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Passing waves from atomistic to continuum

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ABSTRACT

Progress in the development of coupled atomistic–continuum methods for simulations of critical dynamic material behavior has been hampered by a spurious wave reflection problem at the atomistic–continuum interface. This problem is mainly caused by the difference in material descriptions between the atomistic and continuum models, which results in a mismatch in phonon dispersion relations. In this work, we introduce a new method based on atomistic dynamics of lattice coupled with a concurrent atomistic–continuum method to enable a full phonon representation in the continuum description. This permits the passage of short-wavelength, high-frequency phonon waves from the atomistic to continuum regions. The benchmark examples presented in this work demonstrate that the new scheme enables the passage of all allowable phonons through the atomistic–continuum interface; it also preserves the wave coherency and energy conservation after phonons transport across multiple atomistic–continuum interfaces. This work is the first step towards developing a concurrent atomistic–continuum simulation tool for non-equilibrium phonon-mediated thermal transport in materials with microstructural complexity.

1. Introduction

Over the past two decades, extensive research efforts have been devoted to the development of coupled atomistic–continuum methods. A key challenge in nearly all such concurrent multiscale methods has been to interface atomistic models with continuum mechanics. Across this interface there is a change in material description, governing equations and numerical resolution, leading to “ghost forces” in static multiscale methods, and “spurious wave reflections” in dynamic multiscale simulations. While significant progress has been made in reducing or eliminating the ghost forces [1–3], the spurious wave reflection at the atomistic–continuum (A–C) interface is still the major obstacle to the development of dynamic multiscale methods. As a result, most of the efforts in the development of dynamic concurrent multiscale methods, for the modeling of either solid [4–9] or fluid systems [10], have been devoted to minimizing reflected waves or absorbing heat at the atomistic–continuum interface.

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In the field of solid mechanics, one early method that addresses the spurious wave reflection problem is to modify the atomistic equation of motion based on Langevin dynamics using a stadium damping to account for the entropy loss in the coarse-grained (CG) region. Based on the generalized Langevin equation (GLE), Cai et al. [5] calculated the time-history-kernel (THK) matrix to minimize the wave reflection in a one-dimensional (1D) model that couples an atomistic simulation system to linear elastic surroundings. Through a wave-packet test, their approach was shown to significantly reduce wave reflections at the A–C interface. This approach was then employed by Wagner and Liu in the bridging scale method (BSM), also for a 1D case [11]. The THK-based method, although effective in eliminating spurious waves, requires intensive computational cost and is difficult to extend to higher dimensions. Therefore, within the framework of BSM, attempts have been made to derive a compact THK that is computationally much less expensive. However, the compact THK is only effective for linear continua and its extension to nonlinear solids remains challenging [6–8,12]. Another two methods in the category of minimizing the wave reflection at the A–C interface are: (1) to treat the A–C interface issue as an optimization problem [4,9], and (2) to apply the idea of digital filters in the signal processing field to selectively filter out the short-wavelength phonon waves reflected back into the atomistic region [13,14]. In the field of fluid dynamics, given the thermal and material flow characteristics, an Eulerian representation of continuum domain is favored instead of the Lagrangian continuum formulation. Methodologies based on the concept of the hybrid atomistic–continuum interface, or "buffers" has been proposed to alleviate the inconsistency between the atomistic and continuum subdomains [10,15,16] or to evacuate waves out of the computational domain [17,18]; the basic concept of these is similar to the coupling boundary conditions, or handshake regions, that are widely used in multiscale solid mechanics methods [19].

The above mentioned approaches of eliminating spurious wave reflections essentially assume that minimizing, absorbing, or filtering out the unwanted wave reflections at the A–C interface is sufficient for purpose of multiscale materials modeling [20,21]. However, as pointed out by Chirputkar and Qian [22], any interface treatment that involves damping to eliminate wave reflections will also dissipate the fine-scale wave components. The fine-scale wave information needs to be transmitted, instead of simply being minimized or filtered out, from the atomic into the continuum domain [22]. To address this issue, Qian and his coworkers proposed a concurrent multiscale methodology through integrating an enrichment function into the basic framework of a space-time discontinuous Galerkin finite element (FE) [22]. This method was applied to one-dimensional wave propagation and two-dimensional crack propagation problems [23]. The numerical examples demonstrate the robustness of their method in terms of both energy conservation and the almost-nonreflective interface. However, their formulation requires solution for extra degrees of freedom in order to include short-wavelength wave components in the FE region. In addition, at each time step, the enriched interpolation functions must vanish at the FE nodes. As a result, it is difficult to preserve the correct phasing of waves after transmitting across the A–C interface. Therefore, this method is not readily applicable to dynamic problems for which phonon coherency is important, e.g., the transient phonon thermal transport in materials under an ultrashort laser pulse. The ultrashort laser induced heat pulse has been widely used in pump-probe techniques to characterize the thermal transport properties of materials [21–26]. It has been pointed out that coherence is the key property of a laser pulse, and is a general phenomenon that takes place whenever the ultrashort lasers interact with solid materials [24]. Moreover, in such experiments, the phonon-microstructure scattering involves wavelengths at the mesoscale, which are beyond the reach of fully atomistic simulations to date. This necessitates a multiscale method that not only allows all possible phonons to pass the A–C interface, but also maintains the phonon wave coherency.

This work aims to address the spurious phonon wave reflection problem within the framework of the concurrent atomistic–continuum (CAC) method. CAC is a dynamic multiscale method with a unified formulation of balance laws that governs both atomistic and continuum modeling regions [25–27]. Therefore, it reduces the phonon wave reflection problem at the A–C interface to a numerical problem caused by different FE mesh size. This is a well-known and long-standing problem in the use non-uniform FE meshes and was regarded as one of the major unsolved problems of the Finite Element Method (FEM) by Zienkiewicz in his "Achievements and Some Unsolved Problems of the Finite Element Method" [28]. The objective of this work is to formulate and implement a lattice dynamics (LD)-based FE scheme to demonstrate the ability of CAC to accommodate short-wavelength, high-frequency phonon waves in the coarse-grained (CG) domain through the addition of a supplemental basis for the FE solution. The new scheme will facilitate the passage of a full population of phonon waves from the atomistic to the CG region without introducing any extra degrees of freedom. The remainder of this article is organized as follows: in Section 2, we briefly introduce the CAC method and quantify the phonon wave transmission and reflection in CAC models that employ the conventional linear interpolation; in Section 3, we present the formulation of the LD-based FE scheme, the results of the benchmark examples, and the error analysis. The paper then concludes with a brief summary and discussion in Section 4.

2. The CAC method and wave reflections at the A–C interface

The formulation of the CAC method is an extension of Irving–Kirkwood's nonequilibrium statistical mechanical formulation of hydrodynamics equations [29] to a concurrent atomistic–continuum formulation for crystalline materials with a two-level structural description of the materials. In CAC, a crystal is described as a continuous collection of lattice cells, but embedded within each cell is a group of discrete atoms, similar to the two-level material description in Micromorphic Theory [30–33]. The concurrent two-level materials description leads to a multiscale representation of the balance laws [25,26]. Supplemented by the underlying interatomic potential, the reformulated balance laws solve for both the continuous