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Generalized mathematical homogenization of atomistic media at finite temperatures in three dimensions

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Abstract

We derive thermo-mechanical continuum equations from Molecular Dynamics (MD) equations using the Generalized Mathematical Homogenization (GMH) theory developed by the authors for 0 K applications. GMH constructs an array of atomistic unit cell problems coupled with a thermo-mechanical continuum problem. The unit cell problem derived is a molecular dynamics problem defined for the perturbation from the average atomistic displacements subjected to the deformation gradient and temperature extracted from the continuum problem. The coarse scale problem derived is a constitutive law-free continuum thermo-mechanical equation. Attention is restricted to heat transfer by lattice vibration (phonons). The method is verified on several model problems against the reference molecular dynamics solution.

Keywords: Multiscale; Homogenization; Bridging; Atomistic; Continuum

1. Introduction

Constructing thermo-mechanical equations of continuum has been a subject of significant interest in physics, material science and mechanics communities. There are numerous challenges and several major obstacles to overcome before such a link can be fully established. In this section, we outline some of the key difficulties, then briefly overview the state-of-the-art in the field and conclude with the subset of issues we address in the manuscript.

The first difficulty is conceptual in nature; it deals with the fact that physics describing continuum and fine scale phenomena is different. While continuum description of mechanical deformation can be explicitly derived from the atomistics and this at a certain extend, has been successfully demonstrated, the thermal part can be only accounted for phenomenologically in the form of heat transfer equation.

The second difficulty is associated with the formulation of the base fine-scale model required for developing phemenological heat transfer equations. The mechanism by which heat is transferred depends on material system. For instance, gases transfer heat by direct collisions between molecules; non-metallic solids such as ceramics transfer heat by lattice vibrations so that there is no net motion of the media as the energy propagates through. Such heat transfer is often described in terms of "phonons", quanta of lattice vibrations. Metals, on the other hand, have free electrons, which are not bound to any particular atom. As the electrons move, they undergo a series of collisions; the faster electrons (on the hot side of the solid) give off some of their energy to the slower electrons. Conduction through electron collision is more effective than through lattice vibration; this is why metals generally are better heat conductors than ceramic materials, which do not have many free electrons. This implies that for metals the base mathematical model that describes motion of atoms using Newton's laws does not contain sufficient information for developing a complete phemenological

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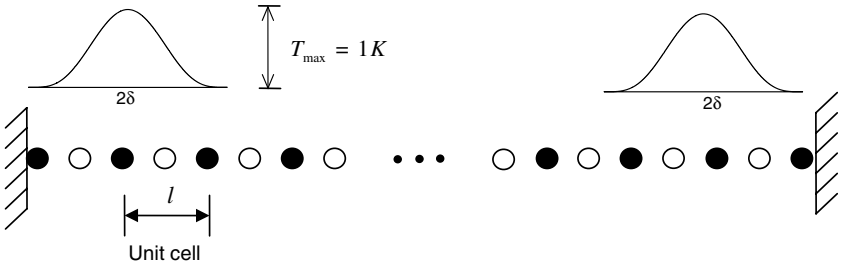

Fig. 1. An atomic chain and a unit cell.

model of heat transfer. Quantum mechanical considerations are unavoidable in this case.

The third difficulty is purely computational. Deterministic atomistic level computations, which solve numerically Newton's equations of motion, can model systems up to the order of 4×10^9 atoms for time scales of the order of nanoseconds [1], still orders of magnitude below continuum length and time scales, being of the order of millimeters and milliseconds. Continuum-level simulations operate in the latter regimes, but do so at the expense of explicit atomistic resolution. This difficulty can be partially circumvented by introducing an intermediate so-called coarse-grained model (or meso-scale model). The well-known examples of such a coarse-grained model are dislocation dynamics and coarse-grained molecular dynamics just to mention a few.

There have been numerous attempts to reconcile between fine scale and continuum thermo-mechanical descriptions. One of the most fundamental approaches is based on statistical mechanics, which converts atomistic data to macroscopic observables such as pressure, energy, heat capacities. In a somewhat related effort, Zhou [2] developed an equivalent deterministic thermo-mechanical continuum theory based on decomposing atomistic velocity into a structural deformation and thermal oscillation parts. A similar starting point has been employed by Li and Weinan [3] within the framework of the Heterogeneous Multiscale Method (HMM) [4]. The method consists of numerical solution of thermo-mechanical equations of continuum and finding the missing constitutive data (mechanical and thermal) by performing atomistic simulations subjected to local boundary conditions extracted from the continuum. An extension of the quasi-continuum method to finite temperature regime has been recently proposed in [5] by incorporating potential of mean force (PMF) originally introduced by Kirkwood in 1935 [6]. Several other noteworthy approaches originally developed for zero-temperature applications have been recently extended to finite temperatures. These include the Coupled Atomistics and Discrete Dislocation (CADD) method [7], the Bridging Scale Method [8] and the Bridging Domain Method [9].

This paper represents an initial effort aimed at deriving thermo-mechanical continuum equations using Generalized Mathematical Homogenization (GMH) theory originally developed by the authors for 0 K applications [10,11]. We only address a subset of aforementioned issues. Since the base model from which we derive continuum equations is molecular dynamics, only heat transfer due to lattice vibration (phonons) is accounted for. We do not introduce an intermediate (meso) scale (see Fig. 1), but rather focus on linking MD (describing motion of atoms or coarse-grained discrete medium) with thermo-mechanical continuum equations. The proposed multiscale approach is somewhat resembles HMM [4] with the main difference being that the coarse scale problem is derived directly from atomistics without making any *a priori* assumption about its mathematical structure. Numerical experiments are conducted to verify the multiscale formulation against the reference molecular dynamics solution.

2. Governing equations

2.1. Molecular dynamics equation of motion

We consider a periodic atomistic medium composed of N atoms. The initial position of atom i in the reference configuration is denoted by $\mathbf{X}_i$, $i = 1,2,\ldots,N$. The displacement of atom i with respect to the reference position is designated by $\mathbf{u}_i$. Upon deformation, the new position of atom i is $\mathbf{x}_i$, given by

$$\mathbf{x}_i = \mathbf{X}_i + \mathbf{u}_i, \quad \mathbf{u}_i = \mathbf{u}_i(\mathbf{X}_i, t). \tag{1}$$

The vector separating two atoms i and j in the reference configuration is given by

$$\mathbf{X}_{ij} = \mathbf{X}_j - \mathbf{X}_i. \tag{2}$$

The corresponding vector separating two atoms in the deformed configuration is

$$\mathbf{x}_{ij} = \mathbf{x}_j - \mathbf{x}_i = \mathbf{X}_{ij} + \mathbf{u}_j(\mathbf{X}_j, t) - \mathbf{u}_i(\mathbf{X}_i, t). \tag{3}$$

Hereafter the Roman subscripts i and j are reserved for atoms labels and will not be subject to summation convention. Spatial directions, for which summation convention over repeated indices is applied, will be denoted by Greek subscripts.

For simplicity, we focus our attention to pairwise potentials. However, the formulation can be extended to other potentials governing nonmetallic materials. For pairwise potentials, the interaction between atoms i and j is depicted by the interatomic potential $\Phi_{ij}(\mathbf{x}_{ij})$. The interatomic force $\mathbf{f}_{ij}$ applied on atom i by atom j is evaluated as

$$\mathbf{f}_{ij} = \frac{\partial \Phi_{ij}(x_{ij})}{\partial x_{ij}} \frac{\mathbf{x}_{ij}}{x_{ij}}, \tag{4}$$