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A Two-Way Interfacial Condition for Lattice Simulations

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Abstract. In this paper, we formulate a two-way interfacial condition for simulating lattice dynamics in one space dimension. With a time history treatment, the incoming waves are incorporated into the motion of the boundary atoms accurately. This condition reduces to the absorbing boundary condition when there is no incoming wave. Numerical tests validate the effectiveness of the proposed condition in treating simultaneously incoming waves and outgoing waves.

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Key words: Interfacial condition, incoming wave, multiscale computation, time history treatment.

1 Introduction

Multiscale computations have become an indispensable tool in exploring fundamental issues in materials science and their applications in micro, nano and multiscale physics for emerging technologies [7]. In concurrent multiscale computations for a crystalline solid, one selects an atomistic region, where full atomistic computations are performed. The atomistic region is typically a tiny portion of the full solid, where detailed dynamics are demanded to understand nonlinearities, defects, and other important physics. In the complementary region, a coarse grid (continuum) description is used, where short waves are neglected. This greatly reduces the computing load and memory requirement.

Due to the domain decomposition, an artificial interface is introduced between the atomistic and the continuum region. On this interface, suitable conditions are needed to avoid spurious wave reflections. Such spurious waves, if not well suppressed, enter the atomistic region and disturb the local physics in a nonlinear manner. Extensive

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efforts have been made in designing interfacial conditions to reduce the spurious reflections. In the literature, many authors adopted a handshaking region between the atomistic and the continuum regions. In this region, a certain dissipative mechanism is introduced [2]. These interfacial conditions are mostly local in time, namely, requires only information from adjacent grid points at the current time step. A suitable amount of dissipation needs to be tuned in such a way to balance the efficiency and accuracy. They are therefore not accurate treatments of the interface. On the other hand, exact-solution-based interfacial conditions have also been developed more recently. For instance, when time information of an interfacial atom is available, one may reconstruct the displacement at a nearby atom for a linear lattice. This time history treatment was proposed by Adelman and Doll [1] for a harmonic lattice, and further developed for multiscale computations in [3, 8–10]. In contrast to absorbing treatments with a handshaking region, the time history treatment resolves exactly the interface for a linear infinite lattice. In numerical implementations, the accuracy may be reached with sufficiently long time history. For careful analysis, please refer to [5].

In all aforementioned numerical interfacial treatments, fine fluctuations in the continuum region are not taken into account. No wave enters the atomistic region unless it is resolved by the coarse grid. We notice that based on the extended space-time finite element, efforts have been made in incorporating fine scale oscillations into coarse scale solutions [4]. In applications, however, fine scale oscillations do exist in the continuum region and may propagate into the atomistic region. Thermal fluctuation is one such case with great importance. To our knowledge, there is yet quite limited knowledge about how to treat accurately thermal fluctuations in a multiscale computation [6, 12]. Unlike for a continuous wave propagation, a two-way interfacial condition for discrete lattices has not been studied so far in the literature.

In this paper, we develop a two-way interfacial condition for treating both incoming and outgoing waves in one space dimension. With this condition, outgoing waves propagate freely across the interfaces without reflection. With numerical tests, we demonstrate that incoming waves enter the atomistic domain effectively.

The rest of this paper is organized as followings. In Section 2, we derive the two-way interfacial condition. Numerical tests are performed for the linear lattice in Section 3. Some concluding remarks are made in Section 4.

2 Interfacial condition

We consider a harmonic lattice in one space dimension. The displacement u_n of the n-th atom away from its equilibrium is governed by the following rescaled Newton's law.

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1}, \quad n \in \mathbb{N}. \tag{2.1}$$

Consider an atomistic region Ω_D containing the atoms $n = 1, \cdots, N$, and the rest as the continuum region Ω_C. For the sake of clarity, we focus on the discussion of the left interface. The approach applies readily to the right interface. Across the interface, we