Peridynamics as a Rigorous Coarse-Graining of Atomistics for Multiscale Materials Design

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

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Problem

Project Purpose and Approach

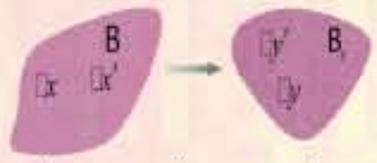
- Derive an energy equation needed for peridynamics
- Mathematical, thermodynamic, and mechanical relation between molecular dynamics and peridynamics
- What is temperature?

Revisions to R&D Goals and Milestones

- Derive and validate a peridynamic first law of thermodynamics
- Verify that the statistical coarse-graining of molecular dynamics into peridynamics is thermodynamically valid
- Continued implementation within LAMMPS

Approach

Kinematics & Peridynamics



$$y = x + u, \quad y' = x' + u'$$

$$x \& x' \in \mathcal{B} \quad y \& y' \in \mathcal{B}'$$

$$\mathbf{y = x + u}, \quad \mathbf{y' = x' + u'}$$

$$\mathbf{x \& x' \in \mathcal{B}} \quad \mathbf{y \& y' \in \mathcal{B}'}$$

$$y' - y = x' - x + u' - u$$

$$= \left(I + \nabla u\right)(x' - x) + O(\| x' - x \|^2)$$

Classical elasticity depends upon the deformation gradient that is a local linear approximation (assuming it's defined) and approximates the true deformation—peridynamics avoids the use of the deformation gradient and so enables complicated deformation to be modeled

Nonlocal continuum internal force

$$y' - y = x' - x + u' - u$$

$$k(y' - y, x', x)$$

Posit a force density per volume representing an "interaction density"

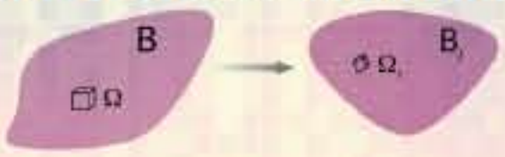
Constitutive relationship: mapping of the deformation to the force density per volume

"Force that material $\mathcal{B}/\Omega$ exerts on material Ω"

$\Omega \subseteq \mathcal{B}$

$$\int_{\Omega} \int_{\mathcal{B}/\Omega} k(y' - y, x', x)\, dx'\, dx$$

Global balance of linear momentum



$$\frac{d}{dt}\int_{\Omega} \rho(x)\dot{u}(x,t)\,dx = \int_{\Omega} \int_{\mathcal{B}/\Omega} k(y' - y, x', x)\, dx'\, dx + \int_{\Omega} b(x,t)\,dx$$

"Force that material $\mathcal{B}/\Omega$ exerts on Ω"

Nonlocal because force occurs over a volume and not at a surface

Irving & Kirkwood procedure

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 18, NUMBER 6 JUNE, 1950

The Statistical Mechanical Theory of Transport Processes.
IV. The Equations of Hydrodynamics*

J. H. Irving and John G. Kirkwood
Gates and Crellin Laboratories of Chemistry, No. 1803, Pasadena, California
(Received November 23, 1949)

The equations of hydrodynamics—continuity equation, equation of motion, and equation of energy transport—are derived by means of the classical statistical mechanics. Transport expressions are obtained

- Seminal paper that provides much of the continuum formalism used by the molecular dynamic community
- Demonstrated that the conservation of linear momentum derived can be generalized (and greatly simplified) by replacing the divergence of stress with the peridynamic integral operator representing internal force density
- Contrasting with our statistical coarse-graining ideas
- Statistical coarse-graining of molecular dynamics into peridynamics (SAND2007-6410)
  - Peridynamic fields determined via a probabilistic representation of atoms
  - Force as an expected value of force
  - Averaging procedure for aggregating atoms
  - Rescaling averaged fields into a larger length scale
  - Can be used for pairwise and multibody potentials

Classical and peridynamic conservation of linear momentum

$$\frac{\partial}{\partial t}\frac{1}{V}L + \nabla\left(\frac{1}{\partial V}\frac{L}{T}\right) = 0, \quad \frac{1}{\partial V}\frac{L}{T}(\nabla U)$$

L "momentum", U "displacement"

V "volume", T "time"

$$\frac{\partial}{\partial t}\frac{1}{V}L + \int \frac{1}{V}\frac{L}{T}\frac{1}{V} = 0, \quad \frac{1}{V}\frac{L}{T}\frac{1}{V}(U)$$

Avoid the assumption of a deformation gradient and so avoid the pitfalls associated with classical continuum mechanics

Peridynamic paradigm and the first law of thermodynamics

Q is "momentum", "mass", "energy", "phase space mass"

$$\frac{\partial}{\partial t}\frac{1}{V}Q + \nabla\left(\frac{1}{\partial V}\frac{Q}{T}\right) = 0, \quad Q = Q(\nabla P)$$

$$\frac{\partial}{\partial t}\frac{1}{V}Q + \int \frac{1}{V}\frac{Q}{T}\frac{1}{V} = 0, \quad Q = Q(P)$$

First law of thermodynamics

$$\mathrm{P_{int}}(t) + \mathrm{Q}(t) = \frac{D}{Dt}\mathrm{E}(t)$$

"Stress power", now have a peridynamic equivalent

"thermal power", developing a peridynamic equivalent

Rate of "internal energy" (due to molecular interactions)

First law for mesoscopic phenomena without standard kinematic assumptions—impact for material failure modeling

Results

Peridynamics implemented within LAMMPS

- SAND2007-7957J
- Provide MD users a computational mechanics capability
- Accepted Comp. Physics Comm.
- Peridynamic states by fall 08
- Statistical coarse-graining ideas to follow
- Enable applications to test-bed our ideas

Significance

Key Accomplishments

- Statistical coarse-graining of molecular dynamics into peridynamics (SAND2007-6410)
- Relationship with Irving & Kirkwood process
- Peridynamic stress power
- Bond-based peridynamics implemented within LAMMPS (SAND2007-7957J)

Significance of Results

Development of a peridynamic model that goes beyond molecular dynamics and classical elasticity enabling mesoscopic next-generation materials modeling

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NNSA National Nuclear Security Administration

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