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A non-equilibrium multiscale simulation of shock wave propagation

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Abstract

A novel non-equilibrium multiscale dynamics (NEMSD) is proposed to simulate non-equilibrium thermal–mechanical processes. The model couples coarse-grain thermodynamics with a fine scale molecular dynamics. A *Distributed Nośe-Hoover Thermostat Network* is used, which regulates the temperature in each coarse scale Voronoi cell according to the finite element (FE) nodal temperature. The atoms in each element-cell, namely Voronoi cell-ensemble, are assumed to be in a local equilibrium state within one coarse scale time step. The change of FE nodal temperature provides a source of random forces, which drive the system out of equilibrium. The proposed NEMSD can successfully simulate shock wave propagation in a cubic lattice.

Keywords: Atomistic simulation; Coarse grain; Multiscale simulation; Nonequilibrium molecular dynamics; Shock wave

1. Introduction

Traditional simulation methods of computational mechanics are confined within a single-scale of physics. For example, finite element methods (FEM) only can deal with problems of continuum mechanics, while molecular dynamics (MD) provides estimation of discrete atomistic motions at the atomistic scale. These ''single-scale'' methods have their limitations, as FEM cannot provide atomistic details while MD cannot simulate a large domain due to its computational cost. The multiscale computation is a new simulation technique that aims to bring the best of the two worlds by using continuum simulation methods in the most part of the domain of interest and using first principle based methods in only places where atomistic precision is required. Many multiscale methods have been proposed in recent years and they have been successful for certain problems. They include Abraham and his co-workers' macroscopic, atomistic, *ab initio* dynamics (MAAD) (1998), Rudd and Broughton's coarse-grained molecular dynamics (CGMD) (1998, 2005), Liu and his co-workers' bridging scale method (Wagner and Liu, 2003; Wagner et al., 2004; Park et al., 2005), E and his co-workers' heterogeneous multiscale method (2001, 2003), and among others.

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This paper presents a novel non-equilibrium multiscale dynamics (NEMSD) method that can simulate non-equilibrium thermal–mechanical coupling process at small scales. The conventional MD and equilibrium MD are unable to simulate non-equilibrium processes. Since early 1980s, the non-equilibrium molecular dynamics (NEMD) has become a major simulation tool for simulations of non-equilibrium processes, which is largely due to the contribution made by Hoover (1983) and Evans and Morriss (1990). According to different ways to drive the system out of equilibrium, there are mainly three types of NEMDs: boundary-driven NEMD (Baranyai, 1996; Müller-Plathe, 1997; Lepri et al., 2003), prescribed-flow-driven NEMD (Evans and Morriss, 1990; Tuckerman et al., 1997; Dressler and Edwards, 2002), and the synthetic NEMD (Evans et al., 1983; Zhang et al., 2000; Bright and Evans, 2005).

The NEMD shares the same difficulties as the conventional MD due to its inability to simulate a realistically sized domain. The advantages of the proposed NEMSD over NEMD are two folds. First, it is a multiscale simulation, so in general it saves computational cost. In the proposed NEMSD, the mean field, or the coarse-grained thermodynamics field, is solved over the entire domain by using FEM with the inputs from both boundary and initial conditions; whereas the fine scale fluctuation is solved via a first-principle based MD model for specific regions where atomistic resolution is desired. The second advantage is in the way non-equilibrium phenomenon is modeled. The traditional NEMD only introduces a constant external field to drive the system out of equilibrium, whereas the proposed NEMSD uses the coarse scale mean field or the nonuniform drift field to drive the fine scale system out of equilibrium. In the proposed NEMSD, a *Distributed Nośe-Hoover Thermostat Network* is used, in which each coarse scale finite element (FE) cell may be viewed as an element ensemble whose statistical properties is regularized by a Nośe-Hoover thermostat according to the current temperature of the FE node inside the cell.

The change of FE nodal temperature provides a source of random force. In turn, the fine scale simulation results are used to update temperature and displacement field at coarse-grain level, and it may also be used to calculate the transport coefficients for the coarse-grain formulation.

2. Multiscale non-equilibrium molecular dynamics

We start with the multiscale decomposition proposed by Wagner and Liu (2003) and Rudd and Broughton (1998), which decomposes the discrete atomistic displacement field, $\mathbf{q}$, into a coarse scale part and a fine scale part: $\mathbf{q} = \bar{\mathbf{q}} + \mathbf{q}\prime$. The symbol $\bar{}$ indicates coarse scale quantities and the symbol $\prime$ indicates their fine scale counterparts. The multiscale displacement decomposition implies similar decompositions for velocities and momentums, i.e. $\mathbf{v} = \bar{\mathbf{v}} + \mathbf{v}\prime$ and $\mathbf{p} = \bar{\mathbf{p}} + \mathbf{p}\prime$. We assume that the coarse scale atomistic displacements can be described by a continuous mean field $\bar{\mathbf{u}}(\mathbf{X})$, which is defined by a FE interpolation field,

$$\bar{\mathbf{u}} = \mathbf{N}(\mathbf{X})\mathbf{d}, \quad \Rightarrow \bar{\mathbf{q}} = \mathbf{N}(\mathbf{X}_\mathrm{a})\mathbf{d} \tag{1}$$

where $\mathbf{d}$ is FE nodal displacement array, $\mathbf{N}(\mathbf{X}_\mathrm{a})$ is the FE shape function matrix evaluated at the position $\mathbf{X}_\mathrm{a}$ of the atom a. With the bridging scale formulation, both the coarse scale components and the fine scale components can be obtained from the total scale variable: $\bar{\mathbf{q}} = \mathbf{P}(\mathbf{X}_\mathrm{a})\mathbf{q}$, $\mathbf{q}' = \mathbf{Q}(\mathbf{X}_\mathrm{a})\mathbf{q}$, where $\mathbf{P}$ and $\mathbf{Q}$ are projection operators defined as $\mathbf{P} = \mathbf{N}\mathbf{M}^{-1}\mathbf{N}^T\mathbf{M}_\mathrm{a}$ and $\mathbf{Q} = \mathbf{I} - \mathbf{P}$, $\mathbf{M}_\mathrm{a}$ is the diagonal mass matrix for atoms and $\mathbf{M} = \mathbf{N}^T\mathbf{M}_\mathrm{a}\mathbf{N}$ is the coarse scale mass matrix.

A conceptual illustration of the multiscale simulation is shown in Fig. 1. The mean field motions are solved by using FEM over the entire domain based on a coarse-grain model. Whereas the fine scale motions are solved via a first-principal based MD model for specific regions where atomistic resolution is desired. For a single cell-ensemble c surrounding the FE node I, the following multiscale adiabatic Hamiltonian can be written

$$H_c^{\mathrm{adia}} = \sum_{i=1}^{n_\mathrm{c}} \frac{1}{2m_i}\bar{\mathbf{p}}_i \cdot \bar{\mathbf{p}}_i + \sum_{i=1}^{n_\mathrm{c}} \frac{1}{2m_i}\mathbf{p}_i' \cdot \mathbf{p}_i' + U(\mathbf{q}) \tag{2}$$

where n_c is the number of atoms in the cell-ensemble c. Note that the coarse scale momentum is orthogonal to the fine scale momentum, i.e.

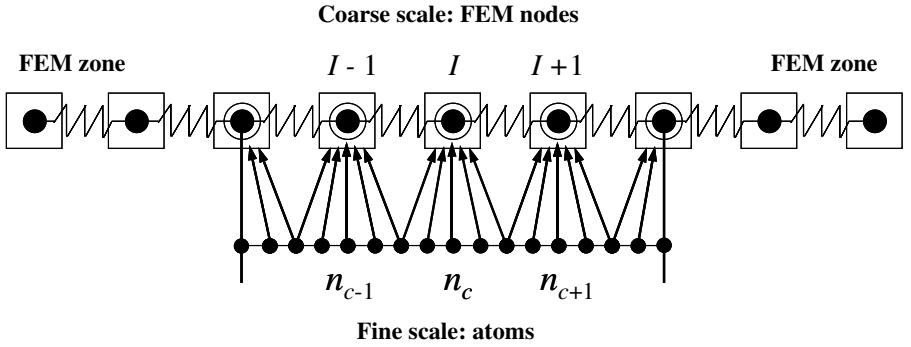

Fig. 1. The structure of distributed Nośe-Hoover thermostat.

$$\sum_i \bar{\mathbf{p}}_i \cdot \mathbf{p}'_i = 0, \quad \Leftarrow \mathbf{PQ} = \mathbf{P}(\mathbf{I} - \mathbf{P}) \equiv 0 \tag{3}$$

The two-scale equations of motion are then given as

$$\dot{\mathbf{q}}_i = \frac{\partial H_c^{\text{adia}}}{\partial \mathbf{p}_i} = \frac{\bar{\mathbf{p}}_i}{m_i} + \frac{\mathbf{p}'_i}{m_i} \quad \text{and} \quad \dot{\mathbf{p}}_i = -\frac{\partial H_c^{\text{adia}}}{\partial \mathbf{q}_i} = -\frac{\partial U(\mathbf{q})}{\partial \mathbf{q}_i} = \mathbf{F}_i \tag{4}$$

$$\dot{\bar{\mathbf{q}}}_i = \frac{\partial H_c^{\text{adia}}}{\partial \bar{\mathbf{p}}_i} = \frac{\bar{\mathbf{p}}_i}{m_i} \quad \text{and} \quad \dot{\bar{\mathbf{p}}}_i = -\frac{\partial H_c^{\text{adia}}}{\partial \bar{\mathbf{q}}_i} = \mathbf{F}_j \frac{\partial \mathbf{q}_j}{\partial \bar{\mathbf{q}}_i} \tag{5}$$

In terms of FE nodal degrees of freedom, Eq. (5) becomes $\mathbf{M}\ddot{\mathbf{d}} = \mathbf{N}^T\mathbf{F}$, whereas the fine scale equations of motion may be expressed in terms of $\mathbf{q}_i$ and $\mathbf{p}'_i$ as follows,

$$\dot{\mathbf{q}}_i = \frac{\bar{\mathbf{p}}_i}{m_i} + \frac{\mathbf{p}'_i}{m_i} \quad \text{and} \quad \dot{\mathbf{p}}'_i = \mathbf{F}_i - \dot{\bar{\mathbf{p}}}_i \tag{6}$$

In the proposed NEMSD, each coarse scale FE node may be viewed as a thermal reservoir. The atoms surrounding each FE node, namely each Voronoi cell-ensemble (see Fig. 2), are assumed to be in a local equilibrium state within the duration of the coarse-grain time scale length. In passing, we note that the length scale of the Voronoic cell-ensemble should be comparable with the phonon mean free path, which may change from place to place due to the presence of defects. To couple the local equilibrium state with the coarse scale heat conduction, we use a local Nośe-Hoover thermostat such that the fine scale equations of motion become

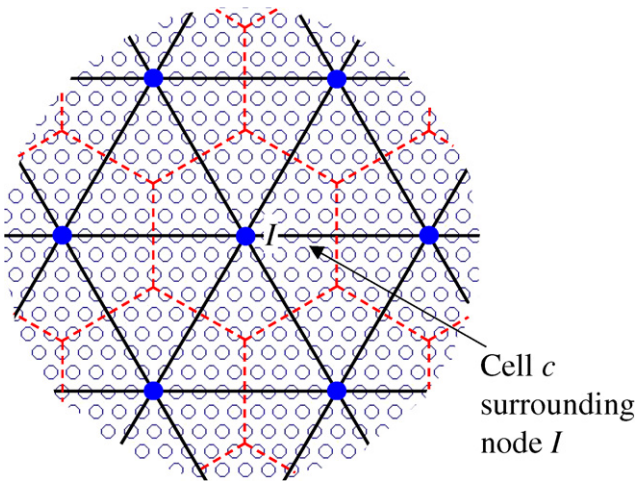

Fig. 2. Coarse-grain FE mesh and Voronoi cell-ensemble.

$$\dot{\mathbf{q}}_i = \frac{\bar{\mathbf{p}}_i}{m_i} + \frac{\mathbf{p}'_i}{m_i} \quad \text{and} \quad \dot{\mathbf{p}}'_i = \mathbf{F}_i - \dot{\bar{\mathbf{p}}}_i - \xi_c \mathbf{p}'_i \tag{7}$$

$\forall i \in \mathbf{n}_c$, $\mathbf{n}_c = \{1,\ldots, n_c\}$ and

$$\dot{\xi}_c = \frac{1}{Q_c}\left(\sum_{i\in\mathbf{n}_c} \frac{\mathbf{p}'_i \cdot \mathbf{p}'_i}{2m_i} - 3n_c k_B T_c\right) \tag{8}$$

where k_B is the Boltzmann constant, Q_c is the pseudo mass of the auxiliary variable ξ_c, and the local cell temperature T_c for each cell-ensemble is the coarse scale thermodynamic temperature at FE node I. Since the FE nodal temperature changes from node to node and time to time, the local temperature differs among different cell-ensembles and from different coarse scale time steps. It results in a distributed Nośe-Hoover thermostat network, which provides right amount random forces or fluctuations to maintain the specified temperature. The authors have proved in a recent paper (Li et al., submitted) that the distributed Nośe-Hoover thermostat network renders the distribution function in each cell-ensemble canonical.

3. Coarse-grain model

In this paper, we adopt non-equilibrium coarse scale thermodynamics, which is associated with a coarse-grained Helmholtz free energy that is based on both the Cauchy–Born rule and the quasi-harmonic approximation (Diestler, 2002; Jiang et al., 2005). The approximated free energy expression allows us to derive macroscopic quantities for coupled thermo–mechanical equations. If the local deformation is homogeneous, the total atomistic potential U_0 can be written as: $U_0 \approx U_0(\bar{\mathbf{F}}^c)$, where $\bar{\mathbf{F}}^c$ is the average deformation gradient within a cell c, which is approximated as the value of the coarse scale deformation gradient evaluated at the node I. According to the harmonic approximation, the Helmholtz free energy in a cell-ensemble c has the form of (Weiner, 1983):

$$\Phi^c(\bar{\mathbf{F}}^c, T_c) = U_0(\bar{\mathbf{F}}^c) + k_B T_c \sum_{i=1}^{n_c}\sum_{k=1}^{3} \log\left[2\sinh\left(\frac{\hbar\omega_{ik}(\bar{\mathbf{F}}^c)}{4\pi k_B T_c}\right)\right] \tag{9}$$

where $\hbar$ is Planck's constant divided by 2π; ω_{ik} are normal mode frequencies for the lattice, which can be determined via harmonic approximation; and T_c is the coarse scale thermodynamic temperature. Note that in the proposed NEMSD, T_c is updated based on fine scale atomistic velocities:

$$T_c = \frac{2}{3(n_c-1)k_B}\left\langle \sum_{i=1}^{n_c} \frac{\mathbf{p}'_i \cdot \mathbf{p}'_i}{2m_i} \right\rangle \tag{10}$$

where $\langle\cdot\rangle$ denotes averaging in time. With Φ^c available, one can derive the expressions for the state variables such as the first Piola–Kirchhoff stress $\mathbf{P}^c$, the specific heat at constant temperature $\mathbf{C}^c_T$ and the specific heat at constant volume C^c_V:

$$\mathbf{P}^c(\bar{\mathbf{F}}^c, T_c) = \frac{1}{\Omega_c}\frac{\partial \Phi^c}{\partial \bar{\mathbf{F}}^c} = \frac{1}{\Omega_c}\left\{U'_0(\bar{\mathbf{F}}^c) + \frac{\hbar}{4\pi}\sum_{i=1}^{n_c}\sum_{k=1}^{3}\left[\coth\left(\frac{\hbar\omega_{ik}(\bar{\mathbf{F}}^c)}{4\pi k_B T_c}\right)\omega'_{ik}(\bar{\mathbf{F}}^c)\right]\right\} \tag{11}$$

$$\mathbf{C}^c_T(\bar{\mathbf{F}}^c, T_c) = -T_c\frac{\partial^2 \Phi^c}{\partial T_c \partial \bar{\mathbf{F}}^c} = \frac{-\hbar^2}{16\pi^2 k_B T_c}\sum_{i=1}^{n_c}\sum_{k=1}^{3}\omega_{ik}(\bar{\mathbf{F}}^c)\omega'_{ik}(\bar{\mathbf{F}}^c)\left(\sinh^2\left(\frac{\hbar\omega_{ik}(\bar{\mathbf{F}}^c)}{4\pi k_B T_c}\right)\right)^{-1} \tag{12}$$

$$C^c_V(\bar{\mathbf{F}}^c, T_c) = -T_c\frac{\partial^2 \Phi^c}{\partial T_c^2} = k_B\sum_{i=1}^{n_c}\sum_{k=1}^{3}\left(\frac{\hbar\omega_{ik}(\bar{\mathbf{F}}^c)}{4\pi k_B T_c}\right)^2\left(\sinh^2\left(\frac{\hbar\omega_{ik}(\bar{\mathbf{F}}^c)}{4\pi k_B T_c}\right)\right)^{-1} \tag{13}$$

The equation of motion at coarse scale is

$$\nabla_{\mathbf{X}}\cdot\mathbf{P} + \rho_0\mathbf{B} = \rho_0\ddot{\bar{\mathbf{u}}}, \forall \mathbf{X} \in \Omega_0 \tag{14}$$

where $\mathbf{P}$ is the first Piola–Kirchhoff stress, ρ_0 is the density in material configuration, $\mathbf{B}$ is the body force, $\nabla_{\mathbf{X}}$ is the material divergence operator, and Ω_0 denotes the whole coarse scale domain. Consider the first law of

thermodynamics: $\dot{w} = \rho_0 z - \mathrm{DIV}\mathbf{Q} + \mathbf{P} : \dot{\bar{\mathbf{F}}}$, where w is the internal energy per unit reference volume, z is the heat source per unit mass and $\mathbf{Q}$ is the heat flux. For the heat flux $\mathbf{Q}$, we exploit Fourier's law: $\mathbf{Q} = -\mathbf{K}_\mathrm{T} \cdot \nabla T$, where $\mathbf{K}_\mathrm{T}$ is the thermal conductivity. Then the first law provides the following heat conduction equation,

$$\frac{\mathbf{C}_T}{\Omega_0} : \dot{\bar{\mathbf{F}}} + \frac{C_V}{\Omega_0}\dot{T} = \rho_0 z + \nabla \cdot \mathbf{K} \cdot \nabla T \tag{15}$$

Eqs. (14) and (15) form the complete set of governing equations for the coarse-grain model. A detailed finite element formulation is presented in (Li et al., submitted).

4. Numerical example

To illustrate the effectiveness of NEMSD, we simulate shock wave propagation in a cubic lattice. The dimension of the simulation domain is $[-100\ h_\mathrm{a},\ 100\ h_\mathrm{a}] \times [-100\ h_\mathrm{a},\ 100\ h_\mathrm{a}]$, where $h_\mathrm{a} = 3.253$ A is the interatomic spacing. By choosing the characteristic length $L_\mathrm{c} = h_\mathrm{a}$, the normalized interatomic spacing is 1, and the normalized dimension of the domain is $[-100,\ 100] \times [-100,\ 100]$. We simulate the problem with 40401 atoms and 800 linear triangle elements. There are total of 441 FE nodes and each of them represents a Voronoi

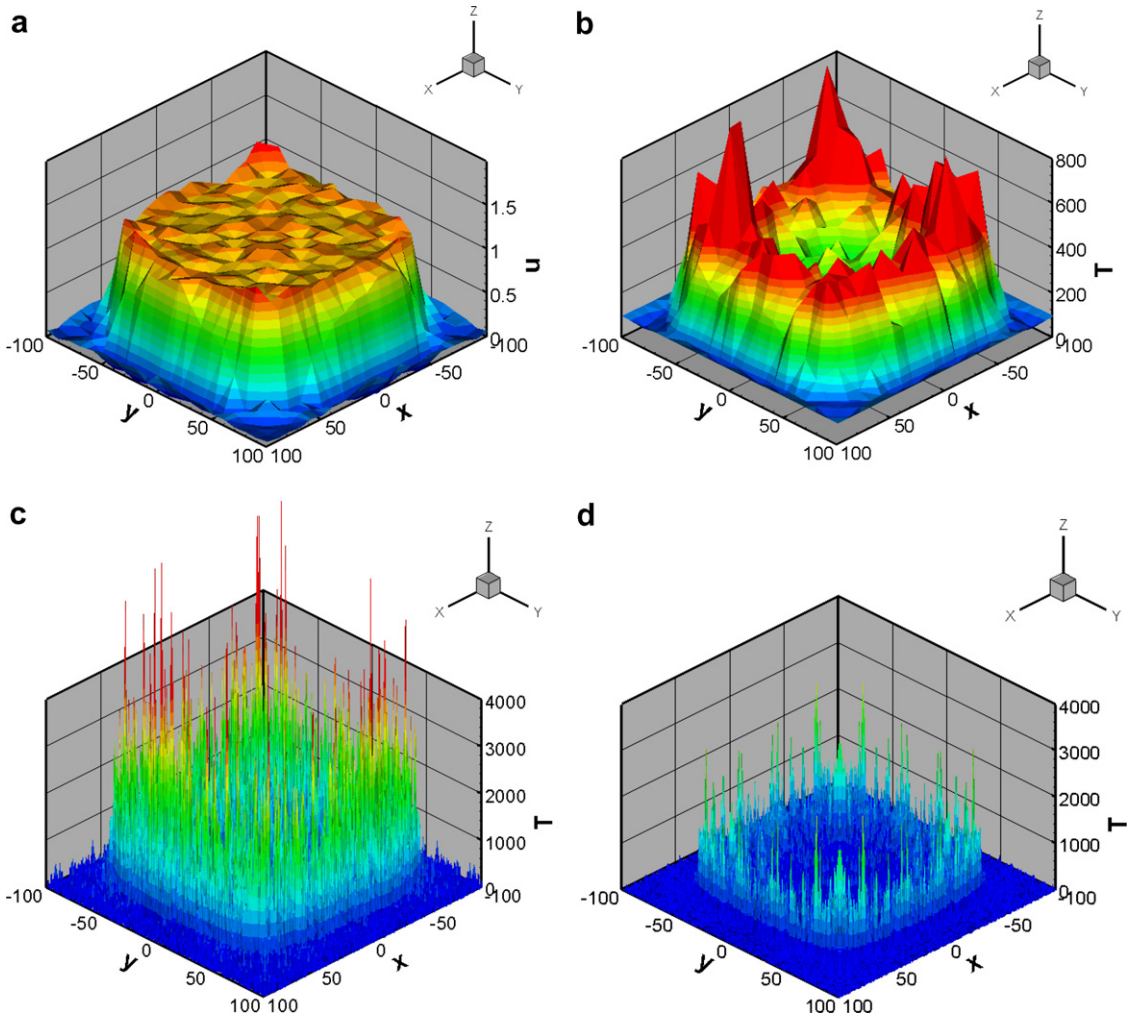

Fig. 3. Shock wave propagation: (a) Displacement solution by NEMSD; (b) Coarse scale temperature profile obtained by NEMSD; (c) Instantaneous temperature profile obtained by NEMSD; (d) Instantaneous temperature profile obtained by equilibrium MD.

cell-ensemble of 100 atoms. An initial dislocation is prescribed as: $q(r) = 1$ for $r \leqslant 20$, where q is out-of-plane displacement. A constant out-of-plane force $f = 0.04$, which is slightly higher than the critical force (the Peierls force), is applied to every atoms. In this example, a special Frenkel–Kontorova potential, or the FPU-β potential (Lepri et al., 2003), is used,

$$U(q) = \sum_i \left(\frac{k}{2}(q_i - q_j)^2 + \frac{K}{2}(q_i - \mathrm{int}(q_i))^2 - \frac{K}{24}(q_i - \mathrm{int}(q_i))^4 \right), \quad |i-j| = 1 \tag{16}$$

The following normalized parameters are used: $k = 1$, $K = 0.7$, $m = 1$, $\tilde{k}_B = k_B t_c^2 / m_c L_c^2$, and $\tilde{\hbar} = \hbar t_c / m_c L_c^2$. The characteristic mass, length and time are chosen as: $m_c = 26.98$ amu, $L_c = 3.253$ Å and $t_c = 2.0 \times 10^{-13}$ s, respectively. The coarse scale time step is 0.2 and the fine scale time step is 0.02. The initial temperature is chosen as $T_0 = 100$ K.

Fig. 3(a)–(c) show the displacement, thermodynamic (coarse scale) temperature and instantaneous kinetic (fine scale) temperature profiles at the 720th coarse scale time step. One can observe that the shock wave moves from the center to the boundaries. Extreme high temperature peak is observed at the shock front, which generates coarse scale heat wave propagation. In Fig. 3(d), we give the instantaneous kinetic temperature profile obtained by thermostated equilibrium MD with the same initial temperature, $T_0 = 100$ K. Comparing Fig. 3(c) with Fig. 3(d), one may find that the thermal fluctuation is highly intense in the case of NEMSD, which suggests that the system is indeed away from equilibrium.

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