

Generalized Mathematical Homogenization: From theory to practice

Aiqin Li, Renge Li, Jacob Fish*

Multiscale Science and Engineering Center, Rensselaer Polytechnic Institute, Troy, NY 12180, United States

Received 23 August 2007; received in revised form 27 November 2007; accepted 10 December 2007

Available online 23 December 2007

Abstract

A Generalized Mathematical Homogenization (GMH) theory for coupling atomistic and continuum descriptions at finite temperature has been extended to account for many-body potentials. GMH gives rise to the constitutive law-free coarse scale equations where coupled continuum thermo-mechanical equations are directly derived from molecular dynamics equations. An integrated computational approach, which seamlessly integrates ABAQUS for coarse scale (finite element method) computations with a molecular dynamics code, has been developed. The accuracy and efficiency of the method has been studied for crystal silicon structures including failure predictions of nanowires.

© 2007 Elsevier B.V. All rights reserved.

Keywords: Generalized Mathematical Homogenization; Constitutive law-free; Thermo-mechanical; Atomistic; Continuum

1. Introduction

Advances in nanosciences have already resulted in new engineering products including catalysts, strain resistant fabrics, sunscreens superior dental materials, printer inks, digital camera displays and high-capacity hard disks. It is anticipated [1] that nanotechnology will revolutionize the way we detect and treat disease, monitor and protect environment, produce and store energy, and build complex structures. Multiscale computational science and engineering has been identified (see page 14 in [1]) as one of the areas critical to future nanotechnology advances. The FY2004 \$3.7-billion-dollar National Nanotechnology Bill (page 14 in [1]) states that: “approaches that integrate more than one such technique (. . .molecular simulations, continuum-based models, etc.) will play an important role in this effort.”

From the computational point of view, the question is what is so unique in nanosystems that have not been successfully handled with existing computational methods? The answer to this question was eloquently articulated by Rudd and Broughton [2] who pointed out that nanosystems do not generally obey continuum principles because they are simply too small; continuum description does not account for predominant surface effects that would result in too stiff behavior. On the other hand, a brute force approach of modeling nanosystems entirely at atomistic scale would necessitate billions of unknowns and consideration of time scales on the order of 10^{-15} s. This suggests a multiscale computational paradigm where important atomistic features are captured at a fraction of computational cost required by atomistic simulation of the entire system.

Multiscale modeling and simulation methods that couple atomistic simulations with continuum description have attracted significant attention and shown great promise with thousands of technical articles published over the past decade. We will not attempt to survey this huge body of literature (see [3–8] for comprehensive survey), but rather pinpoint the unique place of the present manuscript in this larger body of literature.

* Corresponding author. Tel.: +1 518 276 6191.

E-mail address: fishj@rpi.edu (J. Fish).

The method discussed in this manuscript belongs to the category of *information-passing* (sometimes referred to as hierarchical or sequential) methods which evolve a coarse scale (continuum) model by advancing a sequence of fine scale (atomistic) models in small windows (representative volume or unit cell) placed at the Gauss points of the discretized coarse model. The manuscript focuses on the Generalized Mathematical Homogenization (GMH) approach ([9–11]), which is a generalization of a well-known asymptotic homogenization approach (see for instance [12–14]). GMH differs from other information-passing approaches (such as for instance HMM [15]) in that the coarse scale equations are *derived* directly from atomistics without postulating any *a priori* assumptions about their mathematical structure.

The present manuscript extends the previous work on GMH (see [10,11]) in the following two respects: (i) the theory is generalized to account for many-body potentials and (ii) a new computational framework is developed, which seamlessly integrates commercial finite element code of choice with any molecular dynamics code.

The manuscript is organized as follows. The governing MD equations, their rescaling and a multiple space-time asymptotic expansion are introduced in Section 2. The extension of the Generalized Mathematical Homogenization (GMH) to multi-body potentials is detailed in Section 3. Computational aspects of GMH including seamless integration in ABAQUS are discussed in Section 4. Numerical examples including thermo-mechanical response of crystal silicon structures and failure studies of nanowires are presented in Section 5. Conclusion and future research directions conclude the manuscript.

2. Governing equations

2.1. Molecular dynamics equation of motion

In our previous work [11], we derived thermo-mechanical continuum equations from molecular dynamics (MD) equations using the Generalized Mathematical Homogenization (GMH) considering pairwise potential, which is generally inadequate for solids. In the present manuscript, GMH is extended to many-body potentials.

The energy associated with atom i can be written as a sum of energies arising from the pairwise Φ and many-body V terms

$$E_i = \frac{1}{2} \sum_{j \neq i} \Phi(\mathbf{x}_{ij}) + \sum_{(i, n_1, n_2, \dots, n_k)} V(\underbrace{\mathbf{x}_{in_1}, \mathbf{x}_{in_2}, \dots, \mathbf{x}_{in_k}, \mathbf{x}_{n_1 n_2}, \dots}_{k(k+1)/2}), \quad (1)$$

where $\mathbf{x}_{ij} = \mathbf{x}_j - \mathbf{x}_i$ is a vector separating atoms i and j . Hereafter, Roman subscripts i and j are reserved for atoms labels and will not be subject to summation convention. The many-body potentials term V is a function of $k(k+1)/2$ variables. Let the interacting neighboring atoms of atom i be denoted by $n_1, n_2, \dots, n_p, \dots, n_k$, where k is the number of the interacting atoms.

The interatomic force acting on atom i by its neighbors is evaluated as

$$\mathbf{f}_i = -\frac{\partial E_i}{\partial \mathbf{x}_i}.$$

The equation of motion for atom i can be written as

$$m_i \ddot{\mathbf{u}}_i = \mathbf{f}_i = \sum_{j \neq i} \mathbf{f}_{ij}(\mathbf{x}_{ij}) + \sum_{(i, n_1, n_2, \dots, n_k)} \mathbf{S}(\mathbf{x}_{in_1}, \mathbf{x}_{in_2}, \dots, \mathbf{x}_{in_k}, \mathbf{x}_{n_1 n_2}, \dots), \quad (2)$$

where m_i is the mass of atom i ; $\dot{\mathbf{u}}_i = d\mathbf{u}_i/dt$ represents material time derivative of \mathbf{u}_i ; \mathbf{f}_{ij} is a force exerted on atom i by atom j resulting from the pairwise potential Φ and \mathbf{S} is the corresponding force resulting from the many-body potential V . For simplicity, external forces are not considered.

Due to periodic atomistic microstructure, the mass of atom m_i and the interatomic force \mathbf{f}_i are assumed to be periodic functions. Attention is restricted to the case where the wavelength of the traveling signal λ is much larger than the size of the unit cell l , i.e., $l/\lambda \ll 1$.

2.2. Multiple spatio-temporal scales, asymptotic expansions and rescaling of molecular dynamics equations

Due to the rapidly varying interatomic potentials, two distinct *material* coordinates are employed to describe the heterogeneity at the atomistic level: (i) the continuum or coarse scale denoted by \mathbf{X} , at which the atomistic features are invisible and (ii) the atomistic or fine scale, denoted by \mathbf{Y} . The two-scales are related by

$$\mathbf{Y} = \mathbf{X}/\varepsilon, \quad 0 < \varepsilon \ll 1. \quad (3)$$

Download English Version:

<https://daneshyari.com/en/article/499439>

Download Persian Version:

<https://daneshyari.com/article/499439>

[Daneshyari.com](https://daneshyari.com)