``A Theory of Every Scale''
--- A Non-equilibrium Thermodynamics Multiscale Paradigm

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Abstract

Recently, we have developed a novel multiscale Nose-Hoover Langevin dynamics (MNHLD), which is capable of simulating coupled heat conduction and thermal mechanics at both atomistic scale and coarse grain scale in a con-current fashion. The so-called MNHLD is a multiscale paradigm for steady-state non-equilibrium thermodynamic systems. It consists of coupled dynamics at two-scales: (1) a finite-temperature coarse grain description that is based on Cauchy-Born rule and harmonic approximation, and (2) a Langevin molecular dynamics at atomistic scale that can faithfully represent an-harmonic atomistic motions. A distributed Nose-Hoover thermostat couples the two dynamics at two different scales.

The notion of distributed Nose-Hoover thermostat, or a non-uniform distributed thermo-reservoir, is a generalization of classical concept of permanent thermal reservoir. The distributed thermal reservoir is a discrete (both in spatial and temporal) reservoir system, whose temperature is fixed between two macro time steps. By doing so, we create a stochastic (Langevin) force term with zero-mean, whose amplitude is related to temperature at each finite element node.

By bridging these two dynamics, (1) we are able to simulate both micro heat transfer and macro heat transfer induced by mechanical inputs, vice versa, we are able to simulate the thermal effect or the finite temperature effects on the motion of defects at both atomistic scale and mesoscale;

(2) we are able to simulate frozen as well as thermal activation of dislocation motions, and (3) we are able to simulate interactions between harmonic and an-harmonic modes, and their thermal-mechanical contribution.

References

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