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Phonon absorbing boundary conditions for molecular dynamics

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ABSTRACT

With the goal of minimizing the domain size for molecular dynamics (MD) simulations, we develop a new class of absorbing boundary conditions (ABCs) that mimic the phonon absorption properties of an unbounded exterior. The proposed MD-ABCs are extensions of perfectly matched discrete layers (PMDLs), originally developed as an absorbing boundary condition for continuous wave propagation problems. Called MD-PMDL, this extension carefully targets the absorption of phonons, the high frequency waves, whose propagation properties are completely different from continuous waves. This paper presents the derivation of MD-PMDL for general lattice systems, followed by explicit application to one-dimensional and two-dimensional square lattice systems. The accuracy of MD-PMDL for phonon absorption is proven by analyzing reflection coefficients, and demonstrated through numerical experiments. Unlike existing MD-ABCs, MD-PMDL is local in both space and time and thus more efficient. Based on their favorable properties, it is concluded that MD-PMDL could provide a more effective alternative to existing MD-ABCs.

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1. Introduction

Molecular dynamics (MD) is a widely used method to study physical phenomena at the atomic scale. It offers valuable insights into the behavior of certain macroscopic processes like fracture, which are fundamentally triggered at the atomistic scale. One of the major problems in using MD simulation to study such processes is the computational expense involved in simulating a large system. To make the simulation tractable, the MD domain is usually truncated with simple (Dirichlet/Neumann/Periodic) boundary conditions applied at the truncation boundary. However, a simple boundary condition would result in significant energy being artificially reflected back into the region of interest and can completely distort the physical phenomenon being studied. To minimize this error, the simulation domain is taken to be much larger than the region of interest which significantly increases the computational expense of the simulation. This can be avoided by using a more appropriate boundary condition that mimics the effect of the exterior at the truncation boundary. Applying such a boundary condition leads to a much smaller computational domain, thus resulting in significant savings in computational expense.

The problem discussed above is similar to that of suppressing artificial reflections at the truncation boundary of an infinite domain in continuum wave propagation. This problem has been studied extensively and there exist boundary conditions called absorbing boundary conditions (ABCs) that are quite effective in absorbing the incoming energy thus mimicking the exterior [1,2]. It seems natural to extend these boundary conditions to the discrete domains encountered in MD. However,

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since lattice vibrations (phonons) generated in the MD domain have high frequencies and propagate differently from waves in continuous media, continuous ABCs are no longer effective. Instead, ABCs should be derived explicitly for discrete domains to absorb high-frequency phonons. Many ABCs have been developed for this purpose and are summarized in the following paragraphs.

Exact boundary conditions based on the Green's function of the exterior: First developed by Adelman and Doll [3], this approach essentially involves computing the interatomic forces at the truncation boundary through convolution of the boundary response with the exterior Green's function. Cai et al. [4] adopt a similar procedure where the Green's functions for square lattice systems are obtained numerically. Liu and co-workers have extended the idea to more general crystals [5,6]. While these boundary conditions are highly accurate, they are prohibitively expensive and impractical because they involve expensive convolution in time, as well as non-local spatial coupling of boundary atoms.

Rational approximation based methods (rational ABCs): In the context of continuous wave propagation, ABCs are typically derived with the help of rational approximation of the Green's function. These approximations have been directly applied to molecular dynamics simulations [7], but it must be noted that they ignore the discrete dispersion relation and thus cannot accurately absorb high-frequency phonons.

Perfectly matched layer (PML): The PML, also a continuum ABC, involves replacing the exterior with an attenuating medium (PML region) that perfectly matches in impedance with the interior [8], and is truncated using Dirichlet boundary conditions. Due to the impedance matching, there are no reflections at the interface, and due to attenuation in the PML region, the reflection due to truncation is minimal. Owing to its generality and flexibility in applications to complex geometries involving corners, PML is one of the very widely used continuous ABCs, although it has been recently shown that PML may not be as efficient as rational ABCs [9]. PML has been extended to discrete lattice systems in [10], where the interatomic spacing is made complex-valued. This is equivalent to complex stretching in continuous PML that results in wave attenuation (see e.g. [11]). Perfect impedance matching, however, is no longer preserved due to the discrete nature of the problem, leading to significant reflection of high-frequency phonons [12].

Variational boundary condition (VBC): E and co-workers tackle the problem from an optimization view point by using variational principles to minimize the total phonon reflection [13,14]. The basic idea is to increase coupling in the direction normal to the boundary, so as to reduce the extent of coupling in time. The main advantage of VBC is its generality; the procedure is applicable to complex lattice systems. VBC is perhaps the most practical MD-ABC to date in that it is effective in absorbing high-frequency phonons and is more efficient than Green's function based methods. Although the extent of coupling in time is reduced by coupling in space, VBCs still involve convolution operations and are computationally expensive compared to rational ABCs and PMLs. Furthermore, while VBC's stability is ensured through explicit constraints [15], such constraints appear to be sufficient but not necessary for stability, indicating potential degradation of optimal accuracy (for example, the rational ABCs are stable [16] in spite of not satisfying the stability conditions imposed for VBC in [15]). Other minor shortcomings of the method are the lack of transparency in the approximation properties and systematic extension to corners.

In light of the existing ABCs discussed above, it is desirable to obtain a boundary condition that is as accurate as VBCs, as flexible as PMLs (in extension to corners), and as efficient as rational ABCs. To this end, we build on recent research linking continuous PML with rational ABCs [17] to create a class of boundary conditions called perfectly matched discrete layers (PMDLs) [18]. PMDL is essentially PML discretized using linear finite elements with mid-point integration. It has been shown that the integration error exactly cancels the discretization error, thus resulting in perfect matching even after the discretization of the exterior (hence the name, perfectly matched *discrete* layers). Furthermore, PMDL is equivalent to rational ABCs and thus inherits their efficiency while retaining the flexibility of PML. However, PMDL in Refs. [17,18] is developed for continuous wave equation, i.e. PMDL is perfectly matched with the continuous interior, but not with the discrete interior. Thus the continuous PMDL, like other ABCs for wave equation, works well at low frequency limits, but fails in absorbing high frequency phonons. However, we show that the underlying idea of continuous PMDL, namely matching impedance with discrete systems, can be exploited to develop an effective ABC for MD.

Specifically, we show that a PMDL can be viewed as a discrete lattice with nonuniform spacing that has the special property of the characteristic impedance [19] being independent of the atomic spacing. We further show that, for a particular choice of parameters, a PMDL lattice can be made algebraically identical to a general periodic harmonic lattice. Since the PMDL lattice has the additional property of being perfectly matched irrespective of the spacing, any phonon reflections that are introduced due to the truncation of the lattice can be damped out using a few exterior atoms with complex-valued atomic spacing. Named MD-PMDL, the resulting boundary condition is similar in form to continuous PMDL and requires only slightly more computational effort. Compared to existing methods for discrete systems, the proposed method shows promise in providing a more efficient and systematic boundary condition. It should be noted that while MD-PMDL is similar in spirit to continuous PML/PMDL boundary conditions, it is not the same as applying PML/PMDL discretization to the continuum limit equation of the original harmonic lattice. We present both analytical and numerical results that demonstrate this crucial difference.

The outline of the rest of the paper is as follows. The basic problem setup is presented in Section 2 with the help of one-dimensional Frenkel–Kontorova model. Since MD-PMDL is closely related to PMDL, a summary of PMDL ABCs is provided in Section 3, and the extension to a discrete interior is explained in Section 4. The formulation of MD-PMDL including *a-priori* error analysis and a numerical example is presented in Section 5. The extension of MD-PMDL to a square lattice along with numerical examples is presented in Section 6 and the paper is concluded with some closing remarks in Section 7.

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