MULTISCALE MODELING OF MULTI-PHYSICS

Xianqiao Wang*, James D. Lee*[a)] & Jiaoyan (Jenny) Li*
* *Department of Mechanical and Aerospace Engineering, School of Engineering and Applied Science, The George Washington University, Washington D.C., 20052, USA*

Summary Molecular dynamics (MD) and continuum mechanics are two distinct fields, very mature and successful in its own right. However, continuum mechanics is invalid for material systems at nanoscale and, even with a state-of-the-art supercomputer, MD is limited in the length/time scale that it can handle. Our ultimate objective is to bridge the gap between MD and continuum mechanics theoretically and numerically.

NON-EQUILIBRIUM MOLECULAR DYNAMICS

In classical MD simulation (without external force and temperature control), the governing equation for each atom can simply be expressed as

$$m^i \frac{d^2\mathbf{r}^i}{dt^2} = -\frac{\partial V}{\partial \mathbf{r}^i} \qquad i = [1, 2, 3, \cdots N] \tag{1}$$

and the temperature is a dependent variable defined as

$$3Nk_BT = \frac{1}{\Delta t}\int_t^{t+\Delta t} \sum_{i=1}^{N} m^i \{\mathbf{v^i}(\tau) - \bar{\mathbf{v}}(\tau)\}^{\mathbf{2}} \mathbf{d}\tau \tag{2}$$

It can be readily shown that

$$\frac{d}{dt}\{\sum_{i=1}^{N} \frac{1}{2} m^i \mathbf{v}^i \cdot \mathbf{v}^i + V\} = 0 \tag{3}$$

which means total (kinetic and potential) energy is conserved. This implies that, in contrast to continuum theory, there is no energy equation and there is no need for energy equation, since the temperature is just a statistical quantity depending on the velocity field. For non-equilibrium molecular dynamics (considering thermomechanical-electromagnetic coupling effect and temperature control), the governing equation is generalized to [1]

$$m^i \frac{d^2\mathbf{r}^i}{dt^2} = -\frac{\partial V}{\partial \mathbf{r}^i} + q^i\{\mathbf{E}^{ext} + \frac{1}{c}\mathbf{v}^i \times \mathbf{B}^{ext}\} - \chi(t) m^i \{\mathbf{v}^i + \Delta\mathbf{v}^i - \bar{\mathbf{v}}\} \tag{4}$$

where the second term on the right hand side of eq.(4) is the Lorentz force; and the third term may be named as the temperature force which exists only at specified regions where Nose-Hoover thermostat is applied. To ensure that the temperature forces acting on all atoms in the secified region do not cause net linear and angular momenta, let (1) $\bar{\mathbf{v}}$ be the mass-weighted average velocity and (2) $\Delta\mathbf{v}^i$ be systematically and iteratively found such that the total added moment is vanishing. The damping-like coefficient $\chi(t)$ is governed by

$$\dot{\chi} = \frac{1}{\tau^2}\frac{T - T^*}{T^*} \tag{5}$$

where T^* is the desired temperature.

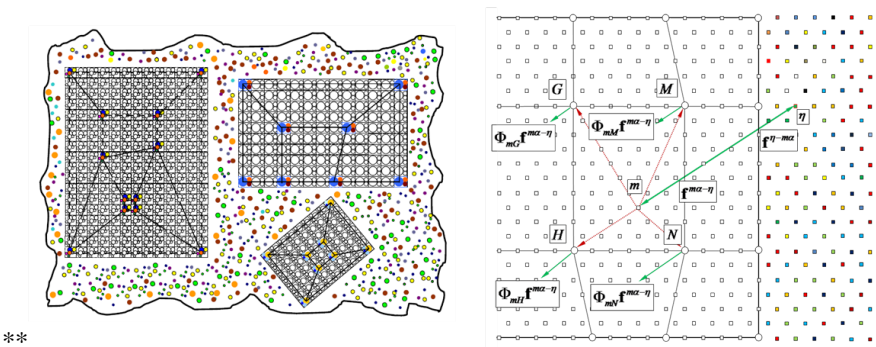

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Figure 1. (a) Schematic diagram of multiphase material system; (b) Interatomic force between atomic region and coarse-grained region

[a)] Corresponding author. E-mail: jdlee@gwu.edu.

MULTISCALE MODELING OF MULTI-PHASE MATERIAL SYSTEM

Here, we present a multiscale modeling and simulation of a multi-phase material system (cf Fig.1a), consisting of several different kinds of single crystals and a large number of differenct kinds of discrete atoms. To be specific, we decomposed the whole region into two subdomains (cf Fig.1b). In the critical region, each atom has its own identity; hence it may be called the atomic region. In the far field, named as coarse-grained region, we impose a kinematic constraint

$$\mathbf{u}^{k\alpha} = \Phi_{kI}\mathbf{U}^{I\alpha} \tag{6}$$

where $\mathbf{u}^{k\alpha}$ stands for the αth atom in the kth unit cell; $\mathbf{U}^{I\alpha}$ is nodal value for the αth atom in the Ith node of an element in which the kth unit cell resides; Φ_{kI} is the corresponding shape function. One may readily prove that, following the kinematic constraint, the force on the αth atom in the Ith node of an element is related to the atomic force $\mathbf{f}^{k\alpha}$ as

$$\mathbf{f}^{k\alpha}\Phi_{kI} = \mathbf{F}^{I\alpha} \tag{7}$$

which enables us to perform the multiscale modeling [2]. It means that (1) each atom in the coarse-grained region loses its identity, so it only serves as a messenger who passes the force to the nodes (cf Fig.1b and eq. (6)), and (2) it acts as a follower according to eq. (5). After eq. (4) is solved for all the atoms in atomic region and for all nodes (each node is a unit cell) in the coarse-grained region, one may calculate the temperature field and induced polarization, voltage, and electric field.

Correspondingly, a multiple time scale numerical procedure should be adopted to go along with a multiple length scale approach. In this work, we use central difference method, may also be called velocity verlet method, to march on in time. Indeed, the time step in the coarse-grained region is greater than that in the atomic region (cf Fig.2).

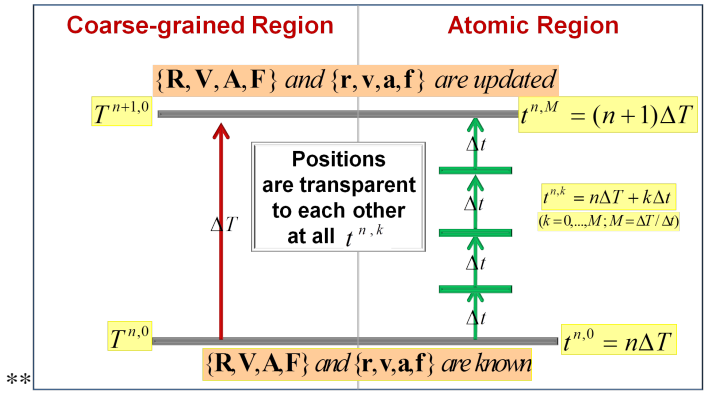

Figure 2. Multiple-time scale algorithm.

CONCLUSION

In this paper, we propose a theory of coarse-grained non-equilibrium molecular dynamics, which bridges the gap between atoms and continua. It has two features: (1) the incorporation of multiple length/time scale modeling, and (2) the incorporation of upgraded Nose-Hoover thermostat and electromagnetic coupling.

References

[1] Wang X.Q., Lee J.D.: Coarse-grained Non-equilibrium Simulation for Crystalline Material at Nano Scale. *Journal of Nanoengineering and Nanosystems* **224**:55–68, 2011.

[2] Wang X.Q., Lee J.D.: Wave Propagating Across Atomic-Continuum Interface. *Philosophical Magazine Letters* **91**:375–386, 2011.