Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 295 (2015) 510–524
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

# A multiscale molecular dynamics method for isothermal dynamic problems using the seamless heterogeneous multiscale method

Manfred H. Ulz

*Institute for Strength of Materials, Graz University of Technology, Kopernikusgasse 24/I, 8010 Graz, Austria*

Received 29 November 2014; received in revised form 11 June 2015; accepted 17 July 2015
Available online 26 July 2015

## Highlights

- We derive the EOM of a multiscale molecular dynamics in a bottom-up approach.
- The model is applicable for isothermal dynamical problems and couples FE and MD.
- We use the seamless HMM to efficiently couple the coarse and the fine scale.
- Dynamical problems (intractable by full MD) are investigated for about a millisecond.

## Abstract

Based on recent developments in Parrinello–Rahman molecular dynamics a hierarchical two-scale molecular dynamics framework is derived that couples a coarse scale local particle dynamics with a fine scale molecular dynamics. This multiscale structure provides a seamless transition from the atomistic to continuum scale for an isothermal problem. The molecular dynamics cells at the fine scale are constrained by the deformation and temperature of the coarse scale grid and supply the coarse scale with the constitutive behaviour of the material computed directly from atomistics. Furthermore, the seamless heterogeneous multiscale method is employed to efficiently perform the time integration by solving the coarse and fine scale equations of motion simultaneously with independent clocks. Numerical examples demonstrate the performance of the proposed multiscale scheme.


*Keywords:* Multiscale; Atomistic; Continuum; Homogenisation; Seamless heterogeneous multiscale method; Generalized mathematical homogenisation

## 1. Introduction

Many phenomena in engineering problems are governed by several scales in space and time. Propagation of acoustic waves, developing microstructures, micro and nano electro-mechanical systems are just a few examples. A sound numerical description of such problems is of great importance for the development of engineering devices. Multiscale models are able to incorporate the physics of the involved scales in a suitable and efficient manner. In particular, two-scale methods employing a continuum-on-atomistic setting have recently become very popular. The information

*E-mail address:* manfred.ulz@tugraz.at.

http://dx.doi.org/10.1016/j.cma.2015.07.019
0045-7825/

exchange between these scales in a numerical simulation permits a classification into two groups: hierarchical (serial or information-passing) and concurrent (simultaneous) methods. In a concurrent coupling of scales, one or a few critical regions of the system are atomistically modelled (*e.g.* to resolve local defects or singularities) and are directly coupled with the surrounding continuum regions. In a hierarchical setting, a fine scale is introduced in the shape of a representative volume element (RVE) (*e.g.* to supply constitutive relations at the coarse scale by averaging over the fine scale) and locally coupled to the coarse scale at integration points.

The coupling of scales in a continuum-on-atomistic setting is extensively debated in the literature [1–5]. The quasi-continuum method [4,6] is one of the most successful models in concurrent coupling. It is based on standard finite elements and constitutive equations derived from atomistic interactions. Next to that, there are the bridging-domain method [7], the bridging-scale method [8,9] and the multiscale continuum field theory [10]. A good review about concurrent schemes is given in Ref. [4], further references are cited therein. The coarse-grained molecular dynamics (CGMD) [11–13] produces equations of motion for the nodal fields of a finite element model, which are derived from an underlying atomistic model at thermodynamic equilibrium. Furthermore, a connection of the micromorphic theory to an atomistic model was studied in the literature [14–16]. The atomistic field theory [17,18] is derived solely from an atomistic model and represents the material in terms of an atomistic field. Such coarse-grained methods are reviewed in a recent paper [19], further references are cited therein. The work documented in Refs. [20,21] developed an approach to embed atomistic physics into a continuum formulation for large scale systems. This was achieved by applying the Cauchy–Born rule [22] to the atomic scale and superposing perturbation displacements at each load increment to the fine scale. A coarse-grained molecular dynamics model [23] for solid systems based on the Mori–Zwanzig projection method is developed in the literature, while an atomistic–continuum coupled model for thermo-mechanics of materials in micro–nano scales is presented in Ref. [24]. A recent publication [25] gives a homogenisation procedure with an emphasis on thermal problems based on a uniform weighted residual approximation method. The so called perfectly matched multiscale simulation [26,27] is another interesting method, which was initially derived to reduce spurious phonon reflections at the multiscale interface. Next to that, a computational multiscale method to couple thermo-mechanical equations at the coarse scale with non-equilibrium molecular dynamics at the fine scale was developed in the literature [28–30].

The heterogeneous multiscale method (HMM) [31–37] is a general top-down approach to design multiscale algorithms. While this method is mainly used for concurrent coupling schemes in the literature, the proposed methodology also applies to a serial coupling. A bottom-up approach denotes the generalized mathematical homogenisation (GMH) method [38–40], which evolves a continuum model by advancing a sequence of fine scale atomistic models in representative volumes placed at the integration points of the discretised continuum model. A framework that combines the serial and concurrent coupling in the generalized mathematical homogenisation method was recently introduced [41].

The HMM is often used for the numerical solution of stiff and highly oscillatory dynamical systems with slow and fast variables [42]. The seamless HMM [43] is a modification to HMM and does not require a reconstruction of the fine scale simulation at each coarse scale time step. A very similar scheme [44] was recently proposed in the literature for dynamic problems by identifying multiple fine scale time steps with one coarse scale time step. The asynchronous coupling of an arbitrary number of models [45], with each model having its own time step size, was recently introduced. A related method is the flow averaging integrators [46], which first turns on the stiff part in the dynamical system over a small fine scale time step and then turns it off during a larger mesoscopic time step. Another variant is the variable step size HMM [47], which uses variable mesoscopic time steps dependent on a function. In Ref. [48] a reduction of simulation time is achieved by interpolating the results of the fine scale simulation over the spatial domain of the coarse scale solver. However, the literature is rather sparse in presenting numerical solutions to time-dependent continuum scale problems as the computational expenses are very high (with exceptions, *e.g.* Refs. [40,49]).

This paper develops a multiscale molecular dynamics (MD) framework suitable to solve time-dependent problems in continuum mechanics. The mechanical continuum equations are solely derived by a bottom-up approach yielding a constitutive-free coarse scale. The proposed scheme is similar in its derivation and results to GMH; however, this work is primarily based on Andersen–Parrinello–Rahman (APR) molecular dynamics [50,51] and recent work in this field [52–55]. Given the difference of being a top-down approach, a resemblance to HMM is recognised. Furthermore, the seamless HMM will be used in the present work to advance the fine scale simulation considerably. We focus our evaluation on two points. Firstly, the equations of motion of a multiscale molecular dynamics suitable for isothermal dynamical problems are derived and solved by the finite element method and MD. Secondly, macroscopic dynamical problems of elasticity intractable by full MD simulations are investigated for the duration of approximately