0}^{\infty} |(Du)_j|^2. \quad (27)$$

For the fourth order term, we get

$$\sum_{j=0}^{\infty} u_j (\Delta \Delta u)_j = \sum_{j=0}^{\infty} |(\Delta u)_j|^2 - u_{-1}(u_1 + u_{-1}) = \sum_{j=0}^{\infty} |(\Delta u)_j|^2 + \lambda(1 - \lambda)u_1^2, \quad (28)$$

where in the last equality, we used $u_{-1} = -\lambda u_1$ in the case $T = 0$ and $u_0 = 0$.

Finally, we have,

$$\langle u, H_0 u \rangle = \kappa \sum_{j=0}^{\infty} |(Du)_j|^2 - \kappa_2 \sum_{j=0}^{\infty} |(\Delta u)_j|^2 - \kappa_2 \lambda(1 - \lambda)u_1^2. \quad (29)$$

By Lemma 1, we have $-\kappa_2 \lambda(1 - \lambda) > 0$ as long as $\kappa_1 > 0$ and $\kappa > 0$. Thus, we have

$$\langle u, H_0 u \rangle \geq \kappa \sum_{j=0}^{\infty} |(Du)_j|^2 - \kappa_2 \sum_{j=0}^{\infty} |(\Delta u)_j|^2 \quad (30)$$

Therefore, the scheme is stable as long as the underlying atomistic model is stable.

For a general traction T , we have

$$\langle u, H_T u \rangle = \langle u, H_0 u \rangle - \frac{\kappa_2}{\kappa}(1 - \lambda)Tu_1. \quad (31)$$

Therefore, the stability follows from the stability in the case of $T = 0$.

Remark 3. *This analysis also shows that if λ in (10) is replaced by an appropriate approximation, i.e., $\tilde{\lambda} \approx \lambda$ satisfying $-\kappa_2 \tilde{\lambda}(1 - \tilde{\lambda}) > 0$, a stable model would also be obtained.*

We show that a careless choice of the BC may lead to instability of the scheme. Instead of (10), let us consider an alternative set of BCs (to distinguish, we use $\tilde{u}$ for the displacement)

$$\tilde{u}_{-1} = (1 + \lambda^{-1})\tilde{u}_0 - \lambda^{-1}\tilde{u}_1 + (\lambda^{-1} - 1)T/\kappa; \quad (32a)$$

$$\tilde{u}_{-2} = (1 + \lambda^{-1})\tilde{u}_{-1} - \lambda^{-1}\tilde{u}_0 + (\lambda^{-1} - 1)T/\kappa. \quad (32b)$$

It is straightforward to check that this set of BC also yields traction T at the boundary

$$-\kappa_1(\tilde{u}_0 - \tilde{u}_{-1}) - \kappa_2(\tilde{u}_0 - \tilde{u}_{-2}) - \kappa_2(\tilde{u}_1 - \tilde{u}_{-1}) = T, \quad (33)$$

and hence consistent with the traction BC in continuum elasticity. However, the resulting scheme with the BC (32) is not stable. In fact, we even lose uniqueness: it is easy to check that $\tilde{u}_j = \lambda^j - 1$ for $j \geq -2$ satisfies

$$-\kappa_2(\tilde{u}_{j+2} - 2\tilde{u}_j + \tilde{u}_{j-2}) - \kappa_1(\tilde{u}_{j+1} - 2\tilde{u}_j + \tilde{u}_{j-1}) = 0, \quad j \geq 0, \quad (34)$$

and also at the boundary

$$\tilde{u}_{-1} = (1 + \lambda^{-1})\tilde{u}_0 - \lambda^{-1}\tilde{u}_1; \quad (35)$$

$$\tilde{u}_{-2} = (1 + \lambda^{-1})\tilde{u}_{-1} - \lambda^{-1}\tilde{u}_0; \quad (36)$$

$$\tilde{u}_0 = 0; \quad (37)$$

$$\limsup_{j \rightarrow \infty} \frac{|\tilde{u}_j|}{j} = 0. \quad (38)$$

2.4. Connection to BCs with applied forces at the boundary

As we alluded to at the beginning of this section, it is also possible to apply forces (T_0 and T_1) directly at the boundary to create a traction. But it is not immediately clear how much forces to apply on each of the two atoms at the boundary. Here we will demonstrate the connection to that approach. In particular, this discussion will also shed light on the selection of the forces.

If we substitute (10) into the force balance equation (11), we get

$$\begin{aligned} -V'(y_3 - y_1) - V'(y_2 - y_1) + V'(y_1 - y_0) &= f_1 + T_1; \\ -V'(y_2 - y_0) - V'(y_1 - y_0) &= f_0 + T_0. \end{aligned}$$

with

$$T_1 = \kappa_2(u_{-1} - u_0) = \kappa_2((1 + \lambda)(u_0 - u_1) + (1 - \lambda)T/\kappa); \quad (39)$$

$$\begin{aligned} T_0 &= \kappa_2(u_{-2} - u_0) + \kappa_1(u_{-1} - u_0) \\ &= \lambda(\kappa_1 + \kappa_2(1 + \lambda))(u_0 - u_1) + (1 - \lambda)(\kappa_1 + \kappa_2(2 + \lambda))T/\kappa. \end{aligned} \quad (40)$$

This provides the formulas for the forces. An important observation, however, is that these forces should depend on the displacement of the atoms at x_0 and x_1 .

Observe that by explicit calculation using the definition (7), we have

$$\kappa_2(1 + \lambda) = -\lambda(\kappa_1 + \kappa_2(1 + \lambda)). \quad (41)$$

Thus we also obtain an energy formulation of the traction boundary condition as

$$\begin{aligned} E_{\text{tbc}} &= \sum_{i \geq 0} (V(y_{i+2} - y_i) + V(y_{i+1} - y_i)) + \frac{\kappa_2}{2}(1 + \lambda)(y_1 - y_0 - 1)^2 \\ &\quad - (1 - \lambda)\kappa_2 \frac{T}{\kappa} y_1 - (1 - \lambda)(\kappa_1 + \kappa_2(2 + \lambda)) \frac{T}{\kappa} y_0 - \sum_{i \geq 0} f_i y_i. \end{aligned} \quad (42)$$

Note that the extra term needed even when the traction $T = 0$.

2.5. Traction BC from the Green's function

To facilitate the extension of the BC to two dimensional systems, we take yet another point of view of the traction BC, from the lattice Green's function perspective.

Let us define the lattice Green's function associated with the model (5),

$$-\kappa_2(G_{j+2} - 2G_j + G_{j-2}) - \kappa_1(G_{j+1} - 2G_j + G_{j-1}) = \delta(j), \quad j \in \mathbb{Z}. \quad (43)$$

In general, the lattice Green's functions are useful analytical and computational tools for studying lattice distortions around defects (see e.g., [44, 50, 51]). A typical route to compute the Green's function is via a Fourier transform,

$$\widehat{G}(\xi) = \sum_{j \in \mathbb{Z}} e^{i\xi j} G_j, \quad \xi \in [-\pi, \pi) \quad (44)$$

with the inverse given by,

$$G_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-i\xi j} \widehat{G}(\xi) d\xi \quad (45)$$

This leads to

$$-\kappa_2(e^{2i\xi} - 2 + e^{-2i\xi})\widehat{G}(\xi) - \kappa_1(e^{i\xi} - 2 + e^{-i\xi})\widehat{G}(\xi) = 1, \quad (46)$$

and

$$\widehat{G}(\xi) = \frac{1}{4\kappa_2 \sin^2(\xi) + 4\kappa_1 \sin^2(\xi/2)}. \quad (47)$$

However, due to the singularity at $\xi = 0$, the integral (45) with $\widehat{G}$ given above is not well defined. A remedy [36] is to modify (45):

$$\begin{aligned} G_j &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\xi j} - 1}{4\kappa_2 \sin^2(\xi) + 4\kappa_1 \sin^2(\xi/2)} d\xi \\ &= -\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{2\sin^2(\xi j/2)}{4\kappa_2 \sin^2(\xi) + 4\kappa_1 \sin^2(\xi/2)} d\xi. \end{aligned} \quad (48)$$

Conceptually, the Green's function (43) is only defined up to a constant, and one can fix $G_0 = 0$ by subtracting a (infinite) constant from (45).

As a result, the integral is now well defined as the integrand is regular as $\xi \rightarrow 0$. The function G_j defined this way still satisfies the equations (43). We now make the connections to the BCs (10).

Lemma 2. For $j \leq 0$,

$$G_{j-1} = (1 + \lambda)G_j - \lambda G_{j+1} \quad (49)$$

Proof. Rewrite (48) using a change of variable $z = \exp(i\xi)$ and the characteristic polynomial associated to the denominator, we get

$$\begin{aligned} G_j &= \frac{1}{2\pi\kappa_2 i} \int_{|z|=1} \frac{(z^{-j} - 1)z}{(z-1)^2(z-\lambda)(z-\lambda^{-1})} dz \\ &= \frac{1}{2\pi\kappa_2 i} \lim_{\epsilon \rightarrow 0} \int_{\gamma_\epsilon} \frac{(z^{-j} - 1)z}{(z-1)^2(z-\lambda)(z-\lambda^{-1})} dz \end{aligned}$$

where the contour γ_ϵ is given by the boundary of $B_1(0) \setminus B_\epsilon(1)$ on the complex plane. The second equality uses the fact that the integrand is regular as $z \rightarrow 1$.

Using this representation, we have

$$\begin{aligned} G_{j-1} - (1 + \lambda)G_j + \lambda G_{j+1} &= \frac{1}{2\pi\kappa_2 i} \lim_{\epsilon \rightarrow 0} \int_{\gamma_\epsilon} \frac{z^{-j}(z^2 - (1 + \lambda)z + \lambda)}{(z-1)^2(z-\lambda)(z-\lambda^{-1})} dz \\ &= \frac{1}{2\pi\kappa_2 i} \lim_{\epsilon \rightarrow 0} \int_{\gamma_\epsilon} \frac{z^{-j}}{(z-1)(z-\lambda^{-1})} dz. \end{aligned}$$

As $j \leq 0$ and $|\lambda| < 1$, the integrand is holomorphic in $B_1(0) \setminus B_\epsilon(1)$ for any ϵ , and hence the integral vanishes for any ϵ by Cauchy's integral theorem. Therefore, (49) holds. $\square$

The equation (49) is exactly in the same form as the BCs (10) when $T = 0$. This is not surprising, since the Green's function represents a special set of solutions. In particular, G_j satisfies the homogeneous difference equations (5). Nevertheless, this simple observation can be employed to determine the coefficients in the BCs by using the Green's functions as test functions. This will be implemented for problems in two-dimensions, and the implementation will be discussed in the next sections.

3. Implementation in two-dimensional models

Here we demonstrate how the BC can be extended to two-dimensional systems.

3.1. The traction BC and the induced boundary value problem

For multi-dimensional problems, the BC is typically non-local [37], in that the displacement of all the atoms at the boundary is coupled. It is also possible to consider nonlocal boundary conditions, for example, in the spirit of the boundary element method for molecular static models by one of the authors [29]. Another alternative is to seek a

local BC [27], in the sense that the position of the ghost atoms are only determined by the positions of nearby atoms in the system. To make the dependence local, we would employ a “local flattening” of the boundary. Roughly speaking, for an atom at the boundary, the position is determined by a homogeneous approximation of the local atom configuration with the local value of the traction tensor.

To better explain the idea, we consider the face-centered cubic (FCC) lattice of Aluminum with the axis aligned in $\langle 110 \rangle$, $\langle 001 \rangle$ and $\langle 1\bar{1}0 \rangle$ orientations. When projected to the $\langle 1\bar{1}0 \rangle$ plane, the lattice spacing in the horizontal and vertical directions are $\frac{a_0}{\sqrt{2}}$ and $\frac{a_0}{2}$, respectively, which makes it look like a triangular lattice, as shown in Fig. 3. Again, we introduce ghost atoms outside the boundary in order to achieve the desired traction condition. They are represented by open circles in Fig. 3.

Figure 3: The projected atomic position of a FCC lattice. Filled circles: Atoms in the interior; Open circles: the ghost atoms introduced outside the boundary. The boxes contain the set of atoms S_j that will be used to determine the displacement of the j th atom (see equation (50)).

Our main goal is to determine the actual position of the ghost atoms based on the displacement of the atoms in the interior and the applied traction T , which is a two-dimensional vector. In this case, it is in general cumbersome to obtain the exact boundary condition [37]. Motivated by the one-dimensional traction BC, we seek an approximate BC in the following form,

$$u_j = \sum_{i \in S_j} B_{ji} u_i + p_j. \quad (50)$$

In this equation, S_j indicates a finite number of close neighbors of the atom j (see e.g., Figure 3). We have introduced a set of unknown parameters including $\{B_{ji}\}$ and p . The

shift vector p is similar to the non-homogeneous term in (10), and it will be determined so that the correct traction is obtained.

Let us first explain the roles of the parameters. In the case when $p = 0$, this boundary condition would coincide with the BCs that model an environment that is at a mechanical equilibrium with zero stress [27, 37]. In principle, an exact BC in this form can be derived, e.g., in [37], which mathematically, is a discrete analogue of the Dirichlet-to-Neumann (DtN) map. The exact expression is typically nonlocal, in that the summation is over all the atoms near the boundary. But here we choose a local approximation, and restrict the summation in (50) to those atoms that are close to the j atoms. These neighbors are collected by the set S_j . Due to the translational symmetry of the lattice, we will use the same set of neighbors when implementing the formula (50), which is also demonstrated in Fig. 3. More specifically, we start with the layer of ghost atoms closest to the boundary and apply the BCs (50). Once the displacement of these atoms are updated, we move to the next layer, and these steps will be repeated until the position of all the ghost atoms are updated.

We now discuss how to determine the coefficients B_{ji} . Since they are independent of the applied traction, they can be computed for the case $T = 0$ and $p = 0$, prior to the simulation. In this case, these coefficients can be determined using an optimization procedure, developed in [27]. More specifically, we choose an objective function as follows,

$$\min h, \quad h = \sum_k |G_{j,k} - \sum_i B_{ji} G_{i,k}|^2. \quad (51)$$

Due to translational symmetry, we can shift the j th atom to the origin. For the current example, we choose the atoms i within radius $4.5a_0$, and k within radius $16a_0$. Here $G_{j,k}$ is the two-dimensional lattice Green's function [50]. The main observation is that the BC should be satisfied by special solutions, especially the lattice Green's functions $G_{i,k}$, which corresponds to the solution of the linearized molecular statics model when a point force is applied on the k th atom. This was already observed for the one-dimensional model. Ideally, the objective function would be zero when the BC is exact. Further, we introduce a constraint,

$$\sum_i B_{ji} = I, \quad (52)$$

so that the constant solutions are admitted. This is also seen in the one-dimensional system: The two coefficients in (10) add up to 1. Problem (51) amounts to a least square problem with about 20 ~ 30 variables. The coefficients $\{B_{ji}\}$ can be easily obtained by using standard LAPACK package.

It remains to estimate the vector p . In principle, it should be determined by requiring the traction to arrive at a prescribed value. The total tractions along the boundary

is given by the sum of the forces [3, 57],

$$t = \sum_{i \in \Omega, j \notin \Omega} f_{ij}. \quad (53)$$

Here, f_{ij} comes from a force decomposition. Namely,

$$f_i = \sum_{j \neq i} f_{ij}, \quad f_{ij} = -f_{ji}. \quad (54)$$

This formula, which was already indicated by (9), is consistent with the intuition of Cauchy. The explicit expressions for the force decomposition (54), especially for multi-body potentials, can be found in [7, 57]. For the embedded atom potential [10, 18], which will be used in the next example, the potential energy is given by

$$V = \frac{1}{2} \sum_{1 \leq i \leq N} \sum_{1 \leq j \leq N, j \neq i} \varphi(r_{ij}) + \sum_{1 \leq i \leq N} E(\rho_i), \quad \rho_i = \sum_{1 \leq j \leq N, j \neq i} \rho(r_{ij}). \quad (55)$$

Here we have adopted the usual notation in molecular simulations: $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and $r_{ij} = |\mathbf{r}_{ij}|$. The corresponding force decomposition is given by,

$$\mathbf{f}_{ij} = -\left\{ \varphi'(r_{ij}) + \rho'(r_{ij})[E'(\rho_i) + E'(\rho_j)] \right\} \frac{\mathbf{r}_{ij}}{r_{ij}}. \quad (56)$$

It clearly satisfies the two conditions in (54), along with other consistency conditions [57].

To control the local traction, we divide the region with ghost atoms into blocks, each denoted by Ω_α^c , $\alpha = 1, 2, \dots, M$. The computational domain is denoted by Ω , and the intersection with Ω_α^c , is written as $\partial\Omega_\alpha$. For each block Ω_α^c , we introduce a shift vector p_α . They are chosen so that the traction along $\partial\Omega_\alpha$ agrees with a prescribed value t_α . This arrangement is illustrated in Fig. 4.

We now put the mathematical models together.

$$\begin{cases} \frac{\partial}{\partial u_i} V = 0, & \forall x_i \in \Omega, \\ u_j = \sum_i B_{ji} u_i + p_\alpha, & \forall x_j \in \partial\Omega_\alpha, \\ \sum_{i \in \Omega, j \in \Omega_\alpha^c} f_{ij} = t_\alpha. \end{cases} \quad (57)$$

The first set of equations represent the force balance in the interior, with potential energy given by V . The remaining equations serve as BCs with prescribed tractions t_α . The unknowns are the atomic displacement, together with the shift vectors p_α . The atomic degrees of freedom associated with the atoms outside Ω has been implicitly taken into account by the second and third equations in (57). In the next section, we will discuss an implementation method.

Figure 4: Imposing tractions along the boundary: Ω indicate the computational domain. The atoms outside the boundary are grouped into blocks Ω_{α}^c with the intersection with the boundary given by $\partial\Omega_{\alpha}$. The traction on each $\partial\Omega_{\alpha}$ is prescribed.

3.2. Numerical implementations

Our reduced model (57) consists of a set of nonlinear algebraic equations. It is therefore natural to make use of iterative methods, such as the quasi-Newton's method. In general, this requires the approximation of the Jacobian matrix, since the analytical form is usually not available. The convergence has been found to be slow, especially when the system is not well prepared.

To find an alternative, we notice that in the domain Ω , the molecular statics model is associated with an energy. Therefore, for Dirichlet BCs, where the atoms outside the boundary are held fixed, the solution to the molecular statics model corresponds to an energy minimization, which is usually more robust and much more efficient than solving the nonlinear equations.

Motivated by this observation, we implement the equations by a domain decomposition approach, and alternate among the three sets of equations in (57). As an example to explain the idea, we consider the coupling of the first two sets of equations and assume that p_{α} is given. To solve these two coupled equations, we create a few overlapping layers, in which the atoms serve as both ghost atoms and interior atoms. This is illustrated by Fig. 5. This is simply the Schwartz iteration [53]) between the two models. Then we incorporate the third equation in (57) to determine the values of p_{α} , using the updated values of the displacement in the interior. The second part is essentially a multiplicative domain decomposition.

Overall, we use the following steps,

1. Update the displacement of all the ghost atoms including those in the overlapping region using (50) (or the second equation in (57));
2. Solve for the displacement of the interior atoms, assuming that other atoms are held fixed (open circles in Fig. 5). This is done by minimizing the energy. Here we

- use the BFGS method [32], which only requires the total energy and the gradient.
3. Go to (4) when convergence is reached. The number of iterations can be used as a criterion.
 4. Solve the third equation in (57) for the values of p_α . Here we use a quasi-Newton method with Jacobian approximated by finite differences.
 5. Return back to (1) until convergence.

Figure 5: An overlapping domain decomposition.

3.3. Results from numerical experiments

3.3.1. A dislocation dipole problem

As a test problem, we consider a dislocation dipole under a shear load. The atoms around the two dislocations with opposite Burgers vectors are shown in Fig. 6. The embedded atom model (EAM) [18] has been used as the interatomic potential.

We first manually control the vector $p = (p_1, 0)$, and observe the influence on the traction changes. As a quasi-static loading, we increase p_1 with small increment and then solve the molecular statics model using the domain decomposition method described in the previous section. For each step, we also compute the traction at the boundary. The history of the total boundary traction is shown in Fig. 7. We observe that the traction increases as p_1 increases. However, when p_1 reaches certain critical

Figure 6: The atoms near the two dislocations.

Figure 7: The history of the traction at the boundary.

Figure 8: The position of the atoms before and after the yield stress.

value, a sudden drop is observed. In this case, the two dislocations move to the boundary, and the entire sample undergoes a complete slip. Fig. 8 shows the atomic positions before and after the slip.

In the next experiment, we apply a uniform traction along the upper and lower boundaries. The simulation box is constructed with width $57.21\text{\AA}$ and height $8.064\text{\AA}$. The third direction is treated with periodic boundary condition to mimic a plane strain condition. Each layer consists of 8000 atoms. In Fig. 9, we show the resulting values of p_1 along the boundary. While, the resulting tractions have reached the prescribed values $(2 \times 10^{-4}, 0)$, it is clear that the values for p are not homogeneous, mainly due to the presence of the dislocations. The displacement is shown in Fig. 10, together with a close-up view of the atomic positions in Fig. 11. All these results suggest that the atomic positions are not uniform. Compared to the simulations of dislocation dipoles using the Parrinello-Rahman method (e.g.,[56]), the current approach does not introduce periodic images of the dislocation dipole. Moreover, the uniform shear stress can be applied without forcing a uniform deformation along the boundaries.

For a better comparison, we first conduct the same simulation, but over a much larger system. In particular, the height is 10 times as large. We then compare the displacement of the atoms in the middle. The side-by-side comparison can be found in Fig. 10. This further confirms that the displacement in this region is not uniform. We also see excellent agreement between the results of the simulation using traction boundary condition with that of the simulation of the much larger system.

We now compare our results with the simulation results of the Parrinello-Rahman method. The result for the same system with height $8.064\text{\AA}$ is shown in Fig. 12, which can be readily compared to the one in Fig. 10. We observe that the displacement along the top and bottom boundaries are uniform, due to the enforced periodic boundary

Figure 9: The traction (top) and the shift vector p_1 (bottom) along the upper boundary.

Figure 10: The displacement u_1 . Left: a simulation for a system with height 8.064 Å. Right: a much larger simulation for a system with height 80.64 Å (only the middle region is shown).

Figure 11: A close-up view of the atoms near the two dislocations (generated in Ovito [48]).

conditions.

At this point, we would like to further comment on the difference between the present method and the Parrinello-Rahman method [41]. First, Parrinello-Rahman method is *not* a method to impose non-homogeneous boundary conditions. Instead, it imposes the average stress on the system, whereas the current method applies general tractions at the boundary. Secondly, the result of the Parrinello-Rahman method is a deformed cell with uniform deformation. The deformation tensor is reflected in the shape of the deformed simulation cell, and it is determined so that the average stress in the system is consistent with the imposed value. Finally, the Parrinello-Rahman uses *periodic* boundary conditions. Therefore, it is not applicable to non-periodic systems, e.g., a single dislocation or an open crack. For comparison, we have implemented the Parrinello-Rahman method for the previous example by minimizing the total energy, including the work induced by the applied stress [41].

3.3.2. A micro-crack under tensile load

As the second application, we consider a micro crack in aluminum. We set up the problem in the same way as the previous experiment. A micro crack is created by removing three layers of atoms in the middle of the sample. The tractions are applied at the top and bottom boundary with prescribed values $(0, 6 \times 10^{-4})$. Figure 13 shows the final position of the atoms after the iterations converged. Also shown in the plot is the vertical component of the displacement u_2 .

We also show the resulting values for the shift vector p and the actual traction t along the boundary in Figure 14.

Figure 12: The displacement u_1 obtained from the Parrinello-Rahman model.

Figure 13: The position of the atoms around the crack (top) and the displacement u_2 (bottom).

Figure 14: The traction (left) and the shift vector p_1 (right) along the upper boundary.

4. Summary and Discussion

We have formulated boundary conditions that impose a traction force on a molecular statics model. These boundary conditions are derived by taking into account the surrounding elastic environment. Hence, the computational domain is part of a much bigger sample, and artificial boundary effects can be eliminated. In the continuum limit, these boundary conditions coincide with the Neumann boundary condition for continuum elasticity models.

Finally, we have restricted our discussions to static problems. Extension to dynamic problems will be considered in future works.

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