



An atomistic-to-continuum molecular dynamics: Theory, algorithm, and applications

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Abstract

To study the connection between atomistic molecular dynamics and macroscale continuum mechanics, we partition the Lagrangian of first-principle molecular dynamics according to its length scales. By doing so, we discover a universal three-scale structure that is embedded in the conventional molecular dynamics formulation, which provides an intrinsic and seamless transition from microscale to macroscale. The multiscale micromorphic molecular dynamics (MMMD) is built on a novel micromorphic multiplicative decomposition that couples a fine scale atomistic dynamics, a mesoscale micromorphic dynamics, and a macroscale particle dynamics of continuum mechanics together in concurrent fashion.

In this work, we discuss the relationship between MMMD and nonlinear continuum mechanics, its computational algorithm, and how to use it to simulate phase transformation under non-equilibrium conditions.

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1. Introduction

The state-of-the-art computer and computation technologies have enabled Molecular Dynamics(MD) to simulate evolutions of atomistic material systems with billions of atoms up to a second time duration. The so-called exascale computing technology (e.g. [1]), which provides at least one exaflops 10^{18} s^{-1} computing speed, may soon allow us to carry out first-principle based molecular dynamics simulation of the material systems with size up to cubic micron and maybe even larger volume. With the new technology innovation, such as quantum computer, it is not a far-fetched idea that in a near future we shall soon be able to use Molecular Dynamics in engineering design and analysis for macroscale objects. For instance, we may soon have the computer power (speed and storage) that enable us using Molecular Dynamics to design semiconductor thin films, integrated circuits and silicon chips, smart phones, or even design aircraft turbine engine blades that are working under extreme conditions.

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This paper attempts to answer a fundamental and theoretical question: can we use the current form of the molecular dynamics to design a macroscale machine or a device component, say a turbine engine blade? The answer is negative! This is because when we design a turbine engine blade we do not (cannot) specify motions of every atom on the surface of the blade! Instead, we design engineering components under specific thermodynamic or statistical conditions, for instance under specific temperature, under given allowable stress or traction state—these are macroscale statistical quantities. One of the main technical challenges of using molecular dynamics in macroscale engineering design is how to apply macroscale boundary conditions to various molecular dynamics ensemble systems, e.g. [2–6]. It is noted that the macroscale mechanical boundary condition is not the fine scale molecular boundary condition for specific atoms at the boundary but the continuum scale boundary condition that we can measure by using macroscale engineering devices.

In fact, one of the focuses of current multiscale simulation research is how to correctly set up the multiscale boundary condition to couple the fine scale atomistic motion with the coarse scale continuum displacement field. In recent years, various multiscale boundary conditions have been proposed e.g. “handshaking condition”, or “non-reflection boundary condition”, e.g. [7–16] and among others. On the other hand, there have been many efforts to formulate multiscale coarse-grained molecular dynamics. Among them, [17–21] are probably most notable contributions. In particular, in a series work [22–24] Chen et al. proposed a multiscale micromorphic dynamics. In fact, the classical micromorphic continuum theory is also a multiscale theory e.g. [25].

Instead of designing a compatible multiscale interface boundary, in this work, we would like to re-exam the molecular dynamics system itself, which, we believed, has already contained an intrinsic multiscale structure. In early 1980s, Andersen [26] first repartitioned the conventional molecular dynamics Lagrangian, and proposed a multiscale isoenthalpic–isobaric ensemble of molecular dynamics (MD) allowing the volume of a cubic lattice cell to vary. Subsequently, Parrinello and Rahman [27,28] extended Andersen’s formalism to the anisotropic case allowing both the volume and the shape of a molecular dynamics (MD) cell to vary, which is in fact an early form of multiscale molecular dynamics. In recent years, there have been renewed interests in revising APR molecular dynamics, e.g. [29–34], which attempted to extend APR MD to non-equilibrium condition or to macroscale simulations.

In a recent work [35–37], by following the Andersen–Parrinello–Rahman approach, the present authors have repartitioned the Lagrangian of the first-principle atomistic molecular dynamics into different scales under the local equilibrium assumption; by doing so, we have discovered that there exists a universal micromorphic multiscale structure in atomistic molecular dynamics, which is an intrinsic mathematical structure of conventional molecular dynamics. The repartitioned first principle molecular dynamics Lagrangian yields three coupled particle dynamics at different scales. The MMMD method allows us: (1) Apply *macroscale boundary conditions* to finite-size molecular dynamics systems, which usually are in the non-equilibrium condition; (2) Calculate non-uniform and inhomogeneous distribution of macroscale field variables of the MD system under applied macroscale boundary conditions, and (3) Bridge microscale molecular dynamics with macroscale continuum mechanics.

In the present work, we are focusing on the following three fundamental and computational issues of MMMD. First by viewing MMMD as a multiscale dynamics from atomistic scale to continuum scale, we discuss what is the relation between MMMD and continuum mechanics. Second, we present a detailed and complete computational algorithms for MMMD, and we discuss the issues on how to implement it in computations. Third, we apply MMMD to simulate the structure phase transition of finite-size crystal systems under applied boundary loadings, which are essentially non-equilibrium boundary flux conditions.

The paper is arranged into five sections. In Section 2, a detailed multiscale partition of first-principle MD Lagrangian and the derivation of the multiscale micromorphic molecular dynamics (MMMD) are presented, in which we focus on the discussion of micromorphic multiplicative decomposition. In Section 3, we derive the dynamical equations of the multiscale micromorphic molecular dynamics (MMMD). In Section 4, a few numerical examples are presented to show how macroscale boundary is applied to simulate crystal structure phase transformation, which validates the proposed multiscale molecular dynamics. Finally, in Section 5, we close the presentation by making few remarks.

2. Multiscale partition of first-principle MD Lagrangian

We first partition the Lagrangian of first-principle molecular dynamics based on domain decomposition and multiscale kinematics of the atom motion.

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