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Multiresolution molecular mechanics: Adaptive analysis

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Abstract

The concurrent atomistic/continuum coupling method Multiresolution Molecular Mechanics (MMM) has been presented for statics (Yang et al., 2013) and dynamics (Biyikli et al., 2014), its convergence and error structure has been analyzed (Yang et al., 2014), and a unified and consistent framework for general finite element shape functions has been introduced (Yang and To, 2014). The current work presents the adaptivity analysis of the MMM method. To start, the rationale and formulation of the MMM method are briefly introduced. Later, two main features of the adaptivity scheme, refinement and coarsening, are discussed and described in detail and step-by-step procedures are outlined. The adaptivity is tested using three numerical examples: (i) 1-D wave propagation, (ii) 2-D dislocation, and (iii) 3-D nanoindentation. The results of numerical examples agree well with those of full atomistic simulations. Furthermore, control parameters of adaptivity schemes offer much flexibility to adjust between accuracy and efficiency. The introduced adaptivity schemes are simple, effective, and accurate owing to the consistency and robustness of MMM.

Keywords: Multiscale; Molecular dynamics; Atomistic/continuum; Dynamics; Adaptivity

1. Introduction

A class of multiscale methods assemble atomistic and continuum scales together in order to take advantage of both approaches. Continuum is the most traditional and common scale that is analytically and computationally investigated in depth. It assumes that matter completely fills the space it occupies, is continuously distributed, and is infinitely divisible into very small pieces. Owing to the extensive research, continuum theories are well established and thus robust, highly efficient, and accurate; however, they usually fail at the atomistic scale for several reasons. To start with, they ignore the inherent discrete structure of the material, particles such as atoms and electrons. Therefore, continuum approaches leave the physical underpinning of their theory weak [1]. Another reason is the fact that different physical phenomena are in play at each scale; for example, quantum effects are not considered at larger scales but they must be accounted for at the nanoscale [2]. A third reason is because the continuum does not allow the material length to vanish to zero; such as at a crack opening [3]. In rare cases where continuum methods are able to handle the

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physical phenomena at the atomistic scale, they lack the precision that the atomistic methods are ready to offer. Compared to continuum, atomistic methods are relatively new and require further exploration since their inherent discrete structure does not fit in the more traditional understanding. The most attractive feature of atomistic methods is their high accuracy. For example, the behavior of individual atoms in a friction event at the nanoscale can be tracked in profound detail [4]. In addition, atomistic approaches naturally achieve formation of cracks and other types of defects by breaking and rearrangement of bonds without any additional effort. In spite of these advantages, atomistic methods are computationally very expensive hence limited to small systems. For example, a typical aluminum grain consists of approximately 10^{13} atoms, which is much larger than the quantity of atoms a typical computer can handle [5]. For another example, Gracie et al. states that a representative volume element should have a volume of 1000 μm^3, which could be resolved by 8.6×10^{13} atoms assuming a lattice constant of 3.6 Å [6]. One of the largest scale simulations is conducted by Abraham et al. in 2002 that includes one billion atoms corresponding to a cube of only 0.3 μm side length [7]. The limitations of computational power is not only restricted to length scale but it is also true for the time scale. For instance, MD is available to only very high experimental strain rates, i.e., 10^6–10^9 s^{-1} [8].

The main purpose of developing a multiscale method is to systematically reduce the total number of degrees of freedom while preserving accuracy. This way simulations can be run in less time with less computational power. Furthermore, larger length and time scales, which are otherwise unfeasible, can be attained. Reduction in the total number of degrees of freedom is best guided with the following insight: only a small portion of atoms are actually interesting and the rest of the atoms are uninformative [9]. Fig. 1 shows a snapshot from a nanoindentation example where only 8% of the atoms that are physically relevant, hence interesting, are made visible. This particular figure best explains how the multiscale model should be constructed. While the informative atoms can be well investigated by highly accurate atomistic methods, the uninformative and much larger rest of the domain can be handled by efficient continuum methods. In that, the premise is that deformation is free from abrupt changes in the continuum region. This way the entire domain is spatially decomposed into atomistic and continuum regions.

The literature includes many multiscale methods each with its own advantages and disadvantages. Among these methods, the most prominent method is Quasicontinuum (QC) method as first introduced by Tadmot et al. [10]. QC method is essentially built upon two assumptions: Kinematic constraints and energy/force approximation [11–13]. In the former, only a small number of atoms, called representative atoms (rep-atoms), are appointed as degrees of freedom of the system and their positions are explicitly accounted for. Utilizing a mesh, positions of rest of the atoms are interpolated from positions of rep-atoms. The second assumption approximates energy/force by sampling energy/force of particular atoms and multiplying their values in proportion to the number of atoms they represent. The Bridging domain (BD) method couples two decomposed domains of different scales via another domain, called bridging domain, hence the name [14–16]. Two domains of different scales meet at an edge or region where the coupling imposes a displacement constraint in order to achieve compatibility between the two scales. The energy (or Hamiltonian) of the handshake region is a weighted sum of energies of fine and coarse scales. The constraint is imposed by using the augmented Lagrange multiplier method that includes the total energy of the system, the constraint, and a penalty term, which augments the constraint. In the Bridging Scale Method (BSM), the key idea is to divide displacement into orthogonal coarse and fine components [17–19]. The coarse scale components are only the FE displacements interpolated by the FE shape functions. The fine scale components are then the difference between the total displacements calculated by the MD simulation and coarse slace components and they are only required in the atomistic region. Two sets of equations of motion are then derived from the coarse and fine components of the displacement. In the coupling of coarse and fine scales, BSM introduces impedance and random forces as specialized boundary conditions on the atomistic region.

The literature also includes the Coupled Atomistic and Discrete Dislocation (CADD) that couples atomistics with linear elastic continuum [20,21]. A prominent feature of this method is to incorporate dislocations in continuum using the Discrete Dislocation (DD) method in order to reach even larger length scales. The Coupled Atomistic–Continuum (CAC) method combines full atomistic with a coarse-grained finite element framework [22,23]. In the method, crystalline materials are modeled as continuous collection of lattice cells with a group of discrete atoms inside and governing equations are derived with balance laws. The advantage of the method is its coarse grained model that let elements glide to represent dislocations in the continuum region. The Atomistic to Continuum (AtC) is a force-based concurrent multiscale method that combines atomistics and continuum [24,25] where atomistic (Virial) and continuum stresses (or equivalent forces) are blended over a handshake region. The compatibility is assured through the displacements in a weak sense. In their method, known as the Macroscopic Atomistic Ab initio Dynamics