Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2018-0303

Vol. **26**, No. 1, pp. 192-205
July 2019

An Effective and Easy-to-Implement Boundary Condition for Molecular Dynamics Simulations

Cheng Yuan[1], Jerry Zhijian Yang[1,2,*] and Xiantao Li[3]

[1] *School of Mathematics and Statistics, Wuhan University, Wuhan, Hubei 430072, P.R. China.*
[2] *Hubei Key Laboratory in Computational Mathematics (Wuhan University), Wuhan, Hubei 430072, P.R. China.*
[3] *Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA.*

Received 17 November 2018; Accepted (in revised version) 16 January 2019

Abstract. This paper presents an absorbing boundary condition for molecular dynamics simulations of materials defects. The purpose of the boundary condition is to eliminates spurious reflections of phonons at the boundary and minimize the finite size effect. In contrast to other existing methods, our emphasis is placed on the ease of implementation. In particular, we propose a method for which the implementation can be done within existing molecular dynamics code, and it is insensitive to lattice structure, the geometry and space dimension of the computational domain. To demonstrate the effectiveness, the results from two test problems are presented.

AMS subject classifications: 70-08

Key words: Molecular dynamics, boundary conditions, dislocation, crack, Krylov space.

1 Introduction

Molecular dynamics (MD) models have emerged in the last few decades as a powerful methodology in studying material properties. In MD, the interactions of the atoms are explicitly taken into account [1]. As a result, assumptions on the strain-stress relation, interface kinetics, geometry of crystal defects etc, are not needed. Expressed as second-order ordinary differential equations (ODEs), the numerical implementation has been standardized, e.g. see [1]. Recent development of more accurate interatomic potentials [2–4] has made MD even more promising. In particular, MD models that are based on fundamental considerations (quantum mechanics) are also available [5].

*Corresponding author. *Email addresses:* zjyang.math@whu.edu.cn (J. Z. Yang), yuancheng@whu.edu.cn (C. Yuan), xli@math.psu.edu (X. Li)

Meanwhile, a fundamental limitation, which will likely remain for many years to come, is the scale of the material systems that it can describe. This difficulty stems from the intrinsic spatial scale of MD, which starts at the Angstrom scale ($10^{-10}m$). As a result, one is often restricted to small systems (e.g., thousands to a few million atoms). In addition, periodic boundary conditions (PBC) have been implemented almost exclusively. The implication of PBC is an infinite system with periodic images, which creates an artificial interactions among the images. Furthermore, applying non-uniform boundary condition under this setting is not possible. More importantly, there are many mechanical systems that can not be embedded into a larger periodic sample, e.g, an open crack.

Fortunately, non-periodic BCs that correctly describe the influences of the surrounding medium has been recently developed by numerous groups [6–10]. The mathematical derivation starts with an infinite system, from which the computational domain is selected. The degrees of freedom associated with the atoms in the surrounding region are eliminated by using Fourier/Laplace transform. The result is that the atoms outside the boundary can be written as an integral that involves the time history of displacement of the atoms inside the computational domain. In principle this gives the correct boundary condition. For planar boundaries, this derivation is particularly simple, and it can be implemented directly [10–12]. In this case, the BCs can also be approximated by minimizing the reflection coefficients [6, 7, 9, 13–15]. Another important application of these BCs can be found in multiscale models that involve MD and continuum models [16–24] to reduce the computational cost. Typical observations are that as defects migrate, lattice waves are generated continuously, and as they arrive at the artificial boundary, reflections may occur. In many cases, the reflected waves interfere with the dynamics of the defects e.g., [25], which is undesirable. This observation is similar to artificial reflections in the simulations of wave propagation problems, where absorbing BCs play a vital role in minimizing the boundary reflection [26–28].

Despite the success of the existing methods, there are several remaining difficulties. First, the implementation of most existing methods requires significant effort to pre-compute the parameters. For example, such preparations include the force constant matrices, crystal orientations, and the geometry of the computational domain. These steps may not be familiar to general MD practitioners. Secondly, most of the calculations are limited to planar boundaries, and the proper extension to corners is highly nontrivial [9, 11]. Thirdly, when the BC is expressed as a memory integral, one needs to store the previous values of the displacement of the atoms near the boundary, and the integrals have to be evaluated at every step in time. This significantly increases the computational cost. Finally, the implementation of the BCs in existing code is not straight-forward. To our knowledge, none of the above mentioned methods has been included in existing MD code.

This paper presents a simple approach to implement an approximation of the absorbing BCs. We first express the exact BC as a convolutional integral where the kernel function is written as a matrix function. Motivated by the success of the Krylov subspace approximation of matrix functions [29–32], we introduce a hierarchical approximation.