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Heat Jet Approach for Atomic Simulations at Finite Temperature

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Abstract. In this paper, we propose a heat jet approach for atomic simulations at finite temperature. Thermal fluctuations are injected into an atomic subsystem from its boundaries, without modifying the governing equations for the interior domain. More precisely, we design a two way local boundary condition, and take the incoming part of a phonon representation for thermal fluctuation input. In this way, non-thermal wave propagation simulations are effectively performed at finite temperature. We further apply this approach to nonlinear chains with the Morse potential. Chains with model parameters fitted to carbon and gold are simulated at room temperature with fidelity.

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Key words: Heat jet, thermostat, atomic simulations, finite temperature.

1 Introduction

Atomic simulations, or molecular dynamics simulations, have become instrumental for materials science and engineering at nano-scale or sub-micron scale. When mechanical behaviors are considered, technical and conceptual difficulties arise and make finite temperature simulations a challenging task. As the simulated system lies away from thermal equilibrium, both theoretical understanding and numerical treatments are still under active investigations in statistical and computational physics.

In a finite temperature atomic simulation, even the definition of temperature can be sophisticated. Consider an atomic lattice shown schematically in Fig. 1. The vast surrounding region represents a heat bath at a certain target temperature. When there are purely thermal fluctuations, the lattice temperature may be calculated from the temporal/ensemble average of the kinetic energy. When non-thermal motion presents, such as

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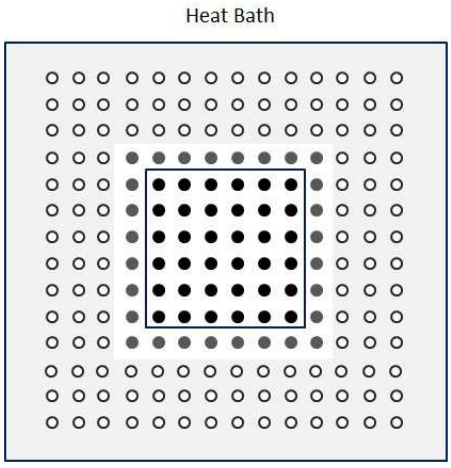

Figure 1: Schematic plot of an atomic lattice: solid dots represent atomic subsystem, gray dots represent boundary atoms, hollow circles represent surrounding atoms, and heat bath is around the outer boundary of the lattice.

in dynamical crack tip propagation, one can hardly decompose the whole motion into a crack part and a thermal part, as they both contain wave components in the full band. In a practical atomic simulation, one usually treats a small subsystem (enclosed by the interior square here) where important physics or mechanical behaviors take place, in order to reduce the numerical cost. Then the deviation between the true temperature and the calculated average kinetic energy can be big, and considerably contaminate the lattice dynamics through nonlinear interactions [1].

In this paper, we pursue a humble goal for finite temperature atomic simulations. While the exact dynamics of the subsystem should be obtained from a finite temperature simulation for the entire lattice, it may be reproduced/approximated if a suitable treatment is supplemented at its numerical boundaries. Here we aim at designing a treatment to accurately resolve non-thermal waves if the subsystem is at zero temperature; meanwhile to maintain a target temperature if there is no non-thermal motion. We assert that a finite temperature atomic simulation may be realized by this algorithm, with both the non-thermal motion and the thermal fluctuations included simultaneously.

There are extensive studies in the literature for both aspects, yet separately. The accurate resolution at zero temperature may be reached by using artificial boundary conditions in atomic simulations, or interfacial treatments for concurrent multiscale simulations [2]. We remark that several concurrent multiscale algorithms tackles with finite temperature, e.g., [3–7]. On the other hand, there are extensive studies on heat baths [8]. To name a few, one may simply rescale the velocity [9], to refresh the velocity of a randomly chosen atom [10], to add a source term together with a damping term satisfying the fluctuation-dissipation relation [11], or to add additional degrees of freedom feeding back acceleration or deceleration [12, 13]. These heat baths modify the dynamics of inte-