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Multiscale coupling of molecular dynamics and peridynamics

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ABSTRACT

We propose a multiscale computational model to couple molecular dynamics and peridynamics. The multiscale coupling model is based on a previously developed multiscale micromorphic molecular dynamics (MMMD) theory, which has three dynamics equations at three different scales, namely, microscale, mesoscale, and macroscale. In the proposed multiscale coupling approach, we divide the simulation domain into atomistic region and macroscale region. Molecular dynamics is used to simulate atom motions in atomistic region, and peridynamics is used to simulate macroscale material point motions in macroscale region, and both methods are nonlocal particle methods. A transition zone is introduced as a messenger to pass the information between the two regions or scales. We employ the "supercell" developed in the MMMD theory as the transition element, which is named as the adaptive multiscale element due to its ability of passing information from different scales, because the adaptive multiscale element can realize both top-down and bottom-up communications. We introduce the Cauchy–Born rule based stress evaluation into state-based peridynamics formulation to formulate atomistic-enriched constitutive relations. To mitigate the issue of wave reflection on the interface, a filter is constructed by switching on and off the MMMD dynamic equations at different scales. Benchmark tests of one-dimensional (1-D) and two-dimensional (2-D) wave propagations from atomistic region to macro region are presented. The mechanical wave can transit through the interface smoothly without spurious wave deflections, and the filtering process is proven to be efficient.

1. Introduction

Computer technology has been transforming scientific and engineering researches. The ever powerful computer and advanced computational algorithms open up opportunities to help us model materials in great details and in unprecedented precisions. For example, the state-of-the-art computational theory and technology, such as ab initio computations and molecular dynamics, e.g. Hohenberg and Kohn (1964), Car and Parrinello (1985), Kohn and Sham (1965), enable us to simulate and predict motions of electrons and atoms with indomitable resolution. Compared with experimental study, computer simulation is fast, cheaper, more efficient, and both informative and flexible, which greatly expands the frontier of researches in many disciplines including materials science, biology, chemistry, etc. The state-of-the-art exascale supercomputer is now capable of handling a molecular system up to sub-millimeter with 110 billion (1.1×10^{11}) atoms (Hou et al., 2012). However, the simulation of a molecular system of macroscale size with 6.022×10^{23} atoms and above is still out of

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reach by even the largest and the faster computers, not to mention the common purpose computers. First principle calculation is even more limited in spatial and time scales because of the calculation of electronic structures. Another challenge is how to analyze and extract useful information from large amount of data that is generated from computer simulations. In engineering research and developments, phenomenological models based finite element analysis and finite difference analysis provide useful tools of simulating continuum objects at macroscopic scale. By virtue of interpolation and discretization of continuum fields, requirements on computer capacity are greatly alleviated. However, macroscale material models usually employ homogenized field variables and adopt empirical assumptions, such as phenomenological constitutive relations, in which some detailed physical information may be lost, making it difficult to understand multiscale physical behaviors of materials, for instance, microscale and mesoscale material defect evolutions.

The limitation of computational model in each scale has motivated the development of various multiscale simulations, concurrent or hierarchical. The goal of a multiscale model is to combine physical theories or mathematical models from different scales in a single framework, so that we can solve the multiscale problem in either a distinctive scale or simultaneously concurrent scales depending on the problems of interest. The possibility of scale division is based on two factors. First, physical nature of materials manifests itself in multiple scales in space and time. Materials defects and flaws are typical multiscale phenomena. For example, microscopic dislocation largely determines the macroscale strength of the material; highly localized region around the crack tip that is characterized by bond breaking and strong discontinuity, but the region where is away from the crack tip may only have moderate or uniform deformation. Second, reliable coupling techniques are required to transfer information among different scales. Cross-scale communication is one of the most challenging issues in both multiscale theory and computer simulations, because quantities in different scales have distinct properties, and a perfect match between them is often difficult. For examples, force in microscale may be described in terms of nonlocal interaction between two or many particles interaction, whereas in macroscale it is often described in terms of local interaction among immediate adjacent particles; and temperature is a concept in macroscale, and its corresponding microscale phenomenon is the random motion of particles.

Several multiscale models have had some success in practice. Among them, the macroscopic, atomistic, ab initio dynamics (MAAD) (Abraham et al., 1998; Broughton et al., 1999) method is one of the earlier works, which spans three scales from quantum mechanics to continuum mechanics. It has been applied to solve dynamical fracture problem of silicon. On the other hand, the issue of numerical wave reflection at interscale boundary can be observed in this method. The quasi-continuum method (Tadmor et al., 1996; Shenoy et al., 1998, 1999; Knap and Ortiz, 2001) is another widely recognized model, in which only representative atoms are being simulated instead of conducting all atom calculations, and it has been successful in solving some quasi-static problems such as nano indentation.

However, MAAD method has interscale boundary impedance mismatch problem, and the quasi-continuum method is restricted to static and quasi-static problems without characterization of dynamics. Moreover, the mismatch of the impedance at the inter-scale boundary forces to introduce a so-called “ghost force”. To resolve the inter-scale boundary mismatch problem, the bridging scale method (Wagner and Liu, 2003; Park et al., 2005a, 2005b; Liu et al., 2006) provides a procedure that can realize the scale transition by a process of projection with minimizing least square error, and it introduces an impedance force that may largely alleviated the inter-scale boundary wave reflection. The coupled atomistic and discrete dislocation (CADD) (Shilkrot et al., 2002, 2004) is advantageous to simulate dislocation-type of defects, and it may involve a priori knowledge of slip systems for dislocation detection and passing through interfaces. The recently proposed Multiscale Crystal Defect Dynamics (MCDD) (Li et al., 2014) employs a similar idea by using information of the lattice microstructure to construct multiscale methods. Other prominent multiscale methods include concurrent atomistic continuum (CAC) method (Chen and Lee, 2005; Xiong et al., 2011), and the perfectly matched multiscale simulation (PMMS) method (To and Li, 2005; Li et al., 2006), among others.

Theoretically speaking, an ideal multiscale method would need to have a two-way cross-scale information passage: the bottom-up and the top-down. This is what is lacking in existing multiscale methods. The bottom-up approach is relatively straightforward, where information from microscale is properly collected and interpreted to describe macroscale phenomena. For example, a macroscale displacement field is the averaged or homogenized field from atomistic displacements, and stress and temperature fields can be calculated from atomistic forces and random velocities according to statistical mechanics. On the other hand, the top-down message passing is more challenging, and requires uncanny physical insights. In specific, we may illustrate the top-down approach through the response of a molecular system when a macroscale boundary condition such as traction is prescribed. This procedure is not trivial, because a single-scale model cannot describe both molecular system and macroscale boundary conditions. To resolve this issue, recently the present authors proposed a micromorphic multiscale molecular dynamics (MMMD) model that has intrinsic multiscale structure and multiscale dynamics (Li and Tong, 2015; Tong and Li, 2015a, 2015b; Li and Urata, 2016), which is a new type of multiscale model that attempts to rigorously resolve the relationship between molecular dynamics and continuum mechanics. The model is derived from and equivalent to classical molecular dynamics, but macroscale quantities such as traction are incorporated into microscale model versus multiscale structure design, and thus the top-down message passing becomes natural.

The present work is to further establish a multiscale coupling paradigm based on the previous multiscale molecular dynamics theory (Li and Tong, 2015; Tong and Li, 2015a). By taking advantage of the previous physical multiscale theory, an adaptive multiscale element is constructed as a messenger to translate information between regions of different scales. The message transition is smooth due to the clearly defined top-down and bottom-up characterizations. In atomistic region, molecular dynamics is the natural choice. In macroscopic region, several models can be employed depending on the