Generalized Mathematical Homogenization of Atomistic Media at Finite Temperatures

Jacob Fish, Wen Chen and Yuye Tang

Rensselaer Polytechnic Institute

Abstract

In this manuscript, we derive thermo-mechanical continuum equations directly from molecular dynamics using the Generalized Mathematical Homogenization (GMH) theory. GMH is a space-time multiple scale asymptotic expansion method, which constructs coupled atomistic unit cell problem and the coarse scale (continuum) problem. The fine scale problem derived can be interpreted as a molecular dynamics problem on a unit cell, subjected to the coarse scale fields including macroscopic deformation gradient and temperature. The coarse scale problem derived is a constitutive law-free continuum thermo-mechanical equation, which calculates the overall stress and thermal flux vector directly from atomistics. Numerical experiments have been conducted to verify the formulation against the reference molecular dynamics solution. Attention is restricted to one-dimensional problems.

1 Introduction

Molecular dynamics (MD) simulations can model systems of up to $4 \times 10^9$ atoms [1] for time scales of the order of nanoseconds, 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 molecular-level resolution. Constructing thermo-mechanical equations of continuum consistent with explicit consideration of motion of atoms has been a subject of significant interest in physics, material science and mechanics communities.

Deterministic atomistic level computations are evolved by numerically solving Newton's equations of motion without any distinction between mechanical and thermal contributions. Such Molecular Dynamics (MD) simulations explicitly track total atomistic displacements. On the other hand, in the thermo-mechanical continuum theories, while mechanical deformation can be explicitly calculated from atomistics, the thermal part can be only accounted for phenomenologically in the form of heat transfer equation. There is obviously a link between transport and momentum balance continuum
equations and certain atomistic features prompting numerous attempts to reconcile between the two descriptions. In the following, we give a brief account of these efforts followed by a new proposition.

The conversion of the atomistic data to macroscopic observables such as pressure, energy, heat capacities, has been provided within the framework of statistical mechanics, which is the formalism that connects thermodynamics to the atomistic world. By this approach, macroscopic behavior of any system can be cast as the sum of properties of many different microstates (representing complete specification of all positions and momenta of all atoms). However, the number of atoms forming the thermodynamic system should be of order $10^{23}$. Consequently, some of the features taken for granted by thermodynamics may fail when applied to smaller systems, such as nanodevices and nanomachines.

An equivalent deterministic thermo-mechanical continuum theory has been recently proposed by Zhou [2]. Continuum equations were derived by decomposing atomistic velocity into a structural deformation and thermal oscillation parts and by relating discrete and continuum descriptions using equivalence of momentum, energy and mass. A similar starting point has been employed by Li and E [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/or thermal) by performing atomistic simulations subjected to the local boundary conditions extracted from the continuum.

One of the best-known scale linking approaches at $0^0K$ is quasicontinuum method (QC). In this method, an approximation to the total potential energy is obtained by making use of interpolation constraints to remove atoms for the deformation field varying slowly on the scale of the lattice parameter. A straightforward extension of this approach to the finite temperature regime can be accomplished by adding kinetic energy to the QC potential energy and interpolating the velocity of any atom from the velocities of the representative atoms. Such an approach [5] has been applied to the dynamic simulation of nanoindentation and crack propagation. Unphysical reflections of waves on non-uniform meshes caused by the inability of the coarse scale model to transmit waves at a wavelength comparable to the discrete features have been observed. While this remains to be the main challenge for the quasicontinuum framework, some progress has been recently made in [6] by incorporating the potential of mean force (PMF) originally introduced by Kirkwood [7].

Variety of other approaches originally developed for zero-temperature applications have been recently extended to finite temperatures. These include the Coupled Atomistics and
Discrete Dislocation (CADD) method [8], the Bridging Scale method [9] and the Bridging Domain method [10].

In this paper, we derive the thermo-mechanical continuum equations directly from the molecular dynamics equations using the Generalized Mathematical Homogenization (GMH) theory originally developed by the first two authors for 0°K applications [11,12]. The fine scale (atomistic) problem derived can be interpreted as a molecular dynamics problem defined over a unit cell domain, subjected to the prescribed coarse scale fields, such as instantaneous deformation gradient and temperature, extracted from the continuum. The coarse scale problem derived is a constitutive law-free thermo-mechanical continuum equation, which calculates the overall stress and the heat flux directly from atomistics. The proposed multiscale approach has some resemblance to the Heterogeneous Multiscale Method with the main difference being that the coarse scale problem is derived directly from atomistics without making any a priori assumption about the mathematical structure of the continuum equations. Numerical experiments have been conducted to verify the multiscale formulation against the reference molecular dynamics solution. Attention is restricted to one-dimensional problems.

2 Governing Equations

2.1 Molecular dynamics equation of motion

Consider a one-dimensional atomic chain composed of \( N \) atoms in a periodic arrangement. The interaction between atoms is governed by the pairwise potentials with a nearest neighbor interaction. The initial position of atom \( i \) in the reference configuration is denoted by \( X_{i}, i=1,2,\cdots,N \). The displacement of atom \( i \) with respect to the reference position is denoted by \( u_{i} \). Upon deformation, the new position of atom \( i \) is \( x_{i} \), given by

\[
x_{i} = X_{i} + u_{i}, \quad u_{i} = u_{i}(X_{i}, t)
\]

The current separation between atoms \( i \) and \( i+1 \) is denoted as \( r_{i,i+1} \) and that between atoms \( i-1 \) and \( i \) is designated as \( r_{i-1,i} \), given by

\[
\begin{align*}
r_{i,i+1} &= x_{i+1} - x_{i} = X_{i+1} - X_{i} + u_{i+1}(X_{i+1}, t) - u_{i}(X_{i}, t) \\
r_{i-1,i} &= x_{i} - x_{i-1} = X_{i} - X_{i-1} + u_{i}(X_{i}, t) - u_{i-1}(X_{i-1}, t)
\end{align*}
\]
Based on the nearest neighbor interaction, the equation of motion for atom $i$ can be written as

$$m_i \ddot{u}_i = f_{i,i+1}(r_{i,i+1}) - f_{i-1,i}(r_{i-1,i})$$  \hspace{1cm} (3)$$

where $m_i$ is the mass of atom $i$; $\dot{u}_i = du_i / dt$ represents the material time derivative of $u_i$; $f_{i,i+1}$ and $f_{i-1,i}$ are interatomic forces between atoms $i$, $i + 1$ and $i - 1$, $i$, respectively. For the pairwise potentials considered, the interaction between atoms $i$ and $j$ is depicted by $\Phi_{ij}(r_{ij})$ and the interatomic forces are evaluated as

$$f_{i,i+1}(r_{i,i+1}) = \frac{d\Phi_{i,i+1}(r_{i,i+1})}{dr_{i,i+1}}, \quad f_{i-1,i}(r_{i-1,i}) = \frac{d\Phi_{i-1,i}(r_{i-1,i})}{dr_{i-1,i}}$$ \hspace{1cm} (4)$$

Due to the periodic atomistic structure, the mass of atom $m_i$ and the interatomic forces $f_{i,i+1}$ and $f_{i-1,i}$ are assumed to be periodic. Attention is restricted to the case where the wavelength of the traveling signal $\lambda$ is much larger than the size of the atomistic unit cell $l$, i.e., $\varepsilon = l / \lambda \ll 1$.

### 2.2 Multiple spatial and temporal scales

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

$$Y = X / \varepsilon \quad 0 < \varepsilon \ll 1$$ \hspace{1cm} (5)$$

The corresponding scales in the spatial (deformed) coordinates are denoted by $x$ and $y$, respectively, and are related by $y = x / \varepsilon$.

In addition to the usual time scale, we introduce the fast time scale $\tau$ in order to capture the high-frequency vibration of atoms at finite temperature. The fast time scale is related to the usual time scale by

$$\tau = t / \varepsilon \quad 0 < \varepsilon \ll 1$$ \hspace{1cm} (6)$$

4
The resulting displacement field and its derivatives are functions of $X,Y,t$ and $\tau$. Prior to carrying out the multiple scale asymptotic analysis it is necessary to rescale the molecular dynamics (MD) Eq. (3) by introducing the following normalized quantity:

$$m_i = m_i / \varepsilon \sim m_i / l \sim \rho \sim O(1)$$

(7)

where $\rho$ is the linear mass density and $l$ the size of the unit cell.

Due to periodicity of masses, we have $m_i = \bar{m}_i(Y)$. The rescaled MD equation of motion can be expressed as:

$$\bar{m}_i \ddot{u}_i(X,Y,t,\tau) = \frac{1}{\varepsilon} [f_{i+1}(r_{i+1}) - f_{i-1}(r_{i-1})]$$

(8)

3 Generalized Mathematical Homogenization

3.1 Multiple-scale asymptotic analysis

We assume that the coarse scale coordinate $X$ takes continuous series of values and displacements $u_i(X,Y,t,\tau)$ are continuous and differentiable in $X$, while the fine scale coordinate $Y$ depicting position of atoms is discrete. We denote the displacement of atom $i$ by $u(X,Y,t,\tau)$ with $X = X_i$. The displacements of the neighboring atoms $u_{i+1}(X_{i+1},Y_{i+1},t,\tau)$ and $u_{i-1}(X_{i-1},Y_{i-1},t,\tau)$ are expanded using Taylor series around the point $X$ as

$$u_{i+1} = u_{i+1}(X_{i+1},Y_{i+1},t,\tau) = u(X,Y_{i+1},t,\tau) + (X_{i+1} - X_i)u_X(X,Y_{i+1},t,\tau) +$$

$$\frac{(X_{i+1} - X_i)^2}{2} u_{XX}(X,Y_{i+1},t,\tau) + \cdots$$

$$u_{i-1} = u_{i-1}(X_{i-1},Y_{i-1},t,\tau) = u(X,Y_{i-1},t,\tau) - (X_i - X_{i-1})u_X(X,Y_{i-1},t,\tau) +$$

$$\frac{(X_i - X_{i-1})^2}{2} u_{XX}(X,Y_{i-1},t,\tau) + \cdots$$

(9)

where $u_X = \partial u / \partial X$ and $u_{XX} = \partial^2 u / \partial X^2$. 

5
Since the coarse and fine scales coordinates are related by Eq. (5), we have

\[ X_{i+1} - X_i = \varepsilon(Y_{i+1} - Y_i), \quad X_i - X_{i-1} = \varepsilon(Y_i - Y_{i-1}) \]  

(10)

From Eqs. (9) and (10) we have

\[ u_{i+1} - u_i = u(X, Y_{i+1}, t, \tau) - u(X, Y_i, t, \tau) + \varepsilon(Y_{i+1} - Y_i)u_X(X, Y_{i+1}, t, \tau) + \]  

\[ \varepsilon^2 \frac{(Y_{i+1} - Y_i)^2}{2} u_{XX}(X, Y_{i+1}, t, \tau) + \ldots \]

\[ u_i - u_{i-1} = u(X, Y_i, t, \tau) - u(X, Y_{i-1}, t, \tau) + \varepsilon(Y_i - Y_{i-1})u_X(X, Y_{i-1}, t, \tau) - \]  

\[ \varepsilon^2 \frac{(Y_i - Y_{i-1})^2}{2} u_{XX}(X, Y_{i-1}, t, \tau) + \ldots \]  

(11)

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

\[ u(X, Y, t, \tau) = u^0(X, t) + \varepsilon u^1(X, Y, t, \tau) + \ldots \]  

(12)

where the leading order term \( u^0 \) is assumed to be independent of the fine scale coordinates \( Y \) and \( \tau \). For \( O(1) \) continuum theory to be derived in this manuscript only the leading two terms in the asymptotic expansion need to be considered.

Substituting the asymptotic expansion (12) into Eq. (11) yields

\[ u_{i+1} - u_i = \varepsilon[u^1(X, Y_{i+1}, t, \tau) - u^1(X, Y_i, t, \tau) + (Y_{i+1} - Y_i)u_X^0(X, t)] + \]  

\[ \varepsilon^2(Y_{i+1} - Y_i)[u_X^1(X, Y_{i+1}, t, \tau) + \frac{Y_{i+1} - Y_i}{2} u_{XX}^0(X, t)] + \ldots \]

\[ u_i - u_{i-1} = \varepsilon[u^1(X, Y_i, t, \tau) - u^1(X, Y_{i-1}, t, \tau) + (Y_i - Y_{i-1})u_X^0(X, t)] + \]  

\[ \varepsilon^2(Y_i - Y_{i-1})[u_X^1(X, Y_{i-1}, t, \tau) - \frac{Y_i - Y_{i-1}}{2} u_{XX}^0(X, t)] + \ldots \]  

(13)

Inserting Eqs. (10) and (13) into (2) yields

\[ r_{i,i+1} = \varepsilon \phi_{i,i+1} + \varepsilon^2 \psi_{i,i+1} + \ldots, \quad r_{i-1,i} = \varepsilon \phi_{i-1,i} + \varepsilon^2 \psi_{i-1,i} + \ldots \]  

(14)
where
\[ \phi_{i,i+1} = [1 + u_X^0(X,t)](Y_{i+1} - Y_i) + u_i^1(X,Y_{i+1},t,\tau) - u^1(X,Y_i,t,\tau) \]
\[ \phi_{i-1,i} = [1 + u_X^0(X,t)](Y_i - Y_{i-1}) + u_i^1(X,Y_i,t,\tau) - u^1(X,Y_{i-1},t,\tau) \]
\[ \psi_{i+1,i} = (Y_{i+1} - Y_i)[u_X^1(X,Y_{i+1},t,\tau) + \frac{Y_{i+1} - Y_i}{2} u_X^0(X,t)] \]
\[ \psi_{i-1,i} = (Y_i - Y_{i-1})[u_X^1(X,Y_i,t,\tau) - \frac{Y_i - Y_{i-1}}{2} u_X^0(X,t)] \] (15)

Since \( \phi_{i,i+1} \sim O(1), \psi_{i,i+1} \sim O(1), \phi_{i-1,i} \sim O(1) \) and \( \psi_{i-1,i} \sim O(1) \), we have
\[ \frac{\varepsilon^2 \psi_{i,i+1}}{\varepsilon \phi_{i,i+1}} \sim O(\varepsilon), \quad \frac{\varepsilon^2 \psi_{i-1,i}}{\varepsilon \phi_{i-1,i}} \sim O(\varepsilon) \] (16)

The interatomic forces can be expanded as
\[
\begin{align*}
\hat{f}_{i+1}(r_{i+1}) &= f_{i+1}(\varepsilon \phi_{i,i+1} + \varepsilon^2 \psi_{i,i+1} + \cdots) \\
&= f_{i+1}(\hat{\phi}_{i,i+1} + \varepsilon f'_{i+1}(\hat{\phi}_{i,i+1})(\psi_{i,i+1} + \cdots) + o(\varepsilon^2 \psi_{i,i+1} + \cdots) \\
\hat{f}_{i-1,i}(r_{i-1,i}) &= f_{i-1,i}(\varepsilon \phi_{i-1,i} + \varepsilon^2 \psi_{i-1,i} + \cdots) \\
&= f_{i-1,i}(\hat{\phi}_{i-1,i} + \varepsilon f'_{i-1,i}(\hat{\phi}_{i-1,i})(\psi_{i-1,i} + \cdots) + o(\varepsilon^2 \psi_{i-1,i} + \cdots) \\
\end{align*}
\] (17)

where
\[ \hat{\phi}_{i+1} = \varepsilon \phi_{i,i+1}, \quad \hat{\phi}_{i-1,i} = \varepsilon \phi_{i-1,i} \] (18)

\[
\begin{align*}
f'_{i+1}(\hat{\phi}_{i,i+1}) &= \frac{\partial f_{i+1}}{\partial \phi_{i,i+1}} \bigg|_{\phi_{i,i+1}} \\
f'_{i-1,i}(\hat{\phi}_{i-1,i}) &= \frac{\partial f_{i-1,i}}{\partial \phi_{i-1,i}} \bigg|_{\phi_{i-1,i}} \\
\end{align*}
\] (19)

We now focus on the inertia term. Utilizing the chain rule, material time derivative(s) can be expressed as
\[ \dot{u}_i(X_i,Y_i,t,\tau) = \dot{u}(X,Y_i,t,\tau) = \frac{\partial u}{\partial t} + \varepsilon^{-1} \frac{\partial u}{\partial \tau} \]
\[ \dot{u}_i(X, Y, t, \tau) = \left( \frac{\partial}{\partial t} + \varepsilon^{-1} \frac{\partial}{\partial \tau} \right) \left( \frac{\partial u}{\partial t} + \varepsilon^{-1} \frac{\partial u}{\partial \tau} \right) \]  
(20)

Inserting the asymptotic expansion (12) into (20) yields

\[ \dot{u}_i(X, Y, t, \tau) = \varepsilon^{-1} \frac{\partial^2 u^1}{\partial \tau^2} + \frac{\partial^2 u^0}{\partial t^2} + 2 \frac{\partial^2 u^1}{\partial t \partial \tau} + \varepsilon \frac{\partial^2 u^1}{\partial t^2} + \cdots \]  
(21)

Substituting Eqs. (17) and (21) into the rescaled MD equation of motion (8) yields

\[ m_i \left[ \varepsilon^{-1} \frac{\partial^2 u^1}{\partial \tau^2} + \frac{\partial^2 u^0}{\partial t^2} + 2 \frac{\partial^2 u^1}{\partial t \partial \tau} + \varepsilon \frac{\partial^2 u^1}{\partial t^2} + \cdots \right] = \frac{1}{\varepsilon} \left[ f_i^{i+1}(\dot{\psi}_{i+1}) + \varepsilon f_i^{i+1}(\dot{\psi}_{i+1})(\psi_{i+1} + \cdots) \right] \]

\[ -f_i^{i-1}(\dot{\psi}_{i-1}) - \varepsilon f_i^{i-1}(\dot{\psi}_{i-1})(\psi_{i-1} + \cdots) + o(\varepsilon^2 \psi_{i+1} - \varepsilon^2 \psi_{i-1} + \cdots) \]  
(22)

Collecting terms of equal power of \( \varepsilon \), gives the momentum balance equations at different orders starting with \( O(\varepsilon^{-1}) \):

\[ O(\varepsilon^{-1}) : \quad m_i \frac{\partial^3 u^1(X, Y, t, \tau)}{\partial \tau^2} = f_i^{i+1}(\dot{\psi}_{i+1}) - f_i^{i-1}(\dot{\psi}_{i-1}) \]  
(23)

\[ O(\varepsilon^{0}) : \quad m_i \left[ \frac{\partial^2 u^0(X, t)}{\partial t^2} + 2 \frac{\partial^2 u^1(X, Y, t, \tau)}{\partial t \partial \tau} \right] = f_i^{i+1}(\dot{\psi}_{i+1})\psi_{i+1} - f_i^{i-1}(\dot{\psi}_{i-1})\psi_{i-1} \]  
(24)

### 3.2 The atomistic unit cell problem

Consider the \( O(\varepsilon^{-1}) \) momentum balance equation (23) first. Substituting the normalized mass (7) into Eq. (23) yields the atomistic unit cell problem

\[ m_i \frac{\partial^2 \dot{u}^1(X, Y, t, \tau)}{\partial \tau^2} = \varepsilon^2 [f_i^{i+1}(\dot{\psi}_{i+1}) - f_i^{i-1}(\dot{\psi}_{i-1})] \quad \forall i \]  
(25)

where

\[ \dot{u}^1(X, Y, t, \tau) = \varepsilon u^1(X, Y, t, \tau) \]  
(26)
\[ \dot{\phi}_{i,i+1} = \varepsilon \dot{\phi}_{i,i+1} = F^0(X,t)(X_{i+1} - X_i) + \dot{u}^1(X,Y_{i+1},t,\tau) - \dot{u}^1(X,Y_i,t,\tau) \]  
\[ \dot{\phi}_{i-1,i} = \varepsilon \dot{\phi}_{i-1,i} = F^0(X,t)(X_i - X_{i-1}) + \dot{u}^1(X,Y_i,t,\tau) - \dot{u}^1(X,Y_{i-1},t,\tau) \] 

and

\[ F^0(X,t) = 1 + u^0_X(X,t) \]

is the deformation gradient.

It can be seen that the atomistic unit cell problem is solved for the fine scale correction \( u^1(X,Y,t,\tau) \) and is subjected to the uniform coarse scale deformation gradient, \( F^0 \). Note that Eq. (25) is in the spirit of molecular dynamics equation where the “inertia” term on the left hand side is expressed in terms of the fine scale correction and the fast time scale. In absence of heterogeneity in masses and interatomic potentials, \( u^1 \) admits a trivial solution. Otherwise, it represents a time-varying correction to the classical Cauchy-Born rule.

### 3.3 The coarse scale equation of motion

We proceed by considering the \( O(\varepsilon^0) \) momentum balance equation (24). Substituting the normalized mass (7) into (24) yields

\[ m_i \frac{\partial^2 u^0(X,t)}{\partial t^2} + 2 \frac{\partial^2 u^1(X,Y,t,\tau)}{\partial t \partial \tau} = \varepsilon [f'_{i,i+1}(\dot{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\dot{\phi}_{i-1,i})\psi_{i-1,i}] \]  
\[ (30) \]

Summing up Eq. (30) for all atoms in the unit cell and dividing the resulting equation by the size of the unit cell, \( l \), yields

\[ \frac{1}{l} \sum_{i=1}^{n} m_i \frac{\partial^2 u^0(X,t)}{\partial t^2} + \frac{2}{l} \frac{\partial}{\partial \tau} \left[ \sum_{i=1}^{n} m_i \frac{\partial u^1(X,Y,t,\tau)}{\partial t} \right] \]

\[ = \frac{\varepsilon}{l} \sum_{i=1}^{n} [f'_{i,i+1}(\dot{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\dot{\phi}_{i-1,i})\psi_{i-1,i}] \]  
\[ (31) \]

We now define the temporal averaging operator as
\[ \langle \chi(\tau) \rangle = \frac{1}{\tau_0} \int_0^{\tau_0} \chi(\tau) d\tau \]  

(32)

where \( \tau_0 \) is a period of function \( \chi(\tau) \).

Applying the temporal averaging operator to Eq. (31) yields

\[ \rho_0 \frac{\partial^2 u^0(X,t)}{\partial t^2} = \frac{\varepsilon}{l} \left( \sum_{i=1}^{n} \left[ f'_{i,i+1}(\phi_{i,i+1}) \psi_{i,i+1} - f'_{i-1,i}(\phi_{i-1,i}) \psi_{i-1,i} \right] \right) \]  

(33)

where the temporal averaging of the second term in Eq. (31) vanishes due to periodicity in the fast time \( \tau \), and

\[ \rho_0 = \frac{1}{l} \sum_{i=1}^{n} m_i \]  

(34)

is the linear mass density. Note that since the above summation is carried out over the unit cell domain, the coarse scale field \( u^0(X,t) \) is taken to be constant for all the atoms in the unit cell.

We now focus on further simplification of Eq. (33). Exploiting the chain rule yields

\[ \frac{\partial f'_{i,i+1}}{\partial X} = \frac{\partial f'_{i,i+1}}{\partial \phi_{i,i+1}} \frac{\partial \phi_{i,i+1}}{\partial X} \]

\[ = f'_{i,i+1}(\phi_{i,i+1}) \left[ u_X^1(X,Y_{i+1},t,t,\tau) - u_X^1(X,Y_i,t,\tau) + (Y_{i+1} - Y_i)u_{XX}^0(X,t) \right] \]  

(35)

\[ \frac{\partial f'_{i-1,i}}{\partial X} = \frac{\partial f'_{i-1,i}}{\partial \phi_{i-1,i}} \frac{\partial \phi_{i-1,i}}{\partial X} \]

\[ = f'_{i-1,i}(\phi_{i-1,i}) \left[ u_X^1(X,Y_i,t,t,\tau) - u_X^1(X,Y_{i-1},t,\tau) + (Y_i - Y_{i-1})u_{XX}^0(X,t) \right] \]  

(36)

From Eqs. (15), (35) and (36), we have

\[ f'_{i,i+1}(\phi_{i,i+1}) \psi_{i,i+1} - f'_{i-1,i}(\phi_{i-1,i}) \psi_{i-1,i} \]
\[ f'_{i,i+1}(\hat{\phi}_{i,i+1})(Y_{i+1} - Y_i)[2u^1_X(X,Y_{i+1},t,\tau) + (Y_{i+1} - Y_i)u^0_{XX}(X,t)] + \]

\[ f'_{i-1,i}(\hat{\phi}_{i-1,i})(Y_i - Y_{i-1})[-2u^1_X(X,Y_{i-1},t,\tau) + (Y_i - Y_{i-1})u^0_{XX}(X,t)] \]

\[ = \frac{1}{2} f'_{i,i+1}(\hat{\phi}_{i,i+1})(Y_{i+1} - Y_i)[u^1_X(X,Y_{i+1},t,\tau) - u^1_X(X,Y_i,t,\tau) + (Y_{i+1} - Y_i)u^0_{XX}(X,t)] + \]

\[ \frac{1}{2} f'_{i-1,i}(\hat{\phi}_{i-1,i})(Y_i - Y_{i-1})[u^1_X(X,Y_i,t,\tau) + u^1_X(X,Y_{i-1},t,\tau)] + \]

\[ \frac{1}{2} f'_{i-1,i}(\hat{\phi}_{i-1,i})(Y_i - Y_{i-1})[u^1_X(X,Y_i,t,\tau) - u^1_X(X,Y_{i-1},t,\tau) + (Y_i - Y_{i-1})u^0_{XX}(X,t)] \]

\[ -\frac{1}{2} f'_{i-1,i}(\hat{\phi}_{i-1,i})(Y_i - Y_{i-1})[u^1_X(X,Y_i,t,\tau) + u^1_X(X,Y_{i-1},t,\tau)] \]

\[ = \frac{1}{2} \frac{\partial}{\partial X}[(Y_{i+1} - Y_i)f_{i,i+1} + (Y_i - Y_{i-1})f_{i-1,i}] + \]

\[ \frac{1}{2} \left\{ f'_{i,i+1}(\hat{\phi}_{i,i+1})(Y_{i+1} - Y_i)[u^1_X(X,Y_i,t,\tau) + u^1_X(X,Y_{i+1},t,\tau)] - \right. \]

\[ \left. f'_{i-1,i}(\hat{\phi}_{i-1,i})(Y_i - Y_{i-1})[u^1_X(X,Y_{i-1},t,\tau) + u^1_X(X,Y_i,t,\tau)] \right\} \] (37)

For a general atomistic unit cell consisting of \( n + 1 \) atoms depicted in Figure 1, the following relation can be proved:
\[
\sum_{i=1}^{n} \{ f_{i,i+1}'(\phi_{i,i+1}) (Y_{i+1} - Y_i) [u^1_X(X, Y_i, t, \tau) + u^1_X(X, Y_{i+1}, t, \tau)] - \\
\]
\[
f_{i-1,i}'(\phi_{i-1,i}) (Y_i - Y_{i-1}) [u^1_X(X, Y_{i-1}, t, \tau) + u^1_X(X, Y_i, t, \tau)] \}
\]
\[
= f_{12}'(\phi_{12}) [u^1_X(Y_1) + u^1_X(Y_2)] (Y_2 - Y_1) - f_{01}'(\phi_{01}) [u^1_X(Y_0) + u^1_X(Y_1)] (Y_1 - Y_0) + \\
f_{23}'(\phi_{23}) [u^1_X(Y_2) + u^1_X(Y_3)] (Y_3 - Y_2) - f_{12}'(\phi_{12}) [u^1_X(Y_1) + u^1_X(Y_2)] (Y_2 - Y_1) + \\
f_{34}'(\phi_{34}) [u^1_X(Y_3) + u^1_X(Y_4)] (Y_4 - Y_3) - f_{23}'(\phi_{23}) [u^1_X(Y_2) + u^1_X(Y_3)] (Y_3 - Y_2) + \\
f_{35}'(\phi_{35}) [u^1_X(Y_4) + u^1_X(Y_5)] (Y_5 - Y_4) - f_{34}'(\phi_{34}) [u^1_X(Y_3) + u^1_X(Y_4)] (Y_4 - Y_3) + \cdots + \\
f_{n-1,n}'(\phi_{n-1,n}) [u^1_X(Y_{n-1}) + u^1_X(Y_n)] (Y_n - Y_{n-1}) - \\
f_{n-2,n-1}'(\phi_{n-2,n-1}) [u^1_X(Y_{n-2}) + u^1_X(Y_{n-1})] (Y_{n-1} - Y_{n-2}) + \\
f_{n,n+1}'(\phi_{n,n+1}) [u^1_X(Y_n) + u^1_X(Y_{n+1})] (Y_{n+1} - Y_n) - \\
f_{n-1,n}'(\phi_{n-1,n}) [u^1_X(Y_{n-1}) + u^1_X(Y_n)] (Y_n - Y_{n-1}) \\
= - f_{01}'(\phi_{01}) [u^1_X(Y_0) + u^1_X(Y_1)] (Y_1 - Y_0) + f_{n,n+1}'(\phi_{n,n+1}) [u^1_X(Y_n) + u^1_X(Y_{n+1})] (Y_{n+1} - Y_n) \\
= 0 \quad (38)
\]

which is the consequence of periodicity

\[
f_{01}'(\phi_{01}) = f_{n,n+1}'(\phi_{n,n+1}), \quad u^1_X(Y_0) = u^1_X(Y_{i,n}), \quad Y_i = Y_{i+n} \quad (39)
\]

Substituting Eqs. (37) and (38) into (33) yields the macroscopic equation of motion
\[
\frac{\rho_0}{t^2} \frac{\partial^2 u^0(X,t)}{\partial t^2} - \frac{\partial \langle P \rangle}{\partial X} = 0
\]

\[
P(X,t,\tau) = \frac{1}{2l} \sum_{i=1}^{n} [(X_{i+1} - X_i)f_{i,i+1}(\dot{\phi}_{i,i+1}) + (X_i - X_{i-1})f_{i-1,i}(\dot{\phi}_{i-1,i})]
\]

where \( P(X,t,\tau) \) is instantaneous (in fast time scale) First Piola-Kirchhoff stress and \( \langle P(X,t,\tau) \rangle \) is the First Piola-Kirchhoff stress.

### 3.4 The thermal equation

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

\[
\mathcal{K} = \sum_{i=1}^{n} \frac{|p_i|^2}{2m_i} = \frac{K_BT}{2} nN_d
\]

where \( p_i \) is the total momentum of atom \( i \) and \( m_i \) is its mass; \( K_B \) the Boltzmann constant and \( T \) the temperature of the ensemble. Based on the equipartition of energy theorem, each degree of freedom contributes equal amount of energy, \( K_BT/2 \). If there are \( n \) atoms, each with \( N_d \) degrees of freedom, the kinetic energy should be equal to \( nN_dK_BT/2 \).

For the 1D system, Eq. (41) reduces to

\[
\mathcal{K} = \sum_{i=1}^{n} \frac{|p_i|^2}{2m_i} = \frac{nK_BT}{2}
\]

The square of the momentum of an atom is given as

\[
|p_i|^2 = m_i^2 \dot{u}_i^2 = m_i^2 \left( \frac{\partial u_i}{\partial t} + \frac{\tau}{\epsilon} \frac{\partial u_i}{\partial \tau} \right)^2
\]

Inserting the asymptotic expansion (12) into (43) yields
\[ p_i^2 = m_i^2 \left[ \left( \frac{\partial u_i^0}{\partial t} + \frac{\partial u_i^1}{\partial \tau} \right)^2 + O(\varepsilon) \right] \]  

(44)

Substituting Eq. (44) into (42) and neglecting terms of \( O(\varepsilon) \) and higher gives

\[ \sum_{i=1}^{n} m_i \left( \frac{\partial u_i^0}{\partial t} + \frac{\partial u_i^1}{\partial \tau} \right)^2 = nK_B T(X,t,\tau) \]  

(45)

where \( T \) is the instantaneous (in fast time scale) temperature.

From Eq. (45) it follows

\[ \frac{\partial}{\partial t} \left[ \sum_{i=1}^{n} m_i \left( \frac{\partial u_i^0}{\partial t} + \frac{\partial u_i^1}{\partial \tau} \right)^2 \right] = nK_B \frac{\partial T}{\partial t} \]  

(46)

which can be rearranged as

\[ \sum_{i=1}^{n} m_i \left[ \frac{\partial u_i^0}{\partial t} \frac{\partial^2 u_i^0}{\partial t^2} + \frac{\partial u_i^0}{\partial t} \frac{\partial^2 u_i^1}{\partial t \partial \tau} + \frac{\partial u_i^1}{\partial \tau} \left( \frac{\partial^2 u_i^0}{\partial t \partial \tau} + \frac{\partial^2 u_i^1}{\partial t \partial \tau} \right) \right] = \frac{nK_B}{2} \frac{\partial T}{\partial t} \]  

(47)

Multiplying both sides of Eq. (30) by \( \frac{\partial u^0}{\partial t} \) and summing up over all atoms in the unit cell yields

\[ \sum_{i=1}^{n} \frac{\partial u_i^0}{\partial t} m_i \left[ \frac{\partial^2 u_i^0}{\partial t^2} + 2 \frac{\partial^2 u_i^1}{\partial t \partial \tau} \right] = \varepsilon \sum_{i=1}^{n} \frac{\partial u_i^0}{\partial t} \left[ f'_{i,i+1}(\hat{\phi}_{i,i+1}) \psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i}) \psi_{i-1,i} \right] \]  

(48)

In view of Eq. (47), Eq. (48) can be written as

\[ \frac{nK_B}{2} \frac{\partial T}{\partial t} + \sum_{i=1}^{n} m_i \left[ \frac{\partial u_i^0}{\partial t} \frac{\partial^2 u_i^1}{\partial t \partial \tau} - \frac{\partial u_i^1}{\partial \tau} \frac{\partial^2 u_i^0}{\partial t \partial \tau} - \frac{\partial u_i^1}{\partial \tau} \frac{\partial^2 u_i^1}{\partial t \partial \tau} \right] = \varepsilon \sum_{i=1}^{n} \frac{\partial u_i^0}{\partial t} \left[ f'_{i,i+1}(\hat{\phi}_{i,i+1}) \psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i}) \psi_{i-1,i} \right] \]  

(49)

Applying the temporal averaging operator to Eq. (49), and exploiting the fact that the second and third terms vanish due to periodicity in the fast time \( \tau \), we have
\[
\frac{nK_B}{2} \frac{\partial \langle T \rangle}{\partial t} = \left\langle \sum_{i=1}^{n} m_i \frac{\partial u^1}{\partial \tau} \frac{\partial^2 u^1}{\partial t \partial \tau} \right\rangle \\
= \varepsilon \frac{\partial u^0}{\partial t} \left\langle \sum_{i=1}^{n} [f'_{i,i+1}(\hat{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i})\psi_{i-1,i}] \right\rangle \tag{50}
\]

where \( \langle T \rangle \) is the fast time average temperature or simply the temperature field. Multiplying both sides of Eq. (30) by \( \partial u^1 / \partial \tau \) and summing up over all atoms in the unit cell yields

\[
\sum_{i=1}^{n} m_i \left[ \frac{\partial u^1}{\partial \tau} \frac{\partial^2 u^0}{\partial t^2} + 2 \frac{\partial u^1}{\partial \tau} \frac{\partial^2 u^1}{\partial t \partial \tau} \right] = \varepsilon \sum_{i=1}^{n} \frac{\partial u^1}{\partial \tau} \left[ f'_{i,i+1}(\hat{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i})\psi_{i-1,i} \right] \tag{51}
\]

Applying the temporal averaging operator to the above equation, and accounting for the fact that the first term on the left hand side vanishes due to periodicity in the fast time \( \tau \), we have

\[
\left\langle \sum_{i=1}^{n} m_i \frac{\partial u^1}{\partial \tau} \frac{\partial^2 u^1}{\partial t \partial \tau} \right\rangle = \frac{\varepsilon}{2} \left\langle \sum_{i=1}^{n} \frac{\partial u^1}{\partial \tau} \left[ f'_{i,i+1}(\hat{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i})\psi_{i-1,i} \right] \right\rangle \tag{52}
\]

Substituting Eq. (52) into (50) yields

\[
\frac{nK_B}{2} \frac{\partial \langle T \rangle}{\partial t} = \varepsilon \left\langle \sum_{i=1}^{n} [2 \frac{\partial u^0}{\partial t} + \frac{\partial u^1}{\partial \tau}] \left[ f'_{i,i+1}(\hat{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i})\psi_{i-1,i} \right] \right\rangle \tag{53}
\]

From Eqs. (37) and (38), we obtain

\[
\varepsilon \left\langle \sum_{i=1}^{n} [2 \frac{\partial u^0}{\partial t} + \frac{\partial u^1}{\partial \tau}] \left[ f'_{i,i+1}(\hat{\phi}_{i,i+1})\psi_{i,i+1} - f'_{i-1,i}(\hat{\phi}_{i-1,i})\psi_{i-1,i} \right] \right\rangle \\
= 2l \frac{\partial u^0}{\partial t} \frac{\partial \langle P \rangle}{\partial X} + \frac{1}{2} \left\langle \sum_{i=1}^{n} u_i(Y) \left\{ \frac{\partial}{\partial X} [(X_{i+1} - X_i)f_{i,i+1} + (X_i - X_{i-1})f_{i-1,i}] \right. \right. \\
+ f'_{i,i+1}(\hat{\phi}_{i,i+1})(X_{i+1} - X_i)[u^1_X(X,Y,t,\tau) + u^1_X(X,Y_{i+1},t,\tau)] -
\]

15
\[ f'_{i+1}(\hat{\phi}_{t,i}) (X_i - X_{i-1}) [u_X'(X,Y_{i-1},t,\tau) + u_X'(X,Y_i,t,\tau)] \] 

(54)

where \( u_i'(Y_i) = \partial u_i'(Y_i) / \partial \tau \). Exploiting the chain rule, we have

\[
\frac{\partial f_{i+1}}{\partial \tau} = \frac{\partial f_{i+1}}{\partial \phi_{i+1}} \frac{\partial \phi_{i+1}}{\partial \tau} = f'_{i+1}(\hat{\phi}_{t,i}) [u_Y'(Y_{i+1}) - u_Y'(Y_i)]
\]

\[
\frac{\partial f_{i-1}}{\partial \tau} = \frac{\partial f_{i-1}}{\partial \phi_{i-1}} \frac{\partial \phi_{i-1}}{\partial \tau} = f'_{i-1}(\hat{\phi}_{t-1,i}) [u_Y'(Y_i) - u_Y'(Y_{i-1})]
\]

(55)

From Eq. (55) it follows

\[
\frac{\partial^2 u_i'(Y_i)}{\partial \tau \partial X} \left[ (X_{i+1} - X_i)f_{i+1} + (X_i - X_{i-1})f_{i-1,i} \right]
\]

\[
= \frac{\partial}{\partial \tau} \{ u_X'(Y_i) [(X_{i+1} - X_i)f_{i+1} + (X_i - X_{i-1})f_{i-1,i}] \} - \\
 u_X'(Y_i) \{ (X_{i+1} - X_i)f'_{i+1}(\hat{\phi}_{t,i}) [u_Y'(Y_{i+1}) - u_Y'(Y_i)] + \\
 (X_i - X_{i-1})f'_{i-1}(\hat{\phi}_{t-1,i}) [u_Y'(Y_i) - u_Y'(Y_{i-1})] \}
\]

(56)

From Eq. (56), we have

\[
\left\{ \sum_{i=1}^{n} u_i'(Y_i) \{ \frac{\partial}{\partial X} [(X_{i+1} - X_i)f_{i+1} + (X_i - X_{i-1})f_{i-1,i}] + \\
 f'_{i+1}(\hat{\phi}_{t,i}) (X_{i+1} - X_i)[u_X'(X,Y_{i-1},t,\tau) + u_X'(X,Y_{i+1},t,\tau)] - \\
 f'_{i-1}(\hat{\phi}_{t-1,i}) (X_i - X_{i-1})[u_X'(X,Y_{i-1},t,\tau) + u_X'(X,Y_i,t,\tau)] \} \right\}
\]

\[
= \left\{ \sum_{i=1}^{n} \frac{\partial}{\partial X} \{ u_i'(Y_i) [(X_{i+1} - X_i)f_{i+1} + (X_i - X_{i-1})f_{i-1,i}] \} - \\
\right\}
\]

16
$$\sum_{i=1}^{n} \frac{\partial^{2} u^{i}(Y_{i})}{\partial \tau \partial X} [(X_{i+1} - X_{i})f_{i,i+1} + (X_{i} - X_{i-1})f_{i,i-1}] +$$

$$\sum_{i=1}^{n} u^{i}_{X}(Y_{i})\{f'_{i,i+1}(\hat{\phi}_{i,i+1})(X_{i+1} - X_{i})[u^{i}_{X}(Y_{i}) + u^{i}_{X}(Y_{i+1})] -$$

$$f'_{i-1,i}(\hat{\phi}_{i-1,i})(X_{i} - X_{i-1})[u^{i}_{X}(Y_{i-1}) + u^{i}_{X}(Y_{i})]\}$$

$$= \left\{ \sum_{i=1}^{n} \frac{\partial}{\partial X} \left\{ u^{i}_{X}(Y_{i})[(X_{i+1} - X_{i})f_{i,i+1} + (X_{i} - X_{i-1})f_{i,i-1}] \right\} \right\} -$$

$$\\frac{\partial}{\partial \tau} \left\{ \sum_{i=1}^{n} u^{i}_{X}(Y_{i})[(X_{i+1} - X_{i})f_{i,i+1} + (X_{i} - X_{i-1})f_{i,i-1}] \right\} +$$

$$\left\{ \sum_{i=1}^{n} u^{i}_{X}(Y_{i})\{f'_{i,i+1}(\hat{\phi}_{i,i+1})(X_{i+1} - X_{i})[u^{i}_{X}(Y_{i}) - u^{i}_{X}(Y_{i+1})] +$$

$$(X_{i} - X_{i-1})f'_{i-1,i}(\hat{\phi}_{i-1,i})[u^{i}_{X}(Y_{i}) - u^{i}_{X}(Y_{i-1})]\} +$$

$$\sum_{i=1}^{n} u^{i}_{X}(Y_{i})\{f'_{i,i+1}(\hat{\phi}_{i,i+1})(X_{i+1} - X_{i})[u^{i}_{X}(Y_{i}) + u^{i}_{X}(Y_{i+1})] -$$

$$f'_{i-1,i}(\hat{\phi}_{i-1,i})(X_{i} - X_{i-1})[u^{i}_{X}(Y_{i-1}) + u^{i}_{X}(Y_{i})]\}$$

$$= \frac{\partial}{\partial X} \left\{ \sum_{i=1}^{n} \left\{ u^{i}_{X}(Y_{i})[(X_{i+1} - X_{i})f_{i,i+1} + (X_{i} - X_{i-1})f_{i,i-1}] \right\} \right\} +$$

$$\left\{ \sum_{i=1}^{n} \left\{ (X_{i+1} - X_{i})f'_{i,i+1}[u^{i}_{X}(Y_{i})u^{i}_{X}(Y_{i+1}) + u^{i}_{X}(Y_{i+1})u^{i}_{X}(Y_{i})] -$$

$$(X_{i} - X_{i-1})f'_{i-1,i}[u^{i}_{X}(Y_{i-1})u^{i}_{X}(Y_{i}) + u^{i}_{X}(Y_{i})u^{i}_{X}(Y_{i-1})]\} \right\}$$

(57)

Similar to the proof of Eq. (38), it can be proved that for the general atomistic unit cell consisting of \(n + 1\) atoms as illustrated in Figure 1, the following summation vanishes.
\[
\sum_{i=1}^{n} \{(X_{i+1} - X_{i}) f_{i+1}' \left[u_{X}^{1}(Y_{i})u_{r}^{1}(Y_{i+1}) + u_{X}^{1}(Y_{i+1})u_{r}^{1}(Y_{i})\right] - (X_{i} - X_{i-1}) f_{i-1}' \left[u_{X}^{1}(Y_{i-1})u_{r}^{1}(Y_{i}) + u_{X}^{1}(Y_{i})u_{r}^{1}(Y_{i-1})\right]\} = 0
\]  

(58)

Substituting Eq. (58) into (57) and the resulting equation into (54) yields

\[
\varepsilon \left\{ \sum_{i=1}^{n} \left[2 \frac{\partial u^{0}}{\partial t} + \frac{\partial u^{1}}{\partial \tau} \right] \left[f_{i+1}'(\hat{\phi}_{i+1}) \psi_{i+1} - f_{i-1}'(\hat{\phi}_{i-1}) \psi_{i-1}\right] \right\} \\
= 2l \frac{\partial u^{0}}{\partial t} \frac{\partial \langle P \rangle}{\partial X} + \frac{1}{2} \frac{\partial}{\partial X} \left\{ \sum_{i=1}^{n} \left\{ u_{r}^{1}(Y_{i}) [(X_{i+1} - X_{i}) f_{i+1} + (X_{i} - X_{i-1}) f_{i-1}] \right\} \right\}
\]

(59)

Inserting Eq. (59) into (53) and utilizing the coarse scale equation of motion (40) yields the thermal equation

\[
q(X, t, \tau) = \frac{1}{2l} \sum_{i=1}^{n} \left\{ u_{r}^{1}(Y_{i}) [(X_{i+1} - X_{i}) f_{i+1} + (X_{i} - X_{i-1}) f_{i-1}] \right\}
\]

(60)

where \( \langle q(X, t, \tau) \rangle \) is the fast-time average heat flux, or simply the heat flux and

\[
C = nK_{B} / l
\]

(61)

Remark: By the Ergodic hypothesis the (fast) time average of the property \( \langle A \rangle \) can be equated to the ensemble average of a property expressed in terms of an average over all microstates (which comprise the ensemble). A given coarse scale property, \( A \), and its fine scale (microscopic) function \( a = a(x_{\lambda}) \), which is a function of the positions and momenta of a system, i.e. the phase space vector, are related by

\[
\langle A \rangle = \frac{1}{N} \sum_{\lambda=1}^{N} a(x_{\lambda})
\]

where \( x_{\lambda} \) is the microstate of the \( \lambda^{th} \) member of the ensemble (see for instance [13]).
4 Verification by a Model Problem and Numerical Results

In this section, we focus on the development, implementation and verification of the generalized mathematical homogenization approach for the model problem of an atomic chain illustrated in Figure 2.

The two-scale problem described by Eqs. (25), (40) and (60) is solved as follows:

i. For every gauss point in the coarse scale solve the unit cell equation of motion for \( \hat{u}^i(X,Y_i,t,\tau) \) subjected to the \( F^0(X,t) \) using Eq. (25) and calculate the First Piola-Kirchhoff stress and heat flux by Eqs. (40) and (60), respectively.

ii. Solve the coarse scale problems (Eqs. (40) with appropriate initial and boundary conditions) using finite element semidiscretization in space and explicit time integration; evaluate the coarse scale deformation gradient \( \Phi^0(X,t) \) and go to i.

4.1 Formulation of the model problem

Consider a chain of initially equally spaced atoms with spacing \( a \) between atoms. The atomic chain is assumed to have a periodic structure with masses \( m_1 \) and \( m_2 \) and nearest neighbor interaction. The chain is subjected to then initial bell-shaped temperature distribution with amplitude \( T_{\text{max}} \) 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 interatomic potential between the first and the second atom in the unit cell is \( \Phi_1 \) and that between the second and the third atom is \( \Phi_2 \) given by

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

where \( \varepsilon_1 \) and \( \varepsilon_2 \) are characteristic energy scales of the interaction and \( \sigma \) the characteristic length scale of the interaction. We assume that the initial configuration of the atomic chain is in equilibrium without external forces so that \( a = 2^{1/6} \sigma \).
Figure 2: An atomic chain with a three-atom unit cell

The interatomic forces are evaluated as

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

(63)

By periodicity, the atomistic unit cell problem (25) reduces to

$$m_1 \frac{\partial^2 \hat{u}^1(Y_2)}{\partial r^2} = \varepsilon^2 [f_{01}(\hat{\phi}_{01}) - f_{12}(\hat{\phi}_{12})], \quad m_2 \frac{\partial^2 \hat{u}^1(Y_1)}{\partial r^2} = \varepsilon^2 [f_{12}(\hat{\phi}_{12}) - f_{01}(\hat{\phi}_{01})]$$

(64)

where

$$\hat{\phi}_{01} = (1 + u_x^0)a + \hat{u}^1(Y_1) - \hat{u}^1(Y_0), \quad \hat{\phi}_{12} = (1 + u_x^0)a + \hat{u}^1(Y_2) - \hat{u}^1(Y_1)$$

(65)

Adding the two equations in (64) yields

$$\frac{\partial^2}{\partial r^2} [m_1 \hat{u}^1(Y_2) + m_2 \hat{u}^1(Y_1)] = 0$$

(66)

From Eq. (66) it follows
\[ m_1 \ddot{u}^1(Y_2) + m_2 \ddot{u}^1(Y_1) = c_1 \tau + c_2 \]  

(67)

where \( c_1 \) and \( c_2 \) are integration constants.

As \( \tau \to \infty \), the left-hand-side of Eq. (67) must be bounded. Therefore

\[ c_1 = 0 \]  

(68)

Without loss of generality, we set \( c_2 = 0 \) as the normalization condition. Thus, we have

\[ m_1 \ddot{u}^1(Y_2) + m_2 \ddot{u}^1(Y_1) = 0 \]  

(69)

and therefore

\[ \ddot{u}^1(Y_0) = \ddot{u}^1(Y_2) = -\frac{m_2}{m_1} \ddot{u}^1(Y_1) \]  

(70)

The dynamic atomistic unit cell problem has only one independent equation

\[ m_2 \frac{\partial^2 \dot{u}^1(Y_1)}{\partial \tau^2} = \varepsilon^2 [f_{12}(\dot{\phi}_{12}) - f_{01}(\dot{\phi}_{01})] \]  

(71)

with

\[ \dot{\phi}_{01} = (1 + u_x^0)a + \frac{m_1 + m_2}{m_1} \dot{u}^1(Y_1), \quad \dot{\phi}_{12} = (1 + u_x^0)a - \frac{m_1 + m_2}{m_1} \dot{u}^1(Y_1) \]  

(72)

The coarse scale equation of motion is

\[ \rho_0 \frac{\partial^2 u^0(X,t)}{\partial t^2} - \frac{\partial \langle P \rangle}{\partial X} = 0 \]  

(73)

with the initial and boundary conditions:

\[ u^0(X,0) = p(X), \quad \frac{\partial u^0}{\partial t}(X,0) = g(X) \]  

(74)

\[ u^0(0,t) = u^0(L,t) = 0 \]  

(75)
The thermal equation is

\[
C \frac{\partial \langle T \rangle}{\partial t} - \frac{\partial \langle q \rangle}{\partial X} = 2\rho_0 \frac{\partial u^0}{\partial t} \frac{\partial^2 u^0}{\partial t^2}
\]  
(76)

with the initial and boundary conditions

\[
\langle T \rangle(X, 0) = \langle T_0 \rangle(X) 
\]  
(77)

\[
\langle T \rangle(0, t) = \langle T \rangle(L, t) = 0 
\]  
(78)

For the three-atom unit cell under consideration, the fast time scale instantaneous first Piola-Kirchhoff stress (40) and the heat flux (60) can be evaluated as

\[
P(X, t, \tau) = \frac{1}{2} [f_{01}(\dot{\phi}_{01})] + f_{12}(\dot{\phi}_{12}), \quad q(X, t, \tau) = \frac{m_1 - m_2}{2m_1} u_\tau(Y_1)P(X, t, \tau) 
\]  
(79)

The linear mass density is given by

\[
\rho_0 = \frac{1}{l} \sum_{i=1}^{2} m_i(Y) = (m_1 + m_2) / l 
\]  
(80)

### 4.2 The harmonic approximation

For the harmonic approximation of the interatomic potentials, the analytical solution to the dynamic atomistic unit cell problem can be constructed and the stress and heat flux can be obtained analytically. In this case, the interatomic potentials reduces to

\[
\Phi_1(r) = \frac{1}{2} k_1 (r - r_0)^2, \quad \Phi_2(r) = \frac{1}{2} k_2 (r - r_0)^2 
\]  
(81)

where \( r_0 = a = 2^{1/6} \sigma \), and

\[
k_1 = \frac{36 \times 4^{1/3} \varepsilon_1}{\sigma^2}, \quad k_2 = \frac{36 \times 4^{1/3} \varepsilon_2}{\sigma^2} 
\]  
(82)
The interatomic forces are evaluated as

\[
\frac{d\Phi_1}{dr} = k_1(r - r_0), \quad \frac{d\Phi_2}{dr} = k_2(r - r_0)
\]  

(83)

Therefore

\[
\begin{align*}
\hat{f}_{01}(\hat{\phi}_{01}) &= k_1[a u_X^0 + \hat{u}_1(Y_1) - \hat{u}_1(Y_0)], \\
\hat{f}_{12}(\hat{\phi}_{12}) &= k_2[a u_X^0 - (\hat{u}_1(Y_1) - \hat{u}_1(Y_0))]
\end{align*}
\]

(84)

\[
\begin{align*}
\hat{f}_{01}'(\hat{\phi}_{01}) &= \varepsilon k_1, \\
\hat{f}_{12}'(\hat{\phi}_{12}) &= \varepsilon k_2
\end{align*}
\]

(85)

The dynamic atomistic unit cell problem (71) becomes

\[
\frac{\partial^2 \hat{u}_1(Y_1)}{\partial \tau^2} + \alpha \hat{u}_1(Y_1) + \beta = 0
\]

(86)

where

\[
\alpha = \frac{\varepsilon^2(k_1 + k_2)(m_1 + m_2)}{m_1 m_2}, \quad \beta = \frac{\varepsilon^2(k_1 - k_2)au_X^0}{m_2}
\]

(87)

Taking the Laplace transform of Eq. (86) with respect to the fast time \(\tau\) yields

\[
s^2 \tilde{u}_1(Y_1, s) - s \hat{u}_0^1 - \hat{u}_0^1 + \alpha \tilde{u}_1(Y_1, s) + \frac{\beta}{s} = 0
\]

(88)

where \(s\) is complex; \(\tilde{u}_1(Y_1, s)\) is the Laplace transform of \(\hat{u}_1(Y_1, \tau)\), and

\[
\begin{align*}
\hat{u}_0^1 &= \hat{u}_1(Y_1, \tau = 0), \\
\hat{u}_{\tau=0} &= \frac{\partial \hat{u}_1}{\partial \tau}(Y_1, \tau = 0)
\end{align*}
\]

(89)

are initial conditions for \(\hat{u}_1(Y_1, \tau)\) in the fast time \(\tau\).

From Eq. (88) it follows

\[
\tilde{u}_1(Y_1, s) = \frac{s \hat{u}_0^1}{s^2 + \alpha} + \frac{\hat{u}_0^1}{s^2 + \alpha} - \frac{\beta}{s(s^2 + \alpha)}
\]

(90)
Taking the inverse Laplace transform of Eq. (90) yields

\[
\hat{u}^1(Y_1, \tau) = (\hat{u}_0^1 - \delta) \cos(\omega \varepsilon \tau) + \frac{\hat{u}_{\varepsilon 0}^1}{\varepsilon \omega} \sin(\omega \varepsilon \tau) + \delta
\]  

(91)

where

\[
\omega = \sqrt{\frac{(k_1 + k_2)(m_1 + m_2)}{m_1 m_2}} \]

\[
\delta = -\beta / \alpha = \frac{m_1 (k_2 - k_1) a u_x^0}{(k_1 + k_2)(m_1 + m_2)}
\]  

(92)

From the solution (91), we can readily identify the period of \( \dot{u}_1(Y_1, \tau) \) in \( \tau \) as

\[
\tau_0 = \frac{2\pi}{\varepsilon \omega} = \frac{2\pi}{\varepsilon} \sqrt{\frac{m_1 m_2}{(k_1 + k_2)(m_1 + m_2)}}^{1/2}
\]  

(93)

The fast time instantaneous first Piola-Kirchhoff stress and heat flux in Eq. (79) become

\[
P(X, t, \tau) = \frac{(k_1 + k_2) a u_x^0}{2} + \frac{(k_1 - k_2)(m_1 + m_2)}{2 m_1} \dot{u}^1(Y_1, \tau)
\]  

(94)

\[
q(X, t, \tau) = \frac{m_1 - m_2}{4 m_1^2} u_x^1(Y_1) [(k_1 + k_2) m_1 a u_x^0 + (k_1 - k_2)(m_1 + m_2) \dot{u}_1(Y_1, \tau)]
\]  

(95)

Substituting the solution (91) into (94) and (95), and recalling

\[
\langle \sin(\omega \varepsilon \tau) \rangle = \langle \cos(\omega \varepsilon \tau) \rangle = \frac{1}{\tau_0} \int_0^{\tau_0} \sin(\omega \varepsilon \tau) d\tau = 0
\]  

(96)

\[
\langle \sin(\omega \varepsilon \tau) \cos(\omega \varepsilon \tau) \rangle = 0, \quad \langle \sin^2(\omega \varepsilon \tau) \rangle = \langle \cos^2(\omega \varepsilon \tau) \rangle = \frac{1}{2}
\]  

(97)

we have

\[
\langle P(X, t, \tau) \rangle = \frac{2 k_1 k_2 a u_x^0}{k_1 + k_2}, \quad \langle q(X, t, \tau) \rangle = 0
\]  

(98)
Therefore, the coarse scale equation of motion (73) and the thermal equation (76) become

\[
\rho_0 \frac{\partial^2 u^0(X, t)}{\partial t^2} - E u^0_{xx} = 0 \tag{99}
\]

\[
C \frac{\partial \langle T \rangle}{\partial t} = 2 \rho_0 \frac{\partial u^0}{\partial t} \frac{\partial^2 u^0}{\partial t^2} \tag{100}
\]

where

\[
E = \frac{2ak_1k_2}{k_1 + k_2} \tag{101}
\]

The thermal equation (100) can be integrated analytically as

\[
C \frac{\partial \langle T \rangle}{\partial t} = \frac{\partial}{\partial t} [\rho_0 (\frac{\partial u^0}{\partial t})^2] \Rightarrow \frac{\partial}{\partial t} [C \langle T \rangle - \rho_0 (\frac{\partial u^0}{\partial t})^2] = 0 \tag{102}
\]

Therefore

\[
\langle T \rangle(X, t) = \frac{m_1 + m_2}{2K_B} \left( \frac{\partial u^0}{\partial t} \right)^2 + A(X) \tag{103}
\]

where \( A(X) \) is an determined by the initial condition as follows.

Based on Eq. (45), the fast time instantaneous temperature at a macroscopic point, which corresponds to a unit cell can be evaluated as

\[
m_2 \left[ \frac{\partial u^0}{\partial t} + \frac{\partial u^1(Y_1)}{\partial \tau} \right]^2 + m_1 \left[ \frac{\partial u^0}{\partial t} + \frac{\partial u^1(Y_2)}{\partial \tau} \right]^2 = 2K_B T(X, t, \tau) \tag{104}
\]

Inserting Eq. (70) into (104) yields

\[
T(X, t, \tau) = \frac{m_1 + m_2}{2K_B} \left( \frac{\partial u^0}{\partial t} \right)^2 + \frac{m_2(m_1 + m_2)}{2K_B m_1} \left[ u_1^0(Y_1) \right]^2 \tag{105}
\]

From Eq. (91), we have

25
\[ u^i_i(Y_1) = -(\hat{u}^i_0 - \delta)\omega \sin(\omega \varepsilon \tau) + \frac{\hat{u}^i_{\tau 0}}{\varepsilon} \cos(\omega \varepsilon \tau) \quad (106) \]

where \( \delta \) corresponds to the static equilibrium position of atom 1 in the unit cell. To illustrate this, we consider the corresponding static unit cell problem of Eq. (71)

\[ f_{12}(\hat{\phi}_{12}) - f_{01}(\hat{\phi}_{01}) = 0 \quad (107) \]

which can be written for the harmonic approximation as

\[ (k_2 - k_1)au^0_x = \frac{(k_1 + k_2)(m_1 + m_2)}{m_1} \hat{u}^1(Y_1) = 0 \quad (108) \]

From the above equation, it follows

\[ \hat{u}^1(Y_1) = \frac{m_2(k_2 - k_1)au^0_x}{(k_1 + k_2)(m_1 + m_2)} = \delta \quad (109) \]

Taking the initial displacement \( \hat{u}^0_0 \) for the dynamic unit cell problem to be the static equilibrium position, i.e., \( \hat{u}^0_0 = \delta \), we have from Eq. (106)

\[ u^i_i(Y_1) = u^i_{i0} \cos(\omega \varepsilon \tau) \quad (110) \]

Inserting Eq. (110) into (105) yields

\[ T(X, t, \tau) = \frac{m_1 + m_2}{2K_B} \left( \frac{\partial u^0_x}{\partial t} \right)^2 + \frac{2m_2(m_1 + m_2)}{2K_B m_1} (u^1_{\tau 0})^2 \cos^2(\omega \varepsilon \tau) \quad (111) \]

At the initial state, we specify

\[ \sum_{i=1}^{\delta} \dot{u}_i = 0 \quad \Rightarrow \quad 2u^0_{i0} + \frac{m_1 - m_2}{m_1} u^1_{i0} = 0 \quad (112) \]

where Eq. (70) has been utilized and

\[ u^0_{i0} = \frac{\partial u^0_x}{\partial t} (t = 0) \quad (113) \]
Inserting Eq. (112) into (111), we have

\[
T_0(X) = T(X,0,0) = \frac{m_1 + m_2}{2K_B} \left(\frac{m_1 + m_2}{2m_1}\right)^2 (u^0_{r_0})^2
\]  

(114)

From Eqs. (114) and (112) it follows

\[
(u^1_{r_0})^2 = \left(\frac{2m_1}{m_1 + m_2}\right)^2 \frac{2K_B T_0(X)}{m_1 + m_2}, \quad (u^0_{r_0})^2 = \left(\frac{m_1 - m_2}{m_1 + m_2}\right)^2 \frac{2K_B T_0(X)}{m_1 + m_2}
\]

(115)

Substituting Eq. (115) into (111) yields

\[
T(X,t,\tau) = \frac{m_1 + m_2}{2K_B} \left(\frac{\partial u^0}{\partial t}\right)^2 + 4m_1 m_2 T_0(X) \frac{\cos^2(\omega \varepsilon \tau)}{(m_1 + m_2)^2}
\]

(116)

\[
\langle T \rangle(X,t) = \frac{m_1 + m_2}{2K_B} \left(\frac{\partial u^0}{\partial t}\right)^2 + \frac{2m_1 m_2 T_0(X)}{(m_1 + m_2)^2}
\]

(117)

Comparing Eq. (117) with (103), it can be seen that

\[
A(X) = \frac{2m_1 m_2 T_0(X)}{(m_1 + m_2)^2}
\]

(118)

### 4.3 The two-scale algorithm

For the general nonlinear interatomic potentials, the coarse scale equation of motion (73) and the thermal equation (76) depend on the fine scale variable \( \hat{u}^1(X, Y_i, t, \tau) \), which is determined by the dynamic atomistic unit cell problem (71) subjected to the periodic boundary conditions (70). The dynamic unit cell problem in turn depends on the coarse scale deformation gradient \( F^0 \), which is obtained from the constitutive law-free coarse scale equation of motion. The coarse scale equation of motion (73), the thermal equation (76) and the dynamic unit cell problem (71) are coupled and have to be solved concurrently.

The two-scale algorithm developed in this Section consists of the finite element semidiscretization in space and explicit time integration for advancing the coarse scale
problems and the explicit fast time integration for solving a sequence of nonlinear
dynamic unit cell problems.

Weak forms of the coarse scale equation of motion and the thermal equation are given as:

For each \( t \in (0, T] \), find \( u^0(X,t) \in \mathcal{U}_t \), \( \langle T \rangle(X,t) \in \mathcal{U}_t \), such that for all \( w(X) \in \mathcal{V} \):

\[
\int_0^L \rho_0 w(X) \frac{\partial^2 u^0(X,t)}{\partial t^2} \, dX - \int_0^L w(X) \frac{\partial \langle P \rangle}{\partial X} \, dX = 0 \tag{119}
\]

\[
\int_0^L Cw(X) \frac{\partial \langle T \rangle}{\partial t} \, dX - \int_0^L w(X) \frac{\partial \langle q \rangle}{\partial t} \, dX = \int_0^L 2\rho_0 w(X) \frac{\partial u^0}{\partial t} \frac{\partial^2 u^0}{\partial t^2} \, dX \tag{120}
\]

subjected to the initial conditions

\[
u^0(X,0) = p(X) = 0, \quad \frac{\partial u^0}{\partial t}(X,0) = g(X) = \frac{m_1 - m_2}{m_1 + m_2} \left[ \frac{2K_p T^0(X)}{m_1 + m_2} \right]^{1/2} \tag{121}
\]

\[
\langle T \rangle(X,0) = \langle T^0 \rangle(X) \tag{122}
\]

where

\[
\mathcal{U}_t = \{ u(X,t) \mid u(X,t) \in H^1(0,L), u(0,t) = u(L,t) = 0 \} \tag{123}
\]

\[
\mathcal{V} = \{ w(X) \mid w(X) \in H^1(0,L), w(0) = w(L) = 0 \} \tag{124}
\]

are the solution space and weighting space, respectively; the Sobolev space \( H^1(0,L) \)
consists of all functions over \( (0,L) \) whose values and first derivatives are square
integrable over the domain.

Integrating Eqs. (119) and (120) by parts, and then introducing the finite element
discretization in space yields the semidiscrete equation of motion and the thermal
equation

\[
M \frac{\partial^2 d(t)}{\partial t^2} + f^n(d(t)) = 0 \tag{125}
\]
\[ C \frac{\partial \theta(t)}{\partial t} + Q''(\theta(t)) = S(t) \]  

(126)

with initial conditions

\[ \mathbf{d}(0) = \mathbf{d}_0 = \mathbf{0}, \quad \frac{\partial \mathbf{d}}{\partial t}(0) = \mathbf{v}_0, \quad \theta(0) = \theta_0 \]  

(127)

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

\[ \mathbf{M} = \sum_{e=1}^{N_e} \int_{k_e} \rho_e \mathbf{N}^T \mathbf{N} dx, \quad \mathbf{C} = \sum_{e=1}^{N_e} \int_{k_e} \mathbf{C} \mathbf{N}^T \mathbf{N} dx \]  

(128)

are the mass and capacity matrices, respectively;

\[ \mathbf{f}^{in}(\mathbf{d}(t)) = \sum_{e=1}^{N_e} \int_{k_e} \mathbf{N}^T \mathbf{P} dx, \quad \mathbf{Q}''(\theta(t)) = \sum_{e=1}^{N_e} \int_{k_e} \mathbf{N}^T (q_x) dx \]  

(129)

are the vectors of internal force and heat flux, respectively;

\[ \mathbf{S}(t) = 2\rho_0 \sum_{e=1}^{N_e} \int_{k_e} \mathbf{N}^T \frac{\partial \mathbf{u}^0}{\partial t} \frac{\partial^2 \mathbf{u}^0}{\partial t^2} dx \]  

(130)

is the vector of heat source arising from equation of motion; \( \mathbf{N} \) is the matrix of finite element shape functions and \( \mathbf{N}_X = d\mathbf{N}/dx \). Since the vectors of internal force \( \mathbf{f}^{in}(\mathbf{d}(t)) \) and heat flux \( \mathbf{Q}''(\theta(t)) \) depend on the displacement and temperature vectors, the semidiscrete equation of motion and thermal equation are coupled nonlinear equations.

The equation of motion (125) and the thermal equation (126) can be integrated using explicit time integration schemes, such as for instance the central difference and forward difference, respectively:

\[ \left(\frac{\partial^2 \mathbf{d}}{\partial t^2}\right)_n = \left(\mathbf{d}_{n-1} - 2\mathbf{d}_n + \mathbf{d}_{n+1}\right) / \Delta t^2 \]  

(131)

\[ \left(\frac{\partial \theta}{\partial t}\right)_n = \left(\theta_{n+1} - \theta_n\right) / \Delta t \]  

(132)
where \( \partial^2 d / \partial t^2 \) = \( \partial^2 d / \partial t^2(t) \) , \( d_n = d(t) \) , \( d_{n-1} = d(t-\Delta t) \) , \( d_{n+1} = d(t+\Delta t) \); 
\( \partial \theta / \partial t \) = \( \partial \theta / \partial t(t) \) , \( \theta_n = \theta(t) \) and \( \theta_{n+1} = \theta(t+\Delta t) \).

Inserting Eqs. (131) and (132) into (125) and (126) yields

\[
d_{n+1} = 2d_n - d_{n-1} - \Delta t^2 M^{-1} f''(d_n) \tag{133}
\]

\[
\theta_{n+1} = \theta_n + \Delta t C^{-1}[S_n - Q''(\theta_n)] \tag{134}
\]

The dynamic atomistic unit cell problem (71) can also be integrated in the fast time employing the central difference scheme as follows:

\[
(\partial^2 \hat{u}^1 / \partial \tau^2) = (\hat{u}^1_{n-1} - 2\hat{u}^1_n + \hat{u}^1_{n+1}) / \Delta \tau^2 \tag{135}
\]

where \( \tau = \epsilon \tau \) , \( \partial^2 \hat{u}^1 / \partial \tau^2(\tau) = (\partial^2 \hat{u}^1 / \partial \tau^2)(\hat{\tau}) \) , \( \hat{u}^1_{n-1} = \hat{u}^1(Y, \hat{\tau} - \Delta \hat{\tau}) \) , \( \hat{u}^1_n = \hat{u}^1(Y, \hat{\tau}) \) , and \( \hat{u}^1_{n+1} = \hat{u}^1(Y, \hat{\tau} + \Delta \hat{\tau}) \).

Substituting Eq. (135) into (71) yields

\[
\hat{u}^1_{n+1} = 2\hat{u}^1_n - \hat{u}^1_{n-1} + \Delta \hat{\tau}^2[f_{12}(\hat{\phi}_{12}) - f_{01}(\hat{\phi}_{01})] / m_2 \tag{136}
\]

with the initial conditions

\[
\hat{u}^1(Y, 0) = \hat{u}^1_0 , \quad \frac{\partial \hat{u}^1}{\partial \tau}(Y, 0) = \frac{\partial u^1}{\partial \tau}(Y, 0) = u^1_{r_0} = \frac{2m_1}{m_1 + m_2} \frac{[2K_B T_0(X)]^{1/2}}{m_1 + m_2} \tag{137}
\]

At each time step, the dynamic atomistic unit cell problem (136) is first solved for \( \hat{u}^1(X, Y, t, \tau) \) , then the stress \( \langle P \rangle \) and heat flux \( \langle q \rangle \) are evaluated according to Eqs. (72) and (79). The vectors of internal force and heat flux are evaluated based on Eq. (129). The time integration proceeds based on Eqs. (133) and (134).
4.4 Verification

We consider an atomic chain consisting of 601 atoms schematically depicted in Figure 2. The interatomic potentials are Lennard-Jones potentials given in Eq. (62). Material parameters are: \( \frac{m_z}{m_1} = 5 \) and \( \frac{\varepsilon_z}{\varepsilon_i} = 2 \). The amplitude of the initial temperature is set to be \( T_{\text{max}} = 2K \).

First, we consider the harmonic approximation of the interatomic potentials. For this case, the coarse scale equation of motion is linear, and the analytical solutions for \( T(X,t,\tau) \) and \( \langle T \rangle \) are given by Eq. (116) and (117), respectively. The coarse scale equation of motion is solved by using the finite element method and the temperature fields are evaluated analytically after the coarse scale velocity \( \partial u^0 / \partial t \) is found.

Figure 3 depicts the plot of \( T(X,t,\tau) \), \( \langle T \rangle \) and the coarse scale displacement evaluated at atom 401 and compares with the results of the molecular dynamics simulation.
It can be observed that the coarse scale displacement predicted by the GMH closely matches the result of the MD simulation. The fast time instantaneous temperature field $T(X, t, \tau)$ is in good agreement with MD simulation, while the fast time average averaged $\langle T \rangle$ correctly predicts the and average value predicted by MD simulation.

Next, we consider the general nonlinear interatomic potentials in the form of Lennard-Jones as depicted in Eq. (62). For this case, the coarse scale equation of motion and the thermal equation are nonlinear and are solved both numerically based on the two-scale algorithm detailed in Section 4.3.
The solutions for the temperature and displacement at atom 401 by the two-scale algorithm based on the GMH and the results of the MD simulation are plotted in Figure 4. It can be seen that the displacement predicted by the GMH closely matches that of the MD, and the temperature field of the GMH correctly predicts the trend and the average values of the temperature field obtained by the molecular dynamics simulation.
Snapshots of temperature and displacement fields at different time instances over the whole atomic chain are also plotted in Figure 5 and Figure 6, respectively. It can be observed that as time increases, the temperatures over the whole atomic chain drop and become smaller and smaller compared with the initial temperature, indicating the heat conduction through the atomic chain, whereas the displacements over the whole atomic chain increase, revealing the thermal expansion driven by the initial temperature gradient. Because the temperature field of the MD simulation is highly oscillatory, the temporally and spatially averaged temperature values of the MD simulation are plotted in Figure 5.
Figure 6: Snapshots of displacements at different time instances

5 Acknowledgment

The financial supports of National Science Foundation under grants CMS-0310596, 0303902, 0408359 and Sandia National Laboratory under contract DE-ACD4-94AL85000 are gratefully acknowledged.

6 References


