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Peridynamic theory of solids from the perspective of classical statistical mechanics

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HIGHLIGHTS

- This work is a classical statistical mechanical framework for peridynamic theory.
- Langevin thermostat is effective for peridynamics at smaller length scales.
- The formalism expands the applicability of peridynamics from macro to nano scales at any temperature.
- The ambiguity related to fluctuation–dissipation in peridynamic theory is unveiled.

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ABSTRACT

In this paper the classical statistical mechanics has been explored in order to develop statistical mechanical framework for peridynamics. Peridynamic equation of motion is known as upscaled Newton's equation. The peridynamic system consists of finite number of nonlocally interacting particles at nano and meso scales. This particle representation of peridynamics can be treated in terms of classical statistical mechanics. Hence, in this work the phase space is constructed based on the PD particle from their evolving momentum $\boldsymbol{p}_i$ and positions $\boldsymbol{x}_i$. The statistical ensembles are derived by defining appropriate *partition functions*. The algorithms for *NVE* and *NPH* implemented in the classical molecular dynamics are revisited for equilibrium peridynamic models. The current work introduces Langevin dynamics to the peridynamic theory through *fluctuation–dissipation* principle. This introduces a heat bath to the peridynamic system which eliminates the ambiguity with the role of temperature in a peridynamic system. Finally, it was seen that the homogenization of a peridynamic model with finite number of particles approaches to a conventional continuum model. The upscaled non-equilibrium peridynamics has potential applications in modeling wide variety of multiscale–multiphysics problems from nano to macro scale or vice versa.

1. Introduction

Peridynamics is a nonlocal continuum theory which is considered to be an upscaled form of molecular dynamics [1–5]. The peridynamic equation of motion is analogous to Newton's equation of motion because classical molecular dynamics solely depends on Newton's equation of motion in order to define position, velocity for each particle in the system. In this context it is clear that the concept of statistical mechanics can be integrated in peridynamics. In the earlier work by Lehoucq and Sears the peridynamic equations for momentum and energy balance were derived based on the concept of non-equilibrium statistical mechanics [6,7]. The mass, momentum and energy densities were defined by coarse graining through

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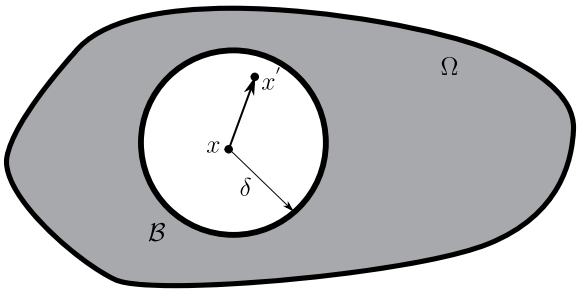

Fig. 1. Schematic of peridynamic body.

Hardy's localization function [8]. This theoretical formulation is the primary work on relating peridynamics and statistical mechanics. The initial concern is the difference between Newton's equation and peridynamic equation as peridynamic equation of motion involves mass and force densities [9]. The typical phase space conjugate variables used in conventional statistical mechanics are the positions and momentums of a finite number of particles. Peridynamic models at nano or meso scales (i.e. equivalent to atomistic or coarse-grain molecular dynamics models) have finite number of particles with non-infinitesimal volume. On the other hand, at macroscale it is known that the particle representation of peridynamic model consists of infinite number of particles with infinitesimal volume (i.e. point particles) [10]. For finite number of peridynamic particles the particle volume needs to be incorporated in order to define the phase-space. So, both the equilibrium and non-equilibrium statistical mechanics need to be outlined specialized for this case.

The concept of temperature is not clear in the current peridynamic formulation and it has not been well justified to apply non-equilibrium statistical mechanics. The nonlinear deformation leads to heat dissipation. So the long term dynamic relaxation of a peridynamic model can be performed by integrating viscous force (i.e. dissipation) with the conservative force [11]. However, during deformation the bond breakage, external fields, irregular spatial distribution of particles etc., lead to deviate the system from dynamic equilibrium state. This requires adaptive energy dissipation process. In a realistic dynamics the energy dissipation and fluctuation coexist [12]. So this issue is resolved by combining *Langevin dynamics* with peridynamic theory [13,12]. As a result, the Langevin dynamics introduces the heat bath into the system. This will lead us to attach a heat bath as well as pressure bath to the system and implement existing molecular dynamics schemes to a peridynamic model. The current work will be able to expand the application of peridynamic theory to multiscale–multiphysics problems [14]. The non-equilibrium peridynamic model will be able to incorporate non-linear deformation, heat conduction, diffusion, etc., under same computational framework. Hence, the current work focuses on defining and validating both equilibrium and non-equilibrium statistical mechanics for peridynamic theory. The peridynamic solver in the open source molecular dynamics code LAMMPS is used throughout the entire work [15,16].

2. Peridynamic theory of solids

The peridynamic theory of solid mechanics [1–3] has been proposed as an alternative to the classical theory, and is offered as a mathematically consistent technique for modeling solid bodies with continuous and discontinuous displacements as well as a method that unifies the mechanics of particles and continuum bodies through the utilization of long-range forces.

The balance equation between rate of change of linear momentum and applied force on a deformable body Ω develops the fundamental equation in classical continuum mechanics is written in Eq. (1)

$$\rho(\boldsymbol{x})\,\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \nabla\cdot\boldsymbol{\sigma} + \boldsymbol{b}(\boldsymbol{x},t)\,. \tag{1}$$

Here, $\boldsymbol{x}\in\Omega$, t is the time, ρ is the mass density, $\ddot{u}$ is the acceleration, $\boldsymbol{\sigma}$ is the stress tensor and b is the body force. This differential equation is not well defined at the discontinuities. The PD formulation of continua introduces integral form of kinematic equation in order to mitigate this issue by calculating the force density on each material point as

$$\rho(\boldsymbol{x})\,\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{\mathcal{B}} \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})\,\mathrm{d}V + \boldsymbol{b}(\boldsymbol{x},t)\,. \tag{2}$$

The deformable body Ω is represented with respect to an arbitrary frame of reference, $\boldsymbol{f}$ is the pairwise force applied on particle at $\boldsymbol{x}$ by a neighborhood particle at $\boldsymbol{x}'$ and $\mathcal{B}$ is a spherical region in the neighborhood of $\boldsymbol{x}$ with radius δ, $\boldsymbol{\xi}=\boldsymbol{x}'-\boldsymbol{x}$ and $\boldsymbol{\eta}=\boldsymbol{u}(\boldsymbol{x}',t)-\boldsymbol{u}(\boldsymbol{x},t)$ are relative position and displacement vectors, respectively (Fig. 1). The relative positions between two bonded points $\boldsymbol{x}$ and $\boldsymbol{x}'$ in the deformed (i.e. current) configuration can be defined as $\boldsymbol{\xi}+\boldsymbol{\eta}=\boldsymbol{y}(\boldsymbol{x}',t)-\boldsymbol{y}(\boldsymbol{x},t)$. For a certain $\delta>0$, $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})=0$ for all $\boldsymbol{\eta}$ when $\|\boldsymbol{\xi}\|>\delta$. This equation may be written more elaborately in terms of bond between $\boldsymbol{x}$ and $\boldsymbol{x}'$ as

$$\rho(\boldsymbol{x})\,\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{\mathcal{B}} \left\{\underline{\boldsymbol{T}}[\boldsymbol{x},t]\left\langle\boldsymbol{x}'-\boldsymbol{x}\right\rangle_{PD} - \underline{\boldsymbol{T}}\left[\boldsymbol{x}',t\right]\left\langle\boldsymbol{x}'-\boldsymbol{x}\right\rangle_{PD}\right\}\mathrm{d}V_{x'} + \boldsymbol{b}(\boldsymbol{x},t)\,. \tag{3}$$