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Traction boundary conditions for molecular static simulations

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Highlights

- We derived traction boundary conditions for molecular statics models.
- The issue comes up due to interactions that extend beyond nearest neighbors.
- Naive treatment of such boundary conditions may lead to boundary layers.
- We analyzed the stability of the resulting boundary value problem.
- We demonstrated the implementation of such boundary conditions.

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; Dislocation dipole

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

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

Meanwhile, many mathematical problems associated with material defects have been formulated as a system under traction. Examples include cracks under mode-I loading [1], where uniform stress can be specified in the far field, and dislocations under shear stress [2], which led to the important concepts of Peierls barrier. Problems of this type cannot simply be treated with BCs that prescribe the displacement of the atoms at the boundary. Another possible approach to introduce traction is the Parrinello–Rahman method [3], where the stress is created by allowing the shape of the simulation cell to change, which is particularly useful when phase transformation processes occur. But the method is limited to periodic cells, and it cannot treat material defects without introducing artificial images.

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

The present approach allows one to simulate a material system with local defects under traction load, which mimics a surround elastic medium. Another potential application is to the atomistic to continuum (AtC) coupling methods, in which the atomistic model is interfaced with a continuum description, e.g., [4–18]. We refer the readers to the review papers [9,10,19] and references therein. We also remark that instead of using the traction boundary condition for the atomistic simulation, an alternative way is to couple the atomistic simulation with a macroscopic model and apply the boundary conditions at the continuum level. This coupling raises issues at the interface between the atomistic and continuum coupling, and leads to similar difficulties as we address in the current work.

The traction boundary condition can be also applied together with methods that are based on domain decomposition (DD), such as [4,20] where the problem is divided into sub-problems, each of which is associated with a sub-domain. In particular, the Dirichlet–Neumann and Neumann–Neumann coupling methods (e.g., see [21]) 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 [22–31,31–33], which is similar to the absorbing BCs in the simulation of wave propagations [34–36]. Such BCs can be derived using the Laplace transform, which reduces the system to a time-independent finite-difference equations [22,23,32,33]. We also point out a very recent work for macroscale mechanical loads in molecular dynamics simulations [37]. 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