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

Jacob Fish [*], Wen Chen, Renge Li

Rensselaer Polytechnic Institute, Troy, NY 12180, USA

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.
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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 phemenologically 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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[*] Corresponding author. Tel.: +1 518 276 6191; fax: +1 518 276 4833.
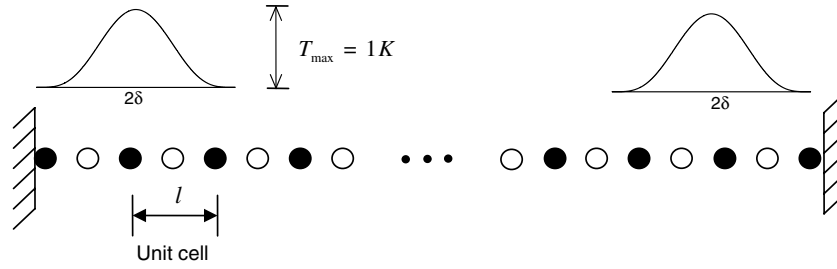 *E-mail address:* fishj@rpi.edu (J. Fish).

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

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

where $x_{ij} = |\mathbf{x}_{ij}|$ is the distance between atoms i and j; $\mathbf{x}_{ij}/x_{ij}$ is the unit vector in the direction of $\mathbf{x}_{ij}$.

The equation of motion for atom i can be written as

$$m_i \ddot{\mathbf{u}}_i = \sum_{j \neq i} \mathbf{f}_{ij}(\mathbf{x}_{ij}), \tag{5}$$

where m_i is the mass of atom i; $\dot{\mathbf{u}}_i = \mathrm{d}\mathbf{u}_i/\mathrm{d}t$ represents material time derivative of $\mathbf{u}_i$. The subscript j denotes the neighboring atoms which interact with atom i, such that $|\mathbf{x}_j - \mathbf{x}_i| < r_c$, with r_c being the cutoff radius. For simplicity, external forces are not considered.

Due to periodic atomistic microstructure, the mass of the atom m_i and the interatomic force $\mathbf{f}_{ij}$ are assumed to be periodic. 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., $\varepsilon = l/\lambda \ll 1$.

2.2. Multiple spatial and temporal scales and rescaling of the MD equations

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

$$\mathbf{Y} = \mathbf{X}/\varepsilon, \quad 0 < \varepsilon \ll 1. \tag{6}$$

The corresponding scales in the spatial coordinates are denoted by $\mathbf{x}$ and $\mathbf{y}$, respectively, and are related by $\mathbf{y} = \mathbf{x}/\varepsilon$.

In addition to the usual time scale, we introduce a fast time scale τ in order to model lattice vibration (phonons) at finite temperature. The fast time scale is related to the usual time scale by

$$\tau = t/\varepsilon, \quad 0 < \varepsilon \ll 1. \tag{7}$$

The resulting displacement field and its derivatives are functions of $\mathbf{X}$, $\mathbf{Y}$, t and τ. Prior to carrying out the multiple scale asymptotic analysis it is necessary *to rescale* the molecular dynamics Eq. (5) so that terms appearing in the equation would be of order one. We start by considering continuum equations of motion, $\rho_0 \ddot{\mathbf{u}}(\mathbf{X}, t) - \nabla_{\mathbf{X}} \cdot \mathbf{P} = 0$, where ρ_0 is the mass density; $\mathbf{P}$ is the first Piola–Kirchhoff stress tensor; $\nabla_{\mathbf{X}} \cdot \mathbf{P} = \mathrm{div}\mathbf{P}$ denotes the divergence of the stress tensor. For homogeneous media, stress derivatives are of order one, whereas for heterogeneous systems, certain components of stresses may be discontinuous, and therefore stress derivatives could be of $O(\varepsilon^{-1})$. Assuming $\rho_0 \sim O(1)$ and the characteristic size of the unit cell $l \sim O(\varepsilon)$ then the volume of the unit cell $\Theta \sim O(\varepsilon^3)$ and $m_i \sim \rho_0 \Theta \sim O(\varepsilon^3)$. Dividing (5) by the volume of the unit cell, yields

$$k_1 \rho_0 \ddot{\mathbf{u}}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) = \frac{1}{k_2 \varepsilon^3} \sum_{j \neq i} \mathbf{f}_{ij}(\mathbf{x}_{ij}), \tag{8}$$

where k_1 and k_2 are $O(1)$ constants. Comparing (8) with the continuum equation of motion it follows that

$$\mathbf{f}_{ij}(\mathbf{x}_{ij}) \sim O(\varepsilon^2). \tag{9}$$

To this end, we introduce the following normalized quantities:

$$\bar{m}_i = m_i/\varepsilon^3 \sim O(1), \quad \bar{\mathbf{f}}_{ij}(\mathbf{x}_{ij}) = \mathbf{f}_{ij}(\mathbf{x}_{ij})/\varepsilon^2 \sim O(1). \tag{10}$$

Due to periodicity of masses, we have $\bar{m}_i = \bar{m}_i(\mathbf{Y}_i)$. The Lagrangian description of the rescaled MD equations of motion is

$$\bar{m}_i(\mathbf{Y}_i) \ddot{\mathbf{u}}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) = \frac{1}{\varepsilon} \sum_{j \neq i} \bar{\mathbf{f}}_{ij}(\mathbf{x}_{ij}), \tag{11}$$

where $\mathbf{u}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) \sim O(1)$ in the stretched coordinate system $\mathbf{Y}$.

3. The generalized mathematical homogenization (GMH) theory

3.1. Multiple-scale asymptotic analysis

We assume that the coarse scale coordinate $\mathbf{X}$ takes continuous series of values and displacements $\mathbf{u}_j(\mathbf{X}_i, \mathbf{Y}_i, t, \tau)$ are continuous and differentiable in $\mathbf{X}$, while the fine scale coordinate $\mathbf{Y}$ is discrete. We denote the displacement of atom i by $\mathbf{u}(\mathbf{X}, \mathbf{Y}_i, t, \tau)$ with $\mathbf{X} = \mathbf{X}_i$. The displacements of the neighboring atoms $\mathbf{u}_j(\mathbf{X}_j, \mathbf{Y}_j, t, \tau)$ can be expanded using Taylor series around the point $\mathbf{X}$ as

$$\begin{aligned}
\mathbf{u}_j &= \mathbf{u}_j(\mathbf{X}_j, \mathbf{Y}_j, t, \tau) \\
&= \mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) + \nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) \cdot \mathbf{X}_{ij} \\
&\quad + \frac{1}{2}\nabla_{\mathbf{X}}\nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) : (\mathbf{X}_{ij} \otimes \mathbf{X}_{ij}) + \cdots,
\end{aligned} \tag{12}$$

where the dot denotes contraction and $\otimes$ designates dyadic or tensor product. In the indicial notation, the components of the gradient of the displacement field $\mathbf{u}$ with respect to the coarse scale reference configuration $\mathbf{X}$ are given as

$$[\nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau)]_{\alpha\beta} = \frac{\partial u_\alpha(\mathbf{X}, \mathbf{Y}_j, t, \tau)}{\partial X_\beta}. \tag{13}$$

From (12) we have

$$\begin{aligned}
\mathbf{u}_j - \mathbf{u}_i &= \mathbf{u}_j(\mathbf{X}_j, \mathbf{Y}_j, t, \tau) - \mathbf{u}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) \\
&= \mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) - \mathbf{u}(\mathbf{X}, \mathbf{Y}_i, t, \tau) + \nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) \cdot \mathbf{X}_{ij} \\
&\quad + \frac{1}{2}\nabla_{\mathbf{X}}\nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) : (\mathbf{X}_{ij} \otimes \mathbf{X}_{ij}) + \cdots
\end{aligned} \tag{14}$$

Since the coarse and fine scales coordinates are related by Eq. (6), we have

$$\mathbf{X}_{ij} = \varepsilon \mathbf{Y}_{ij} = \varepsilon(\mathbf{Y}_j - \mathbf{Y}_i), \tag{15}$$

where $\mathbf{Y}_{ij} \sim O(1)$. Substituting (15) into (14) yields

$$\begin{aligned}
\mathbf{u}_j - \mathbf{u}_i &= \mathbf{u}_j(\mathbf{X}_j, \mathbf{Y}_j, t, \tau) - \mathbf{u}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) \\
&= \mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) - \mathbf{u}(\mathbf{X}, \mathbf{Y}_i, t, \tau) + \varepsilon\nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) \cdot \mathbf{Y}_{ij} \\
&\quad + \frac{\varepsilon^2}{2}\nabla_{\mathbf{X}}\nabla_{\mathbf{X}}\mathbf{u}(\mathbf{X}, \mathbf{Y}_j, t, \tau) : (\mathbf{Y}_{ij} \otimes \mathbf{Y}_{ij}) + \cdots
\end{aligned} \tag{16}$$

A multiple scale asymptotic expansion is employed to approximate the displacement as:

$$\mathbf{u}(\mathbf{X}, \mathbf{Y}, t, \tau) = \mathbf{u}^0(\mathbf{X}, t) + \varepsilon \mathbf{u}^1(\mathbf{X}, \mathbf{Y}, t, \tau) + \cdots, \tag{17}$$

where as usual the leading order term $\mathbf{u}^0$ is assumed to be independent of the fine scale coordinates $\mathbf{Y}$ and τ; only the first two terms in the asymptotic expansion are considered whereas the remaining higher order terms are neglected.

Substituting the asymptotic expansion (17) into (16) yields

$$
\begin{aligned}
\mathbf{u}_j - \mathbf{u}_i &= \mathbf{u}_j(\mathbf{X}_j, \mathbf{Y}_j, t, \tau) - \mathbf{u}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) \\
&= \varepsilon[\mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau) - \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau) + \nabla_{\mathbf{X}} \mathbf{u}^0(\mathbf{X}, t) \cdot \mathbf{Y}_{ij}] \\
&\quad + \varepsilon^2 [\nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau) \cdot \mathbf{Y}_{ij} \\
&\quad + \frac{1}{2} \nabla_{\mathbf{X}} \nabla_{\mathbf{X}} \mathbf{u}^0(\mathbf{X}, t) : (\mathbf{Y}_{ij} \otimes \mathbf{Y}_{ij})] + \cdots
\end{aligned}
\tag{18}
$$

Inserting (15) and (18) into (3) yields

$$
\begin{aligned}
\mathbf{x}_{ij} &= \mathbf{X}_{ij} + \mathbf{u}_j - \mathbf{u}_i \\
&= \varepsilon \boldsymbol{\phi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) + \varepsilon^2 \boldsymbol{\psi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) + \cdots,
\end{aligned}
\tag{19}
$$

where

$$\boldsymbol{\phi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) = \mathbf{F}^0(\mathbf{X}, t) \cdot \mathbf{Y}_{ij} + \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau) - \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau),$$

$$\boldsymbol{\psi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) = \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau) \cdot \mathbf{Y}_{ij} + \frac{1}{2} \nabla_{\mathbf{X}} \nabla_{\mathbf{X}} \mathbf{u}^0(\mathbf{X}, t) : (\mathbf{Y}_{ij} \otimes \mathbf{Y}_{ij}) \tag{20}$$

with

$$\mathbf{F}^0(\mathbf{X}, t) = \mathbf{I} + \nabla_{\mathbf{X}} \mathbf{u}^0(\mathbf{X}, t) \tag{21}$$

being the deformation gradient and $\mathbf{I}$ the identity tensor.

Since $\boldsymbol{\phi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) \sim \mathrm{O}(1)$ and $\boldsymbol{\psi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) \sim \mathrm{O}(1)$, we have

$$\frac{\|\varepsilon^2 \boldsymbol{\psi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau)\|}{\|\varepsilon \boldsymbol{\phi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau)\|} \sim \mathrm{O}(\varepsilon), \tag{22}$$

where $\| \cdot \|$ denotes the vector norm. Following (22) the interatomic force field can be expanded as

$$
\begin{aligned}
\bar{\mathbf{f}}_{ij}(\mathbf{x}_{ij}) &= \bar{\mathbf{f}}_{ij}(\varepsilon \boldsymbol{\phi}_{ij} + \varepsilon^2 \boldsymbol{\psi}_{ij} + \cdots) \\
&= \bar{\mathbf{f}}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) + \frac{\partial \bar{\mathbf{f}}_{ij}}{\partial \hat{\boldsymbol{\phi}}_{ij}} \cdot (\varepsilon^2 \boldsymbol{\psi}_{ij} + \cdots) + \mathrm{O}(\varepsilon^2 \boldsymbol{\psi}_{ij} + \cdots),
\end{aligned}
\tag{23}
$$

where

$$\hat{\boldsymbol{\phi}}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau) = \varepsilon \boldsymbol{\phi}_{ij}(\mathbf{X}, \mathbf{Y}, t, \tau). \tag{24}$$

We further define the normalized gradient, $\bar{\mathbf{f}}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \sim \mathrm{O}(1)$, as

$$\bar{\mathbf{f}}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) = \frac{\partial \bar{\mathbf{f}}_{ij}(\varepsilon \boldsymbol{\phi}_{ij})}{\partial \boldsymbol{\phi}_{ij}} = \varepsilon \frac{\partial \bar{\mathbf{f}}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial \hat{\boldsymbol{\phi}}_{ij}}. \tag{25}$$

Eq. (23) can be rearranged as

$$\bar{\mathbf{f}}_{ij}(\mathbf{x}_{ij}) = \bar{\mathbf{f}}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) + \varepsilon \bar{\mathbf{f}}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot (\boldsymbol{\psi}_{ij} + \cdots) + \mathrm{O}(\varepsilon^2 \boldsymbol{\psi}_{ij} + \cdots). \tag{26}$$

Utilizing the chain rule, we have

$$
\begin{aligned}
\dot{\mathbf{u}}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) &= \dot{\mathbf{u}}(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) = \frac{\partial \mathbf{u}}{\partial t} + \varepsilon^{-1} \frac{\partial \mathbf{u}}{\partial \tau}, \\
\ddot{\mathbf{u}}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) &= \left(\frac{\partial}{\partial t} + \varepsilon^{-1} \frac{\partial}{\partial \tau} \right) \left(\frac{\partial \mathbf{u}}{\partial t} + \varepsilon^{-1} \frac{\partial \mathbf{u}}{\partial \tau} \right).
\end{aligned}
\tag{27}
$$

Inserting the asymptotic expansion (17) into (27) yields

$$\ddot{\mathbf{u}}_i(\mathbf{X}_i, \mathbf{Y}_i, t, \tau) = \varepsilon^{-1} \frac{\partial^2 \mathbf{u}^1}{\partial \tau^2} + \frac{\partial^2 \mathbf{u}^0}{\partial t^2} + 2 \frac{\partial^2 \mathbf{u}^1}{\partial t \partial \tau} + \varepsilon \frac{\partial^2 \mathbf{u}^1}{\partial t^2} + \mathrm{O}(\varepsilon^2). \tag{28}$$

Substituting (26) and (28) into the rescaled MD equations of motion (11) yields

$$
\begin{aligned}
&\bar{m}_i(\mathbf{Y}_i) \left[\varepsilon^{-1} \frac{\partial^2 \mathbf{u}^1}{\partial \tau^2} + \frac{\partial^2 \mathbf{u}^0}{\partial t^2} + 2 \frac{\partial^2 \mathbf{u}^1}{\partial t \partial \tau} + \varepsilon \frac{\partial^2 \mathbf{u}^1}{\partial t^2} + \mathrm{O}(\varepsilon^2) \right] \\
&= \frac{1}{\varepsilon} \sum_{j \neq i} [\bar{\mathbf{f}}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) + \varepsilon \bar{\mathbf{f}}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot (\boldsymbol{\psi}_{ij} + \cdots) + \mathrm{O}(\varepsilon^2 \boldsymbol{\psi}_{ij} + \cdots)].
\end{aligned}
\tag{29}
$$

Collecting terms of equal power of ε, gives the equilibrium equations at different orders starting at $\mathrm{O}(\varepsilon^{-1})$:

$$\mathrm{O}(\varepsilon^{-1}) : \bar{m}_i(\mathbf{Y}_i) \frac{\partial^2 \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)}{\partial \tau^2} = \sum_{j \neq i} \bar{\mathbf{f}}_{ij}(\hat{\boldsymbol{\phi}}_{ij}), \tag{30}$$

$$
\begin{aligned}
\mathrm{O}(\varepsilon^0) :\; &\bar{m}_i(\mathbf{Y}_i) \left[\frac{\partial^2 \mathbf{u}^0(\mathbf{X}, t)}{\partial t^2} + 2 \frac{\partial^2 \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)}{\partial t \partial \tau} \right] \\
&= \sum_{j \neq i} \left[\bar{\mathbf{f}}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \boldsymbol{\psi}_{ij} \right].
\end{aligned}
\tag{31}
$$

3.2. The dynamic atomistic unit cell problem

Consider the $\mathrm{O}(\varepsilon^{-1})$ equilibrium Eq. (30) first. Substituting the normalized mass and interatomic force (10) into (30) yields the dynamic atomistic unit cell problem

$$\boxed{m_i(\mathbf{Y}_i) \frac{\partial^2 \hat{\mathbf{u}}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)}{\partial \tau^2} = \varepsilon^2 \sum_{j \neq i} \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \quad \forall i}, \tag{32}$$

where

$$\hat{\mathbf{u}}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau) = \varepsilon \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau). \tag{33}$$

In the above $\mathbf{u}^1$ can be interpreted as a correction to the classical Cauchy–Born rule. Eq. (32) reflects the fact that when a macroscopically uniform deformation gradient is subjected onto the atomistic unit cell, the deformation field is generally non-uniform, i.e., an internal relaxation occurs and the corresponding inhomogeneous atomic displacements are determined by the equilibrium condition of each atom in the unit cell. Note that the atomistic unit cell problem (32), which describes the lattice vibration (phonons), depends on the fast time coordinate.

3.3. The coarse scale equations of motion

We proceed by considering $O(\varepsilon^0)$ equilibrium Eq. (31). Substituting the normalized mass and interatomic force (10) into (31) yields

$$m_i(\mathbf{Y}_i)\left[\frac{\partial^2 \mathbf{u}^0(\mathbf{X},t)}{\partial t^2} + 2\frac{\partial^2 \mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau)}{\partial t \partial \tau}\right] = \varepsilon \sum_{j\neq i}[\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}]. \tag{34}$$

Summing up Eq. (34) for all atoms in the unit cell and dividing the resulting equation by the volume of the unit cell Θ, yields

$$\frac{1}{\Theta}\sum_{i=1}^{n}\left\{m_i(\mathbf{Y}_i)\left[\frac{\partial^2 \mathbf{u}^0(\mathbf{X},t)}{\partial t^2} + 2\frac{\partial^2 \mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau)}{\partial t \partial \tau}\right]\right\}$$
$$= \frac{\varepsilon}{\Theta}\sum_{i=1}^{n}\sum_{j\neq i}[\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}]. \tag{35}$$

We further define the temporal averaging operator as

$$\langle\chi(\tau)\rangle = \frac{1}{\tau_0}\int_0^{\tau_0}\chi(\tau)\,\mathrm{d}\tau, \tag{36}$$

where τ_0 is a period of the function $\chi(\tau)$.

Applying the temporal averaging operator to (35), we have

$$\left\langle\frac{1}{\Theta}\sum_{i=1}^{n}\left[m_i(\mathbf{Y}_i)\frac{\partial^2 \mathbf{u}^0(\mathbf{X},t)}{\partial t^2}\right]\right\rangle$$
$$= \frac{\varepsilon}{\Theta}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}\left[\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}\right]\right\rangle, \tag{37}$$

where we accounted for the fact that the second term vanishes due to the periodicity in τ. Note that in (37) the term inside the temporal averaging operator on the left-hand-side is independent of the fast time τ and $\mathbf{u}^0(\mathbf{X},t)$ is constant in the atomistic unit cell; therefore, we have

$$\rho_0\frac{\partial^2 \mathbf{u}^0(\mathbf{X},t)}{\partial t^2} = \frac{\varepsilon}{\Theta}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}[\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}]\right\rangle, \tag{38}$$

where

$$\rho_0 = \frac{1}{\Theta}\sum_{i=1}^{n}m_i(\mathbf{Y}_i) \tag{39}$$

is the mass density. Exploiting the chain rule yields

$$\nabla_\mathbf{X}\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) = \frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial \boldsymbol{\phi}_{ij}}\cdot\frac{\partial \boldsymbol{\phi}_{ij}}{\partial \mathbf{X}}$$
$$= \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot[\nabla_\mathbf{X}\nabla_\mathbf{X}\mathbf{u}^0(\mathbf{X},t)\cdot\mathbf{Y}_{ij} + \nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)$$
$$- \nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau)]. \tag{40}$$

From (20) and (40), we have

$$\mathbf{f}'_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\cdot\boldsymbol{\psi}_{ij} = \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot\left[\nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)\cdot\mathbf{Y}_{ij}\right.$$
$$\left.+ \frac{1}{2}\nabla_\mathbf{X}\nabla_\mathbf{X}\mathbf{u}^0(\mathbf{X},t):(\mathbf{Y}_{ij}\otimes\mathbf{Y}_{ij})\right]$$
$$= \frac{1}{2}\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot[2\nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)$$
$$+ \nabla_\mathbf{X}\nabla_\mathbf{X}\mathbf{u}^0(\mathbf{X},t)\cdot\mathbf{Y}_{ij}]\cdot\mathbf{Y}_{ij}$$
$$= \frac{1}{2}\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot[\nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)$$
$$- \nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau) + \nabla_\mathbf{X}\nabla_\mathbf{X}\mathbf{u}^0(\mathbf{X},t)\cdot\mathbf{Y}_{ij}]\cdot\mathbf{Y}_{ij}$$
$$+ \frac{1}{2}\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot[\nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)$$
$$+ \nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau)]\cdot\mathbf{Y}_{ij}$$
$$= \frac{1}{2}\nabla_\mathbf{X}\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\cdot\mathbf{Y}_{ij} + \frac{1}{2}\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot[\nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau)$$
$$+ \nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)]\cdot\mathbf{Y}_{ij}. \tag{41}$$

To proceed with the derivation, we will exploit the following relation

$$\nabla_\mathbf{X}\cdot(\mathbf{v}\otimes\mathbf{w}) = \mathbf{v}\nabla_\mathbf{X}\cdot\mathbf{w} + \nabla_\mathbf{X}\mathbf{v}\cdot\mathbf{w}, \tag{42}$$

where $\mathbf{v}$ and $\mathbf{w}$ are vectors; for the special case of $\mathbf{w}$ being independent of $\mathbf{X}$, we have

$$\nabla_\mathbf{X}\cdot(\mathbf{v}\otimes\mathbf{w}) = \nabla_\mathbf{X}\mathbf{v}\cdot\mathbf{w}. \tag{43}$$

In view of the relation (43), (41) can be written as

$$\mathbf{f}'_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\cdot\boldsymbol{\psi}_{ij} = \frac{1}{2}\nabla_\mathbf{X}\cdot[\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij}] + \frac{1}{2}\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})$$
$$\cdot\nabla_\mathbf{X}[\mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau) + \mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)]\cdot\mathbf{Y}_{ij}. \tag{44}$$

Substituting (44) into (38) yields

$$\rho_0\frac{\partial^2 \mathbf{u}^0(\mathbf{X},t)}{\partial t^2}$$
$$= \frac{1}{2\Theta}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}[\nabla_\mathbf{X}\cdot[\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{X}_{ij}]\right\rangle$$
$$+ \frac{\varepsilon}{2\Theta}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}\{\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij})\cdot\nabla_\mathbf{X}[\mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau) + \mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)]\cdot\mathbf{Y}_{ij}\}\right\rangle. \tag{45}$$

In the remaining of this section we show that the second term in (45) vanishes for a periodic atomistic medium. We start by recalling

$$\mathbf{x}_{ji} = \mathbf{x}_i - \mathbf{x}_j = \mathbf{X}_i - \mathbf{X}_j + \mathbf{u}_i - \mathbf{u}_j = -\mathbf{x}_{ij}$$
$$= \varepsilon\boldsymbol{\phi}_{ji}(\mathbf{X},\mathbf{Y},t,\tau) + \varepsilon^2\boldsymbol{\psi}_{ji}(\mathbf{X},\mathbf{Y},t,\tau) + \cdots, \tag{46}$$

where

$$\boldsymbol{\phi}_{ji}(\mathbf{X},\mathbf{Y},t,\tau) = -\boldsymbol{\phi}_{ij}(\mathbf{X},\mathbf{Y},t,\tau)$$
$$= \mathbf{F}^0(\mathbf{X},t)\cdot\mathbf{Y}_{ji} + \mathbf{u}^1(\mathbf{X},\mathbf{Y}_i,t,\tau) - \mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau), \tag{47}$$

$$\boldsymbol{\psi}_{ji}(\mathbf{X},\mathbf{Y},t,\tau) = -\boldsymbol{\psi}_{ij}(\mathbf{X},\mathbf{Y},t,\tau) = \nabla_\mathbf{X}\mathbf{u}^1(\mathbf{X},\mathbf{Y}_j,t,\tau)\cdot\mathbf{Y}_{ji}$$
$$- \frac{1}{2}\nabla_\mathbf{X}\nabla_\mathbf{X}\mathbf{u}^0(\mathbf{X},t):(\mathbf{Y}_{ji}\otimes\mathbf{Y}_{ji}). \tag{48}$$

The Newton's third law requires

$$\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij}) = -\mathbf{f}_{ji}(\hat{\boldsymbol{\phi}}_{ji}). \tag{49}$$

From (47) and (49) we have the following relation

$$\mathbf{f}'_{ij}(\varepsilon\boldsymbol{\phi}_{ij}) = \frac{\partial\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})}{\partial\boldsymbol{\phi}_{ij}} = -\frac{\partial\mathbf{f}_{ji}(\varepsilon\boldsymbol{\phi}_{ji})}{\partial\boldsymbol{\phi}_{ij}} = -\frac{\partial\mathbf{f}_{ji}(\varepsilon\boldsymbol{\phi}_{ji})}{\partial(-\boldsymbol{\phi}_{ji})}$$

$$= \frac{\partial\mathbf{f}_{ji}(\hat{\boldsymbol{\phi}}_{ji})}{\partial\boldsymbol{\phi}_{ji}} \equiv \mathbf{f}'_{ji}(\hat{\boldsymbol{\phi}}_{ji}). \tag{50}$$

Let the interacting neighbor atoms of atom i be denoted as $n_1, n_2, \ldots, n_p, \ldots, n_k$ where k is the number of the interacting atoms such that $|\mathbf{x}_{n_p} - \mathbf{x} + i| < r_c$, $p = 1, 2, \ldots, k$, with r_c being the cutoff radius. The following summation over the atomistic unit cell can be expanded as

$$\sum_{i=1}^{n}\sum_{j\neq i}\{\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau) + \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau)] \cdot \mathbf{Y}_{ij}\}$$

$$= \sum_{i=1}^{n}\{\mathbf{f}'_{in_1}(\hat{\boldsymbol{\phi}}_{in_1}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_{n_1})] \cdot (\mathbf{Y}_{n_1} - \mathbf{Y}_i)$$

$$+ \mathbf{f}'_{in_2}(\hat{\boldsymbol{\phi}}_{in_2}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_{n_2})] \cdot (\mathbf{Y}_{n_2} - \mathbf{Y}_i)$$

$$+ \mathbf{f}'_{in_3}(\hat{\boldsymbol{\phi}}_{in_3}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_{n_3})] \cdot (\mathbf{Y}_{n_3} - \mathbf{Y}_i) + \cdots$$

$$+ \mathbf{f}'_{in_p}(\hat{\boldsymbol{\phi}}_{in_p}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_{n_p})] \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i) + \cdots$$

$$+ \mathbf{f}'_{in_k}(\hat{\boldsymbol{\phi}}_{in_k}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_{n_k})] \cdot (\mathbf{Y}_{n_k} - \mathbf{Y}_i)\}. \tag{51}$$

The summation in (51) is carried out over all atoms in the unit cell. First, we consider the case that both atom i and any of its interacting neighboring atoms $n_p(p = 1, 2, \ldots, k)$ are in the unit cell. For each interacting atom pair (i, n_p), there are two terms in the summation (51) given by

$$\mathbf{f}'_{in_p}(\hat{\boldsymbol{\phi}}_{in_p}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_{n_p})] \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$+ \mathbf{f}'_{n_pi}(\hat{\boldsymbol{\phi}}_{n_pi}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_{n_p}) + \mathbf{u}^1(\mathbf{Y}_i)] \cdot (\mathbf{Y}_i - \mathbf{Y}_{n_p}) = 0$$

$$(p = 1, 2, \ldots, k). \tag{52}$$

The above identity follows from (50). If any of the interacting atom n_p lies outside the unit cell, by periodicity, the displacement and force vector of atom n_p take the same value as the corresponding atom in the unit cell and thus summation (52) holds.

In view of (51) and (52), we have

$$\sum_{i=1}^{n}\sum_{j\neq i}\{\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau) + \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau)] \cdot \mathbf{Y}_{ij}\} = 0. \tag{53}$$

Substituting (53) into (45) yields the macroscopic equations of motion

$$\boxed{\begin{aligned}&\rho_0 \frac{\partial^2\mathbf{u}^0(\mathbf{X}, t)}{\partial t^2} - \nabla_{\mathbf{X}} \cdot \langle\mathbf{P}\rangle = 0, \\ &\mathbf{P}(\mathbf{X}, t, \tau) = \frac{1}{2\Theta}\sum_{i=1}^{n}\sum_{j\neq i}[\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}],\end{aligned}} \tag{54}$$

where $\mathbf{P}(\mathbf{X}, t, \tau)$ is the First Piola–Kirchhoff stress tensor. It is similar to the virial stress except for the dynamic term, which is absent. The first equation of Eq. (54) is the Lagrangian description of the conservation of the linear momentum.

3.4. The thermal equation

The temperature is directly related to the kinetic energy of the system as follows

$$\mathcal{K} = \sum_{i=1}^{n}\frac{|\mathbf{p}_i|^2}{2m_i} = \frac{k_{\mathrm{B}}T}{2}nN_d, \tag{55}$$

where $\mathbf{p}_i$ is the total momentum of atom i and m_i is its mass; k_{B} is the Boltzmann constant and T is the temperature of the ensemble. According to the theorem of the equipartition of energy, each degree-of-freedom contributes $k_{\mathrm{B}}T/2$. For n atoms, each with N_d degrees-of-freedom, the kinetic energy is $nN_dk_{\mathrm{B}}T/2$.

The square of the momentum of an atom is

$$|\mathbf{p}_i|^2 = \mathbf{p}_i \cdot \mathbf{p}_i = m_i^2\dot{\mathbf{u}}_i \cdot \dot{\mathbf{u}}_i$$

$$= m_i^2\left(\frac{\partial\mathbf{u}_i}{\partial t} + \varepsilon^{-1}\frac{\partial\mathbf{u}_i}{\partial\tau}\right) \cdot \left(\frac{\partial\mathbf{u}_i}{\partial t} + \varepsilon^{-1}\frac{\partial\mathbf{u}_i}{\partial\tau}\right). \tag{56}$$

Inserting the asymptotic expansion (17) into (56) yields

$$|\mathbf{p}_i|^2 = m_i^2\left[\left(\frac{\partial\mathbf{u}_i^0}{\partial t} + \frac{\partial\mathbf{u}_i^1}{\partial\tau}\right) \cdot \left(\frac{\partial\mathbf{u}_i^0}{\partial t} + \frac{\partial\mathbf{u}_i^1}{\partial\tau}\right) + \mathrm{O}(\varepsilon)\right]. \tag{57}$$

Substituting (57) into (55) and neglecting terms of $\mathrm{O}(\varepsilon)$ and higher, we have

$$\sum_{i=1}^{n}\left[m_i\left(\frac{\partial\mathbf{u}_i^0}{\partial t} + \frac{\partial\mathbf{u}_i^1}{\partial\tau}\right) \cdot \left(\frac{\partial\mathbf{u}_i^0}{\partial t} + \frac{\partial\mathbf{u}_i^1}{\partial\tau}\right)\right] = nk_{\mathrm{B}}N_dT(\mathbf{X}, t, \tau), \tag{58}$$

where $\mathbf{u}_i^0 = \mathbf{u}_i^0(\mathbf{X}, t)$ and $\mathbf{u}_i^1 = \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)$.

From (58) follows

$$\frac{\partial}{\partial t}\left[\sum_{i=1}^{n}\left[m_i\left(\frac{\partial\mathbf{u}_i^0}{\partial t} + \frac{\partial\mathbf{u}_i^1}{\partial\tau}\right) \cdot \left(\frac{\partial\mathbf{u}_i^0}{\partial t} + \frac{\partial\mathbf{u}_i^1}{\partial\tau}\right)\right]\right] = nk_{\mathrm{B}}N_d\frac{\partial T}{\partial t} \tag{59}$$

and writing out gives

$$\sum_{i=1}^{n}m_i\left[\frac{\partial\mathbf{u}_i^0}{\partial t} \cdot \frac{\partial^2\mathbf{u}_i^0}{\partial t^2} + \frac{\partial\mathbf{u}_i^0}{\partial t} \cdot \frac{\partial^2\mathbf{u}_i^1}{\partial t\partial\tau} + \frac{\partial\mathbf{u}_i^1}{\partial\tau} \cdot \left(\frac{\partial^2\mathbf{u}_i^0}{\partial t^2} + \frac{\partial^2\mathbf{u}_i^1}{\partial t\partial\tau}\right)\right]$$

$$= \frac{nk_{\mathrm{B}}N_d}{2}\frac{\partial T}{\partial t}. \tag{60}$$

Multiplying both sides of (34) by $\partial\mathbf{u}_i^0/\partial t$ and summing up over all atoms in the unit cell yields

$$\sum_{i=1}^{n}\left[m_i(\mathbf{Y}_i)\frac{\partial\mathbf{u}_i^0}{\partial t} \cdot \left(\frac{\partial^2\mathbf{u}_i^0}{\partial t^2} + 2\frac{\partial^2\mathbf{u}_i^1}{\partial t\partial\tau}\right)\right]$$

$$= \varepsilon\sum_{i=1}^{n}\sum_{j\neq i}\left[\frac{\partial\mathbf{u}_i^0}{\partial t} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \boldsymbol{\psi}_{ij}\right]. \tag{61}$$

In view of (60), (61) can be written as

$$
\frac{nk_{\mathrm{B}}N_d}{2}\frac{\partial T}{\partial t}
$$
$$
+\sum_{i=1}^{n}\left[m_i(\mathbf{Y}_i)\left(\frac{\partial \mathbf{u}_i^0}{\partial t}\cdot\frac{\partial^2 \mathbf{u}_i^1}{\partial t\partial\tau}-\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\frac{\partial^2 \mathbf{u}_i^0}{\partial t^2}-\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\frac{\partial^2 \mathbf{u}_i^1}{\partial t\partial\tau}\right)\right]
$$
$$
=\varepsilon\sum_{i=1}^{n}\sum_{j\neq i}\left[\frac{\partial \mathbf{u}_i^0}{\partial t}\cdot\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}\right].
$$
(62)

Applying the temporal averaging operator to (62), we have

$$
\frac{nk_{\mathrm{B}}N_d}{2}\frac{\partial\langle T\rangle}{\partial t}-\left\langle\sum_{i=1}^{n}m_i(\mathbf{Y}_i)\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\frac{\partial^2 \mathbf{u}_i^1}{\partial t\partial\tau}\right\rangle
$$
$$
=\varepsilon\left\langle\sum_{i=1}^{n}\sum_{j\neq i}\left[\frac{\partial \mathbf{u}_i^0}{\partial t}\cdot\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}\right]\right\rangle,
$$
(63)

where we accounted for the fact that the second and third terms vanish due to periodicity in the fast time τ. Multiplying both sides of (34) by $\partial \mathbf{u}_i^1/\partial\tau$ and summing up over all atoms in the unit cell yields

$$
\sum_{i=1}^{n}\left[m_i(\mathbf{Y}_i)\left(\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\frac{\partial^2 \mathbf{u}_i^0}{\partial t^2}+2\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\frac{\partial^2 \mathbf{u}_i^1}{\partial t\partial\tau}\right)\right]
$$
$$
=\varepsilon\sum_{i=1}^{n}\left[\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\sum_{j\neq i}\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}\right].
$$
(64)

Applying the temporal averaging operator to the above equation and accounting for the fact that the first term vanish due to periodicity in the fast time τ gives

$$
\left\langle\sum_{i=1}^{n}m_i(\mathbf{Y}_i)\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\frac{\partial^2 \mathbf{u}_i^1}{\partial t\partial\tau}\right\rangle=\frac{\varepsilon}{2}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}\left[\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}\right]\right\rangle.
$$
(65)

Substituting (65) into (63) yields

$$
\frac{nk_{\mathrm{B}}N_d}{2}\frac{\partial\langle T\rangle}{\partial t}=\frac{\varepsilon}{2}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}\left[\left(2\frac{\partial \mathbf{u}_i^0}{\partial t}+\frac{\partial \mathbf{u}_i^1}{\partial\tau}\right)\cdot\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\boldsymbol{\psi}_{ij}\right]\right\rangle.
$$
(66)

From (41) and (53) follows

$$
\sum_{i=1}^{n}\sum_{j\neq i}\left[\left(2\frac{\partial \mathbf{u}_i^0}{\partial t}+\frac{\partial \mathbf{u}_i^1}{\partial\tau}\right)\cdot\mathbf{f}_{ij}'(\varepsilon\boldsymbol{\phi}_{ij})\cdot\boldsymbol{\psi}_{ij}\right]
$$
$$
=\sum_{i=1}^{n}\sum_{j\neq i}\left[\frac{\partial \mathbf{u}_i^0(\mathbf{X},t)}{\partial t}\cdot\nabla_{\mathbf{X}}\cdot(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij})\right]
$$
$$
+\frac{1}{2}\sum_{i=1}^{n}\sum_{j\neq i}\left\{\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot[\nabla_{\mathbf{X}}\cdot(\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\otimes\mathbf{Y}_{ij})\right.
$$
$$
\left.+\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\nabla_{\mathbf{X}}(\mathbf{u}^1(\mathbf{Y}_i)+\mathbf{u}^1(\mathbf{Y}_j))\cdot\mathbf{Y}_{ij}\right\}.
$$
(67)

Substituting (67) into (66) and dividing by the volume of the atomistic unit cell yields

$$
\frac{nk_{\mathrm{B}}N_d}{2\Theta}\frac{\partial\langle T\rangle}{\partial t}=\frac{\partial \mathbf{u}^0(\mathbf{X},t)}{\partial t}\cdot\left\langle\frac{1}{2\Theta}\sum_{i=1}^{n}\sum_{j\neq i}[\nabla_{\mathbf{X}}\cdot(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{X}_{ij})]\right\rangle
$$
$$
+\frac{\varepsilon}{4\Theta}\left\langle\sum_{i=1}^{n}\sum_{j\neq i}\left\{\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot[\nabla_{\mathbf{X}}\cdot(\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\otimes\mathbf{Y}_{ij})\right.\right.
$$
$$
\left.\left.+\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\nabla_{\mathbf{X}}(\mathbf{u}^1(\mathbf{Y}_i)+\mathbf{u}^1(\mathbf{Y}_j))\cdot\mathbf{Y}_{ij}]\right\}\right\rangle.
$$
(68)

The second term in (68) can also be recast as the divergence of a vector field. For this reason we utilize the following well-known relations (see [12,13]).

$$
\nabla_{\mathbf{X}}\cdot(\mathbf{S}^T\cdot\mathbf{v})=\mathbf{S}:\nabla_{\mathbf{X}}\mathbf{v}+\mathbf{v}\cdot\nabla_{\mathbf{X}}\cdot\mathbf{S},
$$
(69)
$$
\mathbf{S}\cdot\mathbf{v}=\mathbf{v}\cdot\mathbf{S}^T,
$$
(70)
$$
(\mathbf{u}\otimes\mathbf{v}):\mathbf{S}=\mathbf{u}\cdot\mathbf{S}\cdot\mathbf{v},
$$
(71)

where $\mathbf{S}$ is a second-order tensor; $\mathbf{u}$ and $\mathbf{v}$ are vectors; the superscript T denotes the transpose of a tensor; and $\mathbf{S}:\mathbf{U}=S_{ij}U_{ij}$.

Based on the chain rule, we have

$$
\frac{\partial \mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})}{\partial\tau}=\frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial\boldsymbol{\phi}_{ij}}\cdot\frac{\partial\boldsymbol{\phi}_{ij}}{\partial\tau}
$$
$$
=\mathbf{f}_{ij}'(\hat{\boldsymbol{\phi}}_{ij})\cdot\left[\frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial\tau}-\frac{\partial \mathbf{u}^1(\mathbf{Y}_i)}{\partial\tau}\right]
$$
(72)

and from (69) and (70) follows

$$
\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot\nabla_{\mathbf{X}}\cdot\left[\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\otimes\mathbf{Y}_{ij}\right]
$$
$$
=\nabla_{\mathbf{X}}\cdot\left[(\mathbf{Y}_{ij}\otimes\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij}))\cdot\frac{\partial \mathbf{u}_i^1}{\partial\tau}\right]-[\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij}]:\nabla_{\mathbf{X}}\frac{\partial \mathbf{u}_i^1}{\partial\tau}
$$
$$
=\nabla_{\mathbf{X}}\cdot\left[\frac{\partial \mathbf{u}_i^1}{\partial\tau}\cdot(\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\otimes\mathbf{Y}_{ij})\right]-[\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij}]:\nabla_{\mathbf{X}}\frac{\partial \mathbf{u}_i^1}{\partial\tau}.
$$
(73)

Differentiating $(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij}):\nabla_{\mathbf{X}}\mathbf{u}_i^1$ with respect to fast time gives

$$
\frac{\partial}{\partial\tau}[(\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\otimes\mathbf{Y}_{ij}):\nabla_{\mathbf{X}}\mathbf{u}_i^1]
$$
$$
=\left[\frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial\tau}\otimes\mathbf{Y}_{ij}\right]:\nabla_{\mathbf{X}}\mathbf{u}_i^1+[\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij}]:\nabla_{\mathbf{X}}\frac{\partial \mathbf{u}_i^1}{\partial\tau}.
$$
(74)

From (74) follows

$$
[\mathbf{f}_{ij}(\varepsilon\boldsymbol{\phi}_{ij})\otimes\mathbf{Y}_{ij}]:\nabla_{\mathbf{X}}\frac{\partial \mathbf{u}_i^1}{\partial\tau}
$$
$$
=\frac{\partial}{\partial\tau}\left[(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})\otimes\mathbf{Y}_{ij}):\nabla_{\mathbf{X}}\mathbf{u}_i^1\right]-\left[\frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial\tau}\otimes\mathbf{Y}_{ij}\right]:\nabla_{\mathbf{X}}\mathbf{u}_i^1.
$$
(75)

Substituting (75) into (73) yields

$$\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \nabla_{\mathbf{X}} \cdot [\mathbf{f}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \otimes \mathbf{Y}_{ij}]$$

$$= \nabla_{\mathbf{X}} \cdot \left[\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{Y}_{ij}) \right] - \frac{\partial}{\partial \tau} [(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{Y}_{ij}) : \nabla_{\mathbf{X}} \mathbf{u}_i^1]$$

$$+ \left[\frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial \tau} \otimes \mathbf{Y}_{ij} \right] : \nabla_{\mathbf{X}} \mathbf{u}_i^1. \tag{76}$$

From (76) follows

$$\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \{\nabla_{\mathbf{X}} \cdot [\mathbf{f}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \otimes \mathbf{Y}_{ij}] + \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_j)] \cdot \mathbf{Y}_{ij}\}$$

$$= \nabla_{\mathbf{X}} \cdot \left[\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot (\mathbf{f}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \otimes \mathbf{Y}_{ij}) \right] - \frac{\partial}{\partial \tau} [(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{Y}_{ij}) : \nabla_{\mathbf{X}} \mathbf{u}_i^1]$$

$$+ \left[\frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial \tau} \otimes \mathbf{Y}_{ij} \right] : \nabla_{\mathbf{X}} \mathbf{u}_i^1 + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i)$$

$$+ \mathbf{u}^1(\mathbf{Y}_j)] \cdot \mathbf{Y}_{ij}. \tag{77}$$

Based on (71) and (72), we have

$$\left[\frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial \tau} \otimes \mathbf{Y}_{ij} \right] : \nabla_{\mathbf{X}} \mathbf{u}_i^1 + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_j)] \cdot \mathbf{Y}_{ij}$$

$$= \frac{\partial \mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij} + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_j)] \cdot \mathbf{Y}_{ij}$$

$$= \left[\mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \left(\frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} - \frac{\partial \mathbf{u}^1(\mathbf{Y}_i)}{\partial \tau} \right) \right] \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij}$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_j)] \cdot \mathbf{Y}_{ij}$$

$$= \mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij} - \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_i)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij}$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_i) \cdot \mathbf{Y}_{ij} + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_j) \cdot \mathbf{Y}_{ij}$$

$$= \mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij} + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_j) \cdot \mathbf{Y}_{ij}. \tag{78}$$

Substituting (78) into (77) yields

$$\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \{\nabla_{\mathbf{X}} \cdot [\mathbf{f}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \otimes \mathbf{Y}_{ij}] + \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}[\mathbf{u}^1(\mathbf{Y}_i) + \mathbf{u}^1(\mathbf{Y}_j)] \cdot \mathbf{Y}_{ij}\}$$

$$= \nabla_{\mathbf{X}} \cdot \left[\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot (\mathbf{f}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \otimes \mathbf{Y}_{ij}) \right] - \frac{\partial}{\partial \tau} [(\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{Y}_{ij}) : \nabla_{\mathbf{X}} \mathbf{u}_i^1]$$

$$+ \mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij} + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_j) \cdot \mathbf{Y}_{ij}. \tag{79}$$

From (79) follows

$$\left\langle \sum_{i=1}^n \sum_{j \neq i} \left\{ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot [\nabla_{\mathbf{X}} \cdot (\mathbf{f}_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \otimes \mathbf{Y}_{ij}) + \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}}(\mathbf{u}^1(\mathbf{Y}_i) \right. \right.$$

$$\left. \left. + \mathbf{u}^1(\mathbf{Y}_j)) \cdot \mathbf{Y}_{ij}] \right\} \right\rangle = \nabla_{\mathbf{X}} \cdot \left\langle \sum_{i=1}^n \sum_{j \neq i} \left[\frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{Y}_{ij}) \right] \right\rangle$$

$$+ \left\langle \sum_{i=1}^n \sum_{j \neq i} \left[\mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij} \right. \right.$$

$$\left. \left. + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_j) \cdot \mathbf{Y}_{ij} \right] \right\rangle, \tag{80}$$

where we have made use of the fact that the temporal average of the second term on the right-hand-side of (79) vanishes due to periodicity in the fast time scale.

We proceed to prove that the second term in the right-hand-side of (80) vanishes. As in the previous section, we assume that for atom i, its interacting neighbor atoms are $n_1, n_2, \ldots, n_p, \ldots, n_k$ where k is the number of the interacting atoms such that $|\mathbf{x}_{n_p} - \mathbf{x}_i| < r_c$, $p = 1, 2, \ldots, k$. The following summation over the atomistic unit cell can be expanded as

$$\sum_{i=1}^n \sum_{j \neq i} \left[\mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot \mathbf{Y}_{ij} \right.$$

$$\left. + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_j) \cdot \mathbf{Y}_{ij} \right]$$

$$= \sum_{i=1}^n \left\{ \mathbf{f}'_{in_1}(\varepsilon \boldsymbol{\phi}_{in_1}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_{n_1})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot (\mathbf{Y}_{n_1} - \mathbf{Y}_i) \right.$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{in_1}(\hat{\boldsymbol{\phi}}_{in_1}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_{n_1}) \cdot (\mathbf{Y}_{n_1} - \mathbf{Y}_i)$$

$$+ \mathbf{f}'_{in_2}(\varepsilon \boldsymbol{\phi}_{in_2}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_{n_2})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot (\mathbf{Y}_{n_2} - \mathbf{Y}_i)$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{in_2}(\hat{\boldsymbol{\phi}}_{in_2}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_{n_2}) \cdot (\mathbf{Y}_{n_2} - \mathbf{Y}_i) + \cdots$$

$$+ \mathbf{f}'_{in_p}(\varepsilon \boldsymbol{\phi}_{in_p}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_{n_p})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{in_p}(\hat{\boldsymbol{\phi}}_{in_p}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_{n_p}) \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i) + \cdots$$

$$+ \mathbf{f}'_{in_k}(\hat{\boldsymbol{\phi}}_{in_k}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_{n_k})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot (\mathbf{Y}_{n_k} - \mathbf{Y}_i)$$

$$\left. + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{in_k}(\hat{\boldsymbol{\phi}}_{in_k}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_{n_k}) \cdot (\mathbf{Y}_{n_k} - \mathbf{Y}_i) \right\}. \tag{81}$$

The summation in (81) is carried out over all atoms in the unit cell. First, we consider the case that both atom i and any of its interacting neighboring atoms n_p ($p = 1, 2, \ldots, k$) are in the unit cell. For each interacting atom pair (i, n_p), there are two terms in the summation (81) given by

$$\mathbf{f}'_{in_p}(\varepsilon \boldsymbol{\phi}_{in_p}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_{n_p})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{in_p}(\hat{\boldsymbol{\phi}}_{in_p}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_{n_p}) \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$+ \mathbf{f}'_{n_p i}(\varepsilon \boldsymbol{\phi}_{n_p i}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_i)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_{n_p}^1 \cdot (\mathbf{Y}_i - \mathbf{Y}_{n_p})$$

$$+ \frac{\partial \mathbf{u}_{n_p}^1}{\partial \tau} \cdot \mathbf{f}'_{n_p i}(\hat{\boldsymbol{\phi}}_{n_p i}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_i) \cdot (\mathbf{Y}_i - \mathbf{Y}_{n_p})$$

$$= \mathbf{f}'_{in_p}(\varepsilon \boldsymbol{\phi}_{in_p}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_{n_p})}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_i^1 \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$+ \frac{\partial \mathbf{u}_i^1}{\partial \tau} \cdot \mathbf{f}'_{in_p}(\hat{\boldsymbol{\phi}}_{in_p}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_{n_p}) \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$- \mathbf{f}'_{in_p}(\varepsilon \boldsymbol{\phi}_{in_p}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_i)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}_{n_p}^1 \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i)$$

$$- \frac{\partial \mathbf{u}_{n_p}^1}{\partial \tau} \cdot \mathbf{f}'_{in_p}(\hat{\boldsymbol{\phi}}_{in_p}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_i) \cdot (\mathbf{Y}_{n_p} - \mathbf{Y}_i) = 0$$

$$(p = 1, 2, \ldots, k), \tag{82}$$

where we have exploited the identity $\mathbf{f}'_{in_p}(\varepsilon \boldsymbol{\phi}_{in_p}) = \mathbf{f}'_{n_p i}(\varepsilon \boldsymbol{\phi}_{n_p i})$ as proved in (50).

If any of the interacting neighbor atom n_p lies outside the unit cell, by periodicity, the displacement and force vector of atom n_p take the same value as the corresponding atom in the unit cell and thus summation in (82) also vanishes.

In view of (81) and (82) we have

$$\sum_{i=1}^{n} \sum_{j \neq i} [\mathbf{f}'_{ij}(\varepsilon \boldsymbol{\phi}_{ij}) \cdot \frac{\partial \mathbf{u}^1(\mathbf{Y}_j)}{\partial \tau} \cdot \nabla_{\mathbf{X}} \mathbf{u}^1_i \cdot \mathbf{Y}_{ij}$$
$$+ \frac{\partial \mathbf{u}^1_i}{\partial \tau} \cdot \mathbf{f}'_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \cdot \nabla_{\mathbf{X}} \mathbf{u}^1(\mathbf{Y}_j) \cdot \mathbf{Y}_{ij}] = 0. \tag{83}$$

Substituting (83) into (80) and then the resulting equation into (68) yields

$$\frac{n k_B N_d}{\Theta} \frac{\partial \langle T \rangle}{\partial t} = 2 \frac{\partial \mathbf{u}^0(\mathbf{X}, t)}{\partial t} \cdot \nabla_{\mathbf{X}} \cdot \left\langle \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} [\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}] \right\rangle$$
$$+ \nabla_{\mathbf{X}} \cdot \left\langle \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} \left[\frac{\partial \mathbf{u}^1_i}{\partial \tau} \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}) \right] \right\rangle. \tag{84}$$

We further define

$$C = n k_B N_d / \Theta \tag{85}$$

and make use of the macroscopic equations of motion (54) to obtain the thermal equation

$$\boxed{\begin{aligned} C \frac{\partial \langle T \rangle}{\partial t} - \nabla_{\mathbf{X}} \cdot \langle \mathbf{q}(\mathbf{X}, t, \tau) \rangle &= 2\rho_0 \frac{\partial \mathbf{u}^0(\mathbf{X}, t)}{\partial t} \cdot \frac{\partial^2 \mathbf{u}^0(\mathbf{X}, t)}{\partial t^2}, \\ \mathbf{q}(\mathbf{X}, t, \tau) &= \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} \left[\frac{\partial \mathbf{u}^1_i}{\partial \tau} \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}) \right], \end{aligned}} \tag{86}$$

where we identify $\mathbf{q}(\mathbf{X}, t, \tau)$ as the heat flux vector.

The thermal equation can be rewritten in an alternative form as follows. Recalling the tensor identities (69) and (70) we have

$$\nabla_{\mathbf{X}} \cdot (\mathbf{v} \cdot \mathbf{S}) = \mathbf{S} : \nabla_{\mathbf{X}} \mathbf{v} + \mathbf{v} \cdot \nabla_{\mathbf{X}} \cdot \mathbf{S}. \tag{87}$$

Utilizing (87) we may write

$$\nabla_{\mathbf{X}} \cdot \left(\frac{\partial \mathbf{u}^0}{\partial t} \cdot \langle \mathbf{P} \rangle \right) = \langle \mathbf{P} \rangle : \nabla_{\mathbf{X}} \frac{\partial \mathbf{u}^0}{\partial t} + \frac{\partial \mathbf{u}^0}{\partial t} \cdot \nabla_{\mathbf{X}} \cdot \langle \mathbf{P} \rangle \tag{88}$$

and thus

$$\frac{\partial \mathbf{u}^0}{\partial t} \cdot \nabla_{\mathbf{X}} \cdot \langle \mathbf{P} \rangle = \nabla_{\mathbf{X}} \cdot \left(\frac{\partial \mathbf{u}^0}{\partial t} \cdot \langle \mathbf{P} \rangle \right) - \langle \mathbf{P} \rangle : \nabla_{\mathbf{X}} \frac{\partial \mathbf{u}^0}{\partial t}. \tag{89}$$

Eq. (84) can be written as

$$C \frac{\partial \langle T \rangle}{\partial t} = 2 \frac{\partial \mathbf{u}^0}{\partial t} \cdot \nabla_{\mathbf{X}} \cdot t \langle \mathbf{P} \rangle + \nabla_{\mathbf{X}}$$
$$\cdot \left\langle \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} \left[\frac{\partial \mathbf{u}^1_i}{\partial \tau} \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}) \right] \right\rangle. \tag{90}$$

Inserting (89) into (90) yields

$$C \frac{\partial \langle T \rangle}{\partial t} = 2 \nabla_{\mathbf{X}} \cdot \left(\frac{\partial \mathbf{u}^0}{\partial t} \cdot \langle \mathbf{P} \rangle \right) - 2t \langle \mathbf{P} \rangle : \nabla_{\mathbf{X}} \frac{\partial \mathbf{u}^0}{\partial t}$$
$$+ \nabla_{\mathbf{X}} \cdot \left\langle \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} \left[\frac{\partial \mathbf{u}^1_i}{\partial \tau} \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}) \right] \right\rangle. \tag{91}$$

Making use of the expressions of the First Piola–Kirchhoff stress tensor, macroscopic deformation gradient and the macroscopic equation of motion, we have the following alternative form of the thermal equation

$$\boxed{\begin{aligned} C \frac{\partial \langle T \rangle}{\partial t} - \nabla_{\mathbf{X}} \cdot \langle \tilde{\mathbf{q}}(\mathbf{X}, t, \tau) \rangle &= -2 \langle \mathbf{P}(\mathbf{X}, t, \tau) \rangle : \frac{\partial \mathbf{F}^0}{\partial t}, \\ \tilde{\mathbf{q}}(\mathbf{X}, t, \tau) &= \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} \left[\left(2 \frac{\partial \mathbf{u}^0}{\partial t} + \frac{\partial \mathbf{u}^1_i}{\partial \tau} \right) \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}) \right], \end{aligned}} \tag{92}$$

where $\tilde{\mathbf{q}}(\mathbf{X}, t, \tau)$ is an alternative form of the heat flux vector; $\mathbf{P}(\mathbf{X}, t, \tau)$ is the First Piola–Kirchhoff stress tensor defined in (54). In both forms given in (86) and (92) the unknown field is the temporal average of temperature $\langle T \rangle$. In (92) we recognize the divergence term $\operatorname{div} \tilde{\mathbf{q}}(\mathbf{X}, t, \tau)$ and the work power $\langle \mathbf{P}(\mathbf{X}, t, \tau) \rangle : \partial \mathbf{F}^0 / \partial t$. Note that all quantities appear as time averages and the temporal derivative of $\langle T \rangle$ and F^0 is with respect to the slow time scale t. Numerical experiments reveal that (86) is numerically more stable than (92). For the purpose of numerical verification we adopt the form of the thermal equation given in (86).

4. Finite element implementation and numerical verification

In this Section, we provide implementation details and give some preliminary verification results.

The two-scale problems described by (32), (54) and (86) is solved as follows:

With the initial conditions, for every Gauss point in the coarse scale, calculate the coarse scale deformation gradient $\mathbf{F}^0(\mathbf{X}, t)$; solve the dynamic unit cell problem for $\hat{\mathbf{u}}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)$ using (32); compute the fast temporal average of the First Piola–Kirchhoff stress tensor and heat flux vector using (54b) and (86b), respectively.

Solve the coarse scale problems (54a) and (86a) with appropriate initial and boundary conditions) using finite element semidiscretization in space and explicit time integration; evaluate the coarse scale deformation gradient $\mathbf{F}^0(\mathbf{X}, t)$ and go to I.

4.1. Weak forms and semidiscretization of the macroscopic thermal-mechanical equations

The initial and boundary conditions for the macroscopic equations of motion (54) are chosen as

$$\mathbf{u}^0(\mathbf{X}, 0) = \mathbf{p}(\mathbf{X}), \quad \frac{\partial \mathbf{u}^0}{\partial t}(\mathbf{X}, 0) = \mathbf{g}(\mathbf{X}), \tag{93}$$

$$\mathbf{u}^0(\mathbf{X}, t) = \bar{\mathbf{u}}(\mathbf{X}, t) \text{ on } \Gamma_u; \quad t \langle \mathbf{P} \rangle \cdot \mathbf{n} = \bar{t} \text{ on } \Gamma_t \tag{94}$$

where $\bar{\mathbf{u}}(\mathbf{X}, t)$ and $\bar{t}$ are vectors of prescribed displacement and traction, respectively; $\Gamma_u \cap \Gamma_t = \emptyset$, $\Gamma_u \cup \Gamma_t = \Gamma$ is the boundary of the domain under consideration; $\mathbf{n}$ is the outward norm of the boundary.

The initial and boundary conditions for the macroscopic thermal Eq. (86) are chosen as

$$\langle T \rangle(\mathbf{X}, 0) = \langle T_0 \rangle(\mathbf{X}) \tag{95}$$

$$\langle T \rangle(\mathbf{X}, t) = \overline{T}(\mathbf{X}, t) \text{ on } \Gamma_T; \quad \langle \mathbf{q} \rangle \cdot \mathbf{n} = \bar{q}(\mathbf{X}, t) \text{ on } \Gamma_q \tag{96}$$

where $\overline{T}(\mathbf{X}, t)$ and $\bar{q}(\mathbf{X}, t)$ are the prescribed temperature and boundary heat flux, respectively; $\Gamma_T \cap \Gamma_q = \emptyset$, $\Gamma_T \cup \Gamma_q = \Gamma$.

The weak form of the thermo-mechanical equation is stated as follows:

For $t \in (0, T^{\text{in}}]$, find $\mathbf{u}^0(\mathbf{X}, t) \in \mathscr{U}_t^d$, $\langle T \rangle(\mathbf{X}, t) \in \mathscr{U}_t^\theta$, such that for all $\mathbf{w}^d(\mathbf{X}) \in \mathscr{V}^d$, $w^\theta(\mathbf{X}) \in \mathscr{V}^\theta$ the following holds:

$$\int_\Omega \rho_0 \mathbf{w}^d(\mathbf{X}) \cdot \frac{\partial^2 \mathbf{u}^0(\mathbf{X}, t)}{\partial t^2} \, d\Omega - \int_\Omega \mathbf{w}^d(\mathbf{X}) \cdot \nabla_\mathbf{X} \cdot \langle \mathbf{P} \rangle \, d\Omega = 0, \tag{97}$$

$$\int_\Omega C w^\theta(\mathbf{X}) \frac{\partial \langle T \rangle}{\partial t} \, d\Omega - \int_\Omega w^\theta(\mathbf{X}) \nabla_\mathbf{X} \cdot \langle \mathbf{q} \rangle \, d\Omega$$
$$= 2\rho_0 \int_\Omega w^\theta(\mathbf{X}) \frac{\partial \mathbf{u}^0}{\partial t} \cdot \frac{\partial^2 \mathbf{u}^0}{\partial t^2} \, d\Omega \tag{98}$$

subjected to the initial conditions (93) and (95), where

$$\mathscr{U}_t^d = \{\mathbf{u}^0(\mathbf{X}, t) | \mathbf{u}^0(\mathbf{X}, t) \in H^1(\Omega), \mathbf{u}^0(\mathbf{X}, t) = \bar{\mathbf{u}}(\mathbf{X}, t) \text{ on } \Gamma_u\}, \tag{99}$$

$$\mathscr{U}_t^\theta = \{\langle T \rangle(\mathbf{X}, t) | \langle T \rangle(\mathbf{X}, t) \in H^1(\Omega), \langle T \rangle(\mathbf{X}, t) = \overline{T}(\mathbf{X}, t) \text{ on } \Gamma_T\} \tag{100}$$

are the trial solution spaces, and

$$\mathscr{V}^d = \{\mathbf{w}(\mathbf{X}) | \mathbf{w}(\mathbf{X}) \in H^1(\Omega), \mathbf{w}(\mathbf{X}) = \mathbf{0} \text{ on } \Gamma_u\}, \tag{101}$$

$$\mathscr{V}^\theta = \{w(\mathbf{X}) | w(\mathbf{X}) \in H^1(\Omega), w(\mathbf{X}) = 0 \text{ on } \Gamma_T\} \tag{102}$$

are the weight function spaces. The Sobolev space $H^1(\Omega)$ consists of all functions over domain Ω whose values and their first derivatives are square integrable.

Exploiting the relations

$$\mathbf{w}^d(\mathbf{X}) \cdot \nabla_\mathbf{X} \cdot \langle \mathbf{P} \rangle = \nabla_\mathbf{X} \cdot (\mathbf{w}^d(\mathbf{X}) \cdot \langle \mathbf{P} \rangle) - \langle \mathbf{P} \rangle : \nabla_\mathbf{X} \mathbf{w}^d(\mathbf{X}), \tag{103}$$

$$w^\theta(\mathbf{X}) \nabla_\mathbf{X} \cdot \langle \mathbf{q} \rangle = \nabla_\mathbf{X} \cdot (w^\theta(\mathbf{X}) \langle \mathbf{q} \rangle) - \langle \mathbf{q} \rangle \cdot \nabla_\mathbf{X} w^\theta(\mathbf{X}) \tag{104}$$

we have from (97), (98), (103) and (104) by making use of the divergence theorem and the boundary conditions (94) and (96)

$$\int_\Omega \rho_0 \mathbf{w}^d(\mathbf{X}) \cdot \frac{\partial^2 \mathbf{u}^0(\mathbf{X}, t)}{\partial t^2} \, d\Omega + \int_\Omega \langle \mathbf{P} \rangle : \nabla_\mathbf{X} \mathbf{w}^d(\mathbf{X}) \, d\Omega = \int_{\Gamma_t} \mathbf{w}^d(\mathbf{X}) \cdot \bar{t} \, d\Gamma, \tag{105}$$

$$\int_\Omega C w^\theta(\mathbf{X}) \frac{\partial \langle T \rangle}{\partial t} \, d\Omega + \int_\Omega \langle \mathbf{q} \rangle \cdot \nabla_\mathbf{X} w^\theta(\mathbf{X}) \, d\Omega$$
$$= \int_{\Gamma_q} w^\theta(\mathbf{X}) \bar{q}(\mathbf{X}, t) \, d\Gamma + 2\rho_0 \int_\Omega w^\theta(\mathbf{X}) \frac{\partial \mathbf{u}^0}{\partial t} \cdot \frac{\partial^2 \mathbf{u}^0}{\partial t^2} \, d\Omega. \tag{106}$$

After introducing the finite element discretization in space, we have the following semidiscrete thermo-mechanical equations

$$\mathbf{M} \frac{\partial^2 \mathbf{d}(t)}{\partial t^2} + \mathbf{f}^{\text{in}}(\mathbf{d}(t)) = \mathbf{f}^{\text{ex}}(t), \tag{107}$$

$$\mathbf{C} \frac{\partial \boldsymbol{\theta}(t)}{\partial t} + \mathbf{Q}^{\text{in}}(\boldsymbol{\theta}(t)) = \mathbf{S}(t) \tag{108}$$

with the initial conditions

$$\mathbf{d}(0) = \mathbf{d}_0, \quad \frac{\partial \mathbf{d}}{\partial t}(0) = \mathbf{v}_0, \quad \boldsymbol{\theta}(0) = \boldsymbol{\theta}_0, \tag{109}$$

where $\mathbf{d}(t)$ and $\boldsymbol{\theta}(t)$ are vectors of nodal displacements and temperatures, respectively;

$$\mathbf{M} \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \left(\int_{\Omega_e} \rho_0 \mathbf{N}_d^{eT} \mathbf{N}_d^e \, d\Omega_e \right) \mathscr{L}^e,$$

$$\mathbf{C} = \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \left(\int_{\Omega_e} C \mathbf{N}_\theta^{eT} \mathbf{N}_\theta^e \, d\Omega_e \right) \mathscr{L}^e \tag{110}$$

are the mass and capacity matrices, respectively; $\mathscr{L}_e$ is the scatter operator relating element and global solution vectors.

$$\mathbf{f}^{\text{in}}(\mathbf{d}(t)) = \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \int_{\Omega_e} \mathbf{B}_d^{eT} \langle \mathbf{P} \rangle \, d\Omega_e,$$

$$\mathbf{Q}^{\text{in}}(\boldsymbol{\theta}(t)) = \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \int_{\Omega_e} \mathbf{B}_\theta^{eT} \langle \mathbf{q} \rangle \, d\Omega_e \tag{111}$$

are nodal internal force and heat flux vectors, respectively;

$$\mathbf{f}^{\text{ex}}(t) = \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \int_{\Gamma_t} \mathbf{N}_d^{eT} \bar{t} \, dS, \tag{112}$$

$$\mathbf{S}(t) = \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \int_{\Gamma_q} \mathbf{N}_\theta^{eT} \bar{q} \, d\Gamma + 2\rho_0 \sum_{e=1}^{\text{nel}} \mathscr{L}^{eT} \int_{\Omega_e} \mathbf{N}_\theta^{eT} \frac{\partial \mathbf{u}^0}{\partial t} \cdot \frac{\partial^2 \mathbf{u}^0}{\partial t^2} \, d\Omega_e \tag{113}$$

are nodal external force and heat source vectors, respectively; N_d^e and N_θ^e are matrices of finite element shape functions for displacements and temperatures, respectively; $B_{dA\alpha}^e = N_{dA,\alpha}^e$, $B_{\theta C\alpha}^e = N_{\theta C,\alpha}^e$ with A and C denoting finite element degrees-of-freedom and $\alpha = 1, 2, 3$ for 3D case (or $\alpha = 1, 2$ for 2D case); superscript e denoted finite element numbers. Since nodal internal force $\mathbf{f}^{\text{in}}(\mathbf{d}(t))$ and heat flux $\mathbf{Q}^{\text{in}}(\boldsymbol{\theta}(t))$ vectors depend on the displacement and temperature fields, the semidiscrete equation of motion and thermal equation are coupled.

The semidiscrete equations of motion (107) and the thermal Eq. (108) can be integrated using explicit time integration schemes, such as for instance the central difference and forward difference, respectively

$$\left(\frac{\partial^2 \mathbf{d}}{\partial t^2} \right)_n = (\mathbf{d}_{n-1} - 2\mathbf{d}_n + \mathbf{d}_{n+1})/\Delta t^2, \tag{114}$$

$$\left(\frac{\partial \boldsymbol{\theta}}{\partial t} \right)_n = (\boldsymbol{\theta}_{n+1} - \boldsymbol{\theta}_n)/\Delta t, \tag{115}$$

where $(\partial^2 \mathbf{d}/\partial t^2)_n = \partial^2 \mathbf{d}/\partial t^2(t)$, $\mathbf{d}_n = \mathbf{d}(t)$, $\mathbf{d}_{n-1} = \mathbf{d}(t - \Delta t)$, $\mathbf{d}_{n+1} = \mathbf{d}(t + \Delta t)$; $(\partial \boldsymbol{\theta}/\partial t)_n = \partial \boldsymbol{\theta}/\partial t(t)$, $\boldsymbol{\theta}_n = \boldsymbol{\theta}(t)$ and $\boldsymbol{\theta}_{n+1} = \boldsymbol{\theta}(t + \Delta t)$.

Inserting (114) and (115) into (107) and (108) yields

$$\mathbf{d}_{n+1} = 2\mathbf{d}_n - \mathbf{d}_{n-1} - \Delta t^2 \mathbf{M}^{-1}[\mathbf{f}^{\text{ex}}(t) - \mathbf{f}^{\text{in}}(\mathbf{d}_n)], \tag{116}$$

$$\boldsymbol{\theta}_{n+1} = \boldsymbol{\theta}_n + \Delta t \mathbf{C}^{-1}[\mathbf{S}_n - \mathbf{Q}^{\text{in}}(\boldsymbol{\theta}_n)]. \tag{117}$$

Similarly, the dynamic atomistic unit cell problem (32) is integrated in the fast time using the central difference scheme.
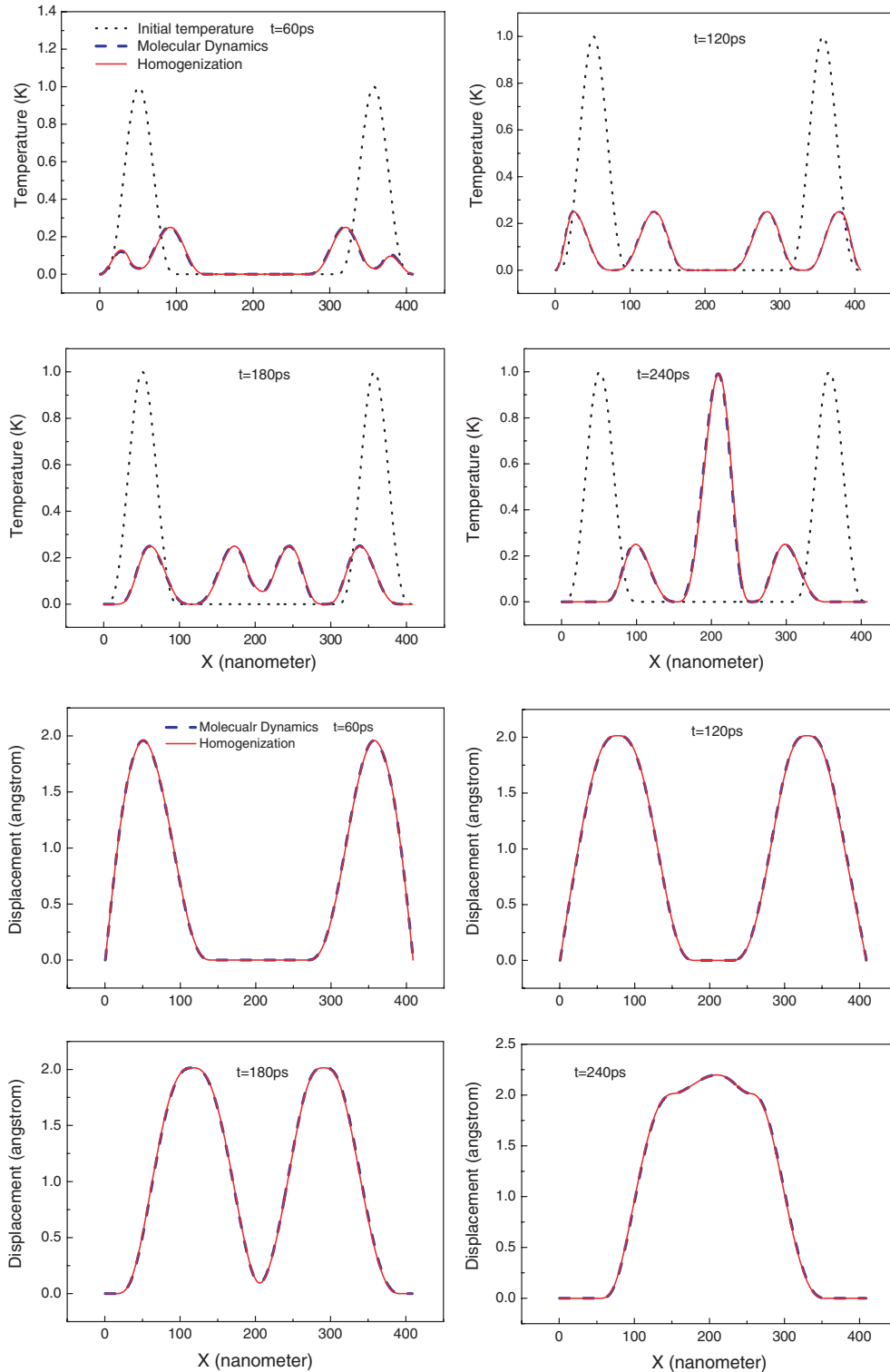
Fig. 2. Snapshots of temperature and displacements along the atomistic chain at different time instances.

4.2. Verification

We firstly consider a model problem of an atomistic chain consisting of 1201 atoms schematically depicted in Fig. 1. Suppose that the atoms are initially equally spaced with spacing a and each atom interacting with its nearest neighbors. The atomistic chain is assumed to possess periodic microstructure with a unit cell of length l composed of three atoms with masses m_1 and m_2. The chain is subjected to two initial bell-shaped temperature distribution at both ends with amplitude T_{max} and width $2\delta = 1/4L$, where L is the total length of the atomic chain. The temperatures at the two ends of the atomistic chain are constant in time. The interatomic potentials take the form of the Lennard-Jones potential. The interatomic potential between the first and the second atom in the unit cell is Φ_1 and that between the second and the third atom is Φ_2 given by

$$\Phi_1(r) = 4\varepsilon_1\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right],$$
$$\Phi_2(r) = 4\varepsilon_2\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right], \tag{118}$$

where ε_1 and ε_2 are characteristic energy scales of the interaction and σ the characteristic length scale of the interaction. We assume that the initial configuration of the atomistic chain is in equilibrium without external forces so that $a = 2^{1/6}\sigma$.

The interatomic forces are evaluated as

$$f_{01} = \frac{d\Phi_1}{dr} = \frac{24\varepsilon_1}{\sigma}\left[\left(\frac{\sigma}{r}\right)^7 - 2\left(\frac{\sigma}{r}\right)^{13}\right],$$
$$f_{12} = \frac{d\Phi_2}{dr} = \frac{24\varepsilon_2}{\sigma}\left[\left(\frac{\sigma}{r}\right)^7 - 2\left(\frac{\sigma}{r}\right)^{13}\right]. \tag{119}$$

For the three-atom unit cell under consideration, the instantaneous First Piola–Kirchhoff stress (54b) and the heat flux (86b) are

$$P(X, t, \tau) = \frac{1}{2}[f_{01}(\varepsilon\phi_{01})] + [f_{12}(\varepsilon\phi_{12})],$$
$$q(X, t, \tau) = \frac{m_1 - m_2}{2m_1}u_\tau^1(Y_1)P(X, t, \tau), \tag{120}$$

where

$$\hat{\phi}_{01} = (1 + u_X^0)a + \frac{m_1 + m_2}{m_1}\hat{u}^1(Y_1),$$
$$\hat{\phi}_{12} = (1 + u_X^0)a - \frac{m_1 + m_2}{m_1}\hat{u}^1(Y_1). \tag{121}$$

The linear mass density is given by

$$\rho_0 = \frac{1}{l}\sum_{i=1}^{2}m_i(Y) = (m_1 + m_2)/l. \tag{122}$$

Material parameters are $m_2/m_1 = 5$ and $\varepsilon_2/\varepsilon_1 = 2$. The amplitude of the initial temperature is set to be $T_{max} = 1$ K.

The snapshots of temperature and displacement fields at different time instances over the atomic chain are plotted in Fig. 2. As expected, the maximum temperatures drops compared with the initial temperature as the wave propagates towards the center.

The CPU time of homogenization in comparison with that of Molecular Dynamics at different atomistic chain sizes is plotted in Fig. 3. For all cases considered, the continuum mesh was sufficiently fine to resolve the macroscopic solution gradients. It can be observed that as chain size increases, the ratio of the CPU time between GMH MD simulations are increased without compromising on
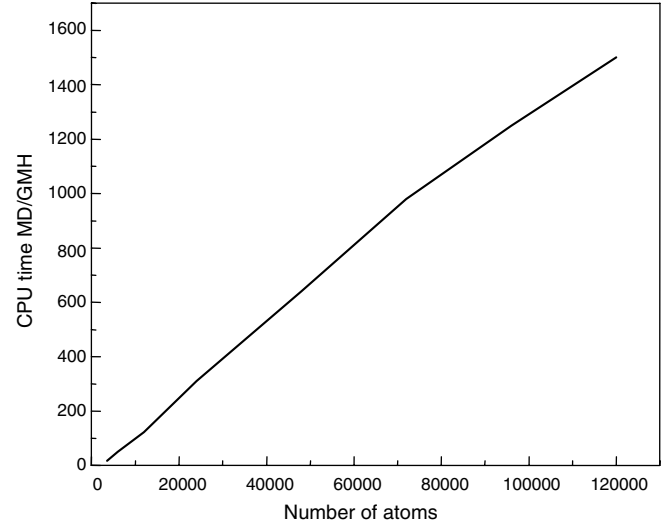

Fig. 3. The speed-up of GMH over MD in terms of CPU time for atomistic chains of different length.
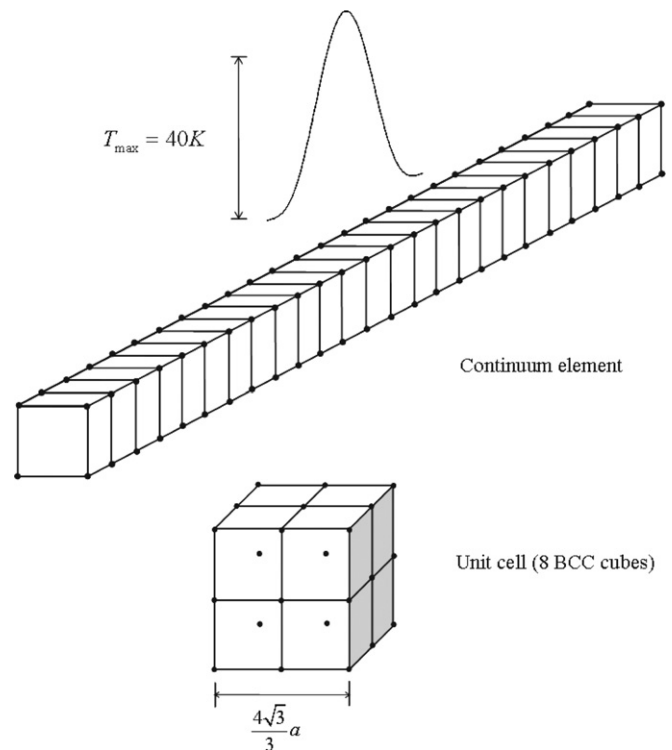

Fig. 4. Continuum and atomistic unit cell models.

solution accuracy. For atomistic chain of 120,001 atoms the speed-up factor is approximately 1500.

We have investigated the ratio of m_2/m_1 on accuracy and CPU ratio between MD and GMH. We have kept m_1 constant and varied the ratio m_2/m_1 from 1 to 100. Results predicted by GMH remained accurate, while the CPU ratio remained practically unaffected.

For the second example, we consider a three-dimensional model of a beam consisting of $100 \times 10 \times 10$ body-centered cubic lattice structure schematically depicted in Fig. 4. The total number of atoms occupying the volume of the beam is 22221. All atoms are assumed to have equal mass m. The beam is clamped at the two ends and is subjected to an initial bell-shaped temperature distribution with amplitude $T_{max} = 40$ K and width $2\delta = L$, where L is the total length of the atomic chain. The interatomic potentials take the form of the Lennard-Jones potential.

The continuum was discretized with 25 hexahedral elements whereas the atomistic unit is composed of 35 atoms as shown in Fig. 5. We considered hexahedral elements with eight-point Gauss quadrature and one-point Gauss-

quadrature with stabilization [14]. In comparison to MD, the CPU speed-up factor was approximately 190 in case of eight-point quadrature, and over 1350 in case of one-point quadrature with stabilization.

The axial displacement solution of a center atom at the cross $x = 3/5L$ as obtained by the GMH and the reference MD solution are plotted in Fig. 5. It can be observed that the coarse scale displacement predicted by GMH closely matches that of the MD. Fig. 6 shows that the temperature field at $x = 3/5L$ obtained by GMH is in good agreement with that obtained by MD.

The snapshots of temperature fields at different time instances over the atomic chain are plotted in Fig. 7. It can be seen that as time increases, the temperature in the middle area drops, whereas temperatures at the two ends increases.

5. Conclusions and future research directions

The primary goal of this paper was to develop a mathematical framework aimed at reconciling between fine scale and continuum thermo-mechanical descriptions. We
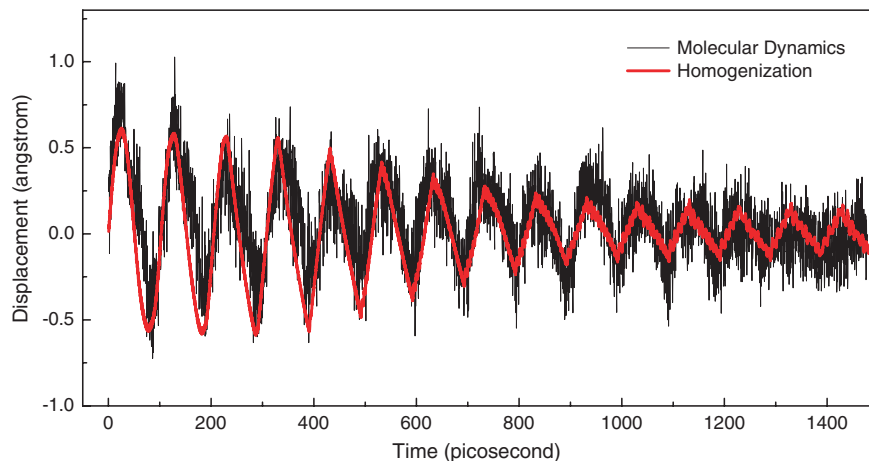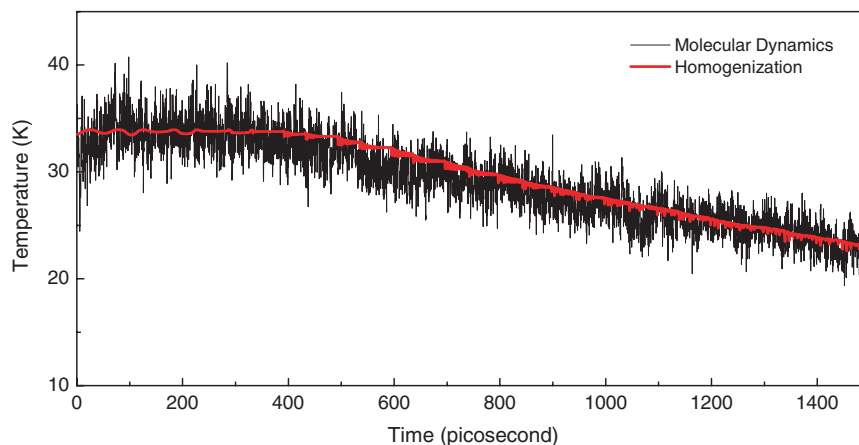

Fig. 5. Displacements of one atom.

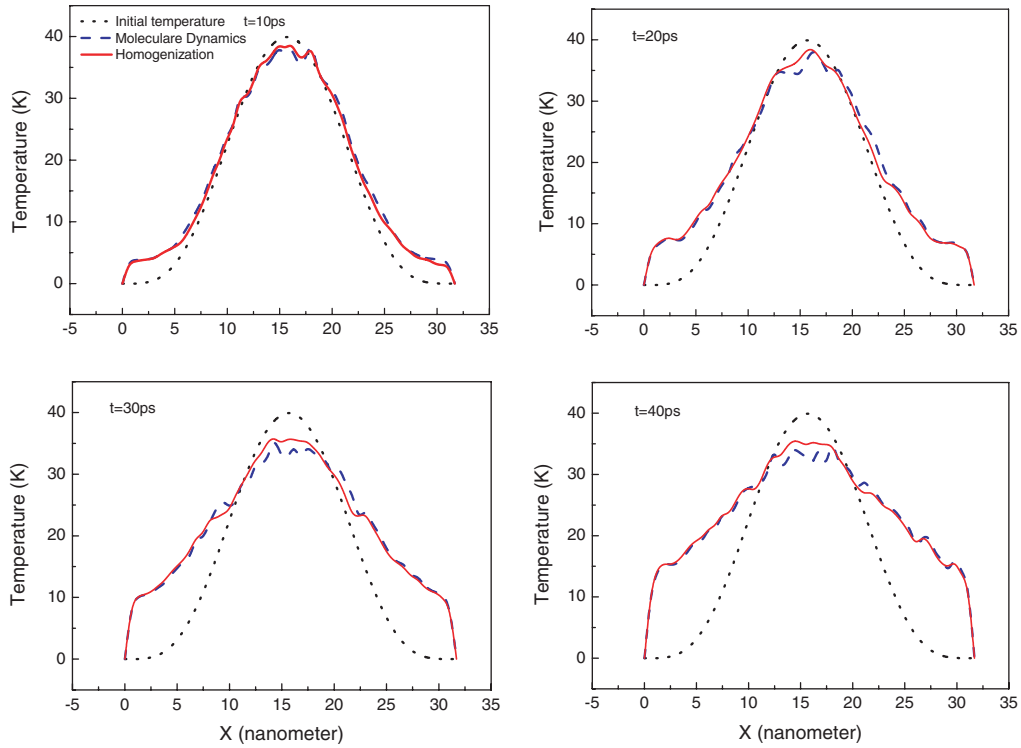Fig. 6. Temperatures at observation area.

Fig. 7. Snapshots of temperatures along the long axis.

derived a dynamic atomistic unit cell problem for the perturbation $\hat{\mathbf{u}}^1$

$$
m_i(\mathbf{Y}_i)\frac{\partial^2 \hat{\mathbf{u}}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)}{\partial \tau^2} = \varepsilon^2 \sum_{j \neq i} \hat{\mathbf{f}}_{ij}(\mathbf{F}^0(\mathbf{X}, t) \cdot \mathbf{X}_{ij})
$$
$$
+ \varepsilon \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_j, t, \tau)
$$
$$
- \varepsilon \mathbf{u}^1(\mathbf{X}, \mathbf{Y}_i, t, \tau)) \quad \forall i
$$

coupled with thermo-mechanical continuum equations for $\langle T \rangle$ and $\mathbf{u}^0$ given as

$$
\rho_0 \frac{\partial^2 \mathbf{u}^0(\mathbf{X}, t)}{\partial t^2} - \nabla_{\mathbf{X}} \cdot \langle \mathbf{P} \rangle = 0
$$
$$
\mathbf{P}(\mathbf{X}, t, \tau) = \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} [\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}],
$$

$$
C\frac{\partial \langle T \rangle}{\partial t} - \nabla_{\mathbf{X}} \cdot \langle \tilde{\mathbf{q}}(\mathbf{X}, t, \tau) \rangle = -2\langle \mathbf{P}(\mathbf{X}, t, \tau) \rangle : \frac{\partial \mathbf{F}^0}{\partial t}\tilde{\mathbf{q}}(\mathbf{X}, t, \tau)
$$
$$
= \frac{1}{2\Theta} \sum_{i=1}^{n} \sum_{j \neq i} \left[\left(2\frac{\partial \mathbf{u}^0}{\partial t} + \frac{\partial \mathbf{u}_i^1}{\partial \tau} \right) \cdot (\mathbf{f}_{ij}(\hat{\boldsymbol{\phi}}_{ij}) \otimes \mathbf{X}_{ij}) \right].
$$

These equations have a familiar structure. The expression of stress is similar to the virial stress formula except for the inertia term, which is absent. It is important to note that this form of stress is not new. Many investigators including Srolovitz et al. [15], Horstemeyer and Baskes [16] and Alber et al. [17] among others adopted this form as a measure of the continuum stress. Perhaps the only expression that we were not able to trace the origin of is that of flux.

We have considered pairwise potentials only, which are usually inadequate for modeling of solids. The methodology developed, however, is generic and is not limited to pair potentials. For three-body potentials, the final expressions will be more complex (see for instance Appendix in Ref. [3] for additional terms arising from the Stillinger–Webber and Tersoff potential.

Despite of some of the encouraging results, development of a complete mathematical and computational framework aimed at linking continuum thermo-mechanical and fine scale descriptions remains an elusive task. The conceptual challenge remains; can the electronic scale be brought into the atomistic description in the form of interatomic potentials and/or as an additional term in MD so that the mathematical framework proposed could be extended to conductors? The computational complexity has been only partially addressed. The number of Gauss points in the continuum could be of order of thousands if not millions. The atomistic unit cell may include millions of atoms if defects to be included. The two-scale algorithm outlined is fully coupled, i.e., at every slow time step, the solution at every unit cell has to be advanced. This creates a tremendous computational challenge that can be only addressed by a combination of innovative scale bridging approaches (such as GMH, HMM or others), coarse-grained models and parallel machines.

Acknowledgements

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