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Dynamical Coupling Atomistic and Continuum Simulations

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Abstract. We propose a new multiscale method that couples molecular dynamics simulations (MD) at the atomic scale and finite element simulations (FE) at the continuum regime. By constructing the mass matrix and stiffness matrix dependent on coarsening of grids, we find a general form of the equations of motion for the atomic and continuum regions. In order to improve the simulation at finite temperatures, we propose a low-pass phonon filter near the interface between the atomic and continuum regions, which is transparent for low frequency phonons, but dampens the high frequency phonons.

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Key words: Multiscale method, finite element, phonon filter method.

1 Introduction

Multiscale modeling makes simulations at large length and time scales possible. The concurrent multiscale methods [1–7] usually combine different physical length scales together, such as atomic scale described by interatomic potentials or by a tight binding model and the continuum scale usually described by elastic mechanics. Such methods have made their success in the simulation of static [8–10] or quasistatic [11] properties. However, the coupling between two length scales inevitably introduces an artificial interface, and the existence of such an interface can cause the spurious reflection of phonons [12–14]. The reflection can interfere with the dynamics in the atomic region and thus prohibit the application of the concurrent multiscale methods to properly simulate dynamical properties. Recently, some hybrid methods have taken a step towards in the

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treatment of dynamical processes [15] by introducing suitable boundary conditions (BC) placed at the coupling interface, such as stadium BC [16,17], exact BC [18–20] and absorbing BC [21], or perfectly matched layer (PML) [22, 23]. Such boundary conditions adopt either a time-dependent [18] or position dependent damping term [16], with which all waves are dampened near the interface region.

However, although the physics properties at two length scales themselves are different, the low frequency phonons can exist in both length scale, while the high frequency phonons can only exist in the atomic region. Meanwhile the low frequency phonon plays a significant role in understanding the long range interaction related to mechanical deformation. Hence, the boundary condition should be frequency dependent, and it should be transparent for the phonon with the frequency as high as possible. The previously proposed algorithms [16, 18, 24] dampen all phonons for the computational convenience. Therefore it is essential to construct a realistic algorithm to couple atomic and continuum simulations.

In this paper, an atomic-based finite element method (AFEM) is introduced, which can be merged seamlessly with an atomistic region in order to enable energy transferring through the coupling interface. Meanwhile, we design a new damping method near the interface to absorb the spurious reflections of high frequency, while keeping low frequency phonons transparent.

2 Theoretical method and analysis

We first consider a one-dimensional (1D) model which can be spatially composed of MD region, FE region and linking region (LR), as shown in Fig. 1. We adopt Lagrangian mechanics to describe the MD region, which is shown without the external force as

$$L(\mathbf{u},\dot{\mathbf{u}}) = \frac{1}{2}\dot{\mathbf{u}}^T \mathbf{M}_A \dot{\mathbf{u}} - V(\mathbf{u}), \tag{2.1}$$

where $\mathbf{M}_A$ is diagonal mass matrix denoted by atomic mass m_μ and $\mathbf{u}$ is discrete atomic displacement. The MD simulation can be numerically implemented in terms of Newton's equation by solving Eq. (2.1).

The FE region is divided into two-node elements with different length from the lattice length a_μ, which is gradually scaled up to $h_l = n_l a_\mu$ ($n_l = 1,2,\cdots,$) into the macroscale, as shown in the left part of Fig. 1. The linear basis functions are set up on the FE region which is linked with the MD systems nearby the most dense elements. Under the Cauchy-Born rule [25], the atomic displacement $\mathbf{u}$ is the linear mapping of the nodal displacement $\mathbf{d}$, expressed as $\mathbf{u} = \mathbf{J}\mathbf{d}$, where $\mathbf{J}$ is Jacobi matrix of the linear interpolation function which provides the atomic displacement within the element. Substituting this relation into Eq. (2.1), by solving the corresponding Lagrangian equation, the equation of motion can be written as

$$[\mathbf{M}][\ddot{\mathbf{d}}] = -[\mathbf{K}][\mathbf{d}], \tag{2.2}$$