Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 306 (2016) 452–478
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

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

Shaofan Li[a,*], Shingo Urata[a,b]

[a] *Department of Civil and Environmental Engineering, University of California, Berkeley, CA 94720, USA*
[b] *Innovative Technology Research Center, Asahi Glass Co., Ltd., Yokohama-shi, Kanagawa 230-0045, Japan*

Received 29 December 2015; received in revised form 4 March 2016; accepted 30 March 2016
Available online 13 April 2016

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.
© 2016 Elsevier B.V. All rights reserved.

Keywords: Continuum mechanics; Molecular dynamics; Multiscale simulation; Non-equilibrium molecular dynamics; Phase transition

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.

* Corresponding author.
E-mail address: shaofan@berkeley.edu (S. Li).

http://dx.doi.org/10.1016/j.cma.2016.03.048
0045-7825/© 2016 Elsevier B.V. All rights reserved.