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A Dynamical Concurrent Multiscale Method Employing a Transmitting Boundary to Minimize Wave Reflections at the Domain Interface

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Abstract. In this work, we present a reformulation of a concurrent multi-scale computation method, previously developed and demonstrated in a static setting at zero temperature, to extend the method for dynamic cases. Additionally, within the context of dynamics, a well-known problem faced in multi-scale simulations pertains to the spurious wave reflections that occur at the artificially introduced interface between the atomistic domain and the coarse scale domain. To address this computational issue, we derive and demonstrate from first principles a simple yet effective solution to mitigate the manifestation of such nonphysical wave reflections at the surface of an artificially truncated domain. We obtain an explicit relationship between the displacement and the velocity terms of the terminal atom and the additional force that needs to be applied on this atom in order to absorb any incident wave. We present how the proposed transmitting boundary can be implemented within the multi-scale formulation for dynamic cases and include numerical examples to verify the efficacy of the methods.

AMS subject classifications: 65C20, 37M05

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1 Introduction

A considerable amount of research is being directed at present towards gaining insight into the relationships between properties of materials at the atomistic level and their

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macro-scale behavior. Studies at the atomistic scale, typically undertaken using molecular mechanics or molecular dynamics (MD) simulations, are currently restricted to small domain sizes owing to the prohibitive computational costs associated with increasing degrees of freedom. On the other hand, the macro-scale properties of materials are generally probed using either experimental techniques (which are often destructive in nature and thus not favored), or continuum approximations which *ipso facto* cannot capture atomistic phenomena. In order to circumvent the limitations intrinsic to each of these two scales of study, researchers have resorted to the use of multi-scale simulations, in which atomistic level detail is retained in locations where it is absolutely necessary (e.g., at crack tips, strain localization regions, etc,) and, farther away from such locations, various methods of homogenization (or "coarse-graining") are employed to decrease the degrees of freedom and the corresponding computational cost. Examples of multi-scale algorithms in the context of solid mechanics include the quasi-continuum (QC) method [1], the generalized mathematical homogenization (GMH) method [2,3], the bridging domain method [4], the Arlequin technique [5], etc.

Many multi-scale techniques are developed first in the setting of static equilibrium and zero temperature, and subsequently extended to account for dynamic/inertial terms and finite temperature. While analyses under static conditions are usually undertaken by searching for the configuration that minimizes the total potential energy of the domain, dynamic simulations proceed by evolving Newton's law of motion through time using some time-stepping algorithm and then tracking particle trajectories. Previously, in [6–8], a multi-scale algorithm, based on the so-called "pseudo-amorphous cell" (PAC), was proposed to perform concurrent simulations on amorphous cells. The central idea of the PAC-based method involved the development of a transformation matrix that could map the displacements of the PAC vertices (henceforth referred to as "nodes") onto the displacements of atoms housed inside that PAC. In this manner, the degrees of freedom of the simulation domain could be decreased, leading to lowered computational costs. It is noted that such PACs are to be distributed judiciously in locations where the strain fields are expected to be small in magnitude, and full atomistic descriptions are retained in regions where high strains are expected. Since previous applications of the PAC-based method were restricted to static conditions, it is imperative to extend the idea to incorporate dynamical loading scenarios like propagation of stress waves and high-strain rate simulations.

The introduction of an artificial boundary between the atomistic and the coarse-grained domains may lead to the manifestation of spurious behavior inside the atomistic domain. One such outstanding and still unresolved problem pertains to the reflection of outgoing waves at the boundary of the domain, an issue which may blemish the accuracy of the solution being computed. For example, in a simulation of an indentation of an atomistic domain at finite temperature, thermal (high frequency) waves may be generated at the indentation site, which may travel outwards towards the artificial interface and then reflect back, thereby resulting in a nonphysical accumulation of heat within the region under investigation. The principal cause of the spurious reflection of these high