Peridynamic theory of solids from the perspective of classical statistical mechanics

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Primary motivation: Multiscale modeling
Background

- Heterogeneity (i.e. nonlocality) gradually increases at smaller length scales: $\delta_{A_0}, \delta_{S_{n-1}} \cdots \delta_{S_n}$.
- It is challenging to link amorphous or heterogeneous microstructure with conventional continuum solvers (e.g. Difficult to link FEA mesh and atoms from polymers...).
- **We need a simple and robust multiscale modeling scheme which can address heterogeneity while bridging multiple length scales.**
- Peridynamics is a nonlocal continuum theory.
- In this context peridynamics can be used at meso or nanoscale by incorporating heterogeneity through pre-existing damages and randomly distributed particles..... JUST LIKE Coarse-grained MD !!
**Peridynamics and Hierarchical Multiscale modeling**

- Peridynamics (nonlocal continuum formulation) acts as coarse-grained MD model at meso or nanoscale. i.e. **Based on Micromorphic theory → Micoscale PD system is a finitely many particle system**

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Peridynamics and Hierarchical Multiscale modeling

- Conventional coarse-graining schemes are typically limited to similar cutoff distances for fine and coarse scale models... similar resolution.

- In the PD based hierarchical model the cutoff distance (i.e. \( \delta \)) varies among wide range of length scales: e.g. between nm to mm ....

- We do not need any multibody potential for each length scale since PD nonlocal force density depends on material’s bulk properties.

- PD can be used as DPD or MD at meso or nanoscales, respectively: \( PD_{nano \ or \ meso} \equiv PD_{macro} + \text{Random noise} \).

Thermostat for a peridynamic system

- Shrinking down the length scale from macro to nano level \(\Rightarrow\) phase-space approaches to be finite (\(N\) particle system).
- Thermal noise \(\eta_{MD} \equiv \eta_{PD}\) at atomistic level.
- **Fluctuation-dissipation** mechanism can be incorporated in PD formulation through stochastic thermostating, i.e. Langevin dynamics ... Introduce effect of TEMPERATURE?

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Thermostat for a peridynamic system

- Attach thermostat to each PD particle instead of using global velocity scaling.
- Simple options: i) NVE + Langevin thermostat, ii) NPH or NPT + Langevin thermostat.
- (In Fig) The stochastic thermostat keeps the temperature stable around $T_{\text{expected}} = 1.0K$.
- Bond breakage or randomly distributed particles causes the PD model to be unstable under global thermostat.
Few notes: Upscaling of fluctuation-dissipation

- The fluctuation-dissipation is re-defined such that $\sigma^* = 2\gamma^* \rho k_B T^*$. $\sigma^*$, $\gamma^*$ and $T^*$ are the amplitude of the random “kick”, frictional co-efficient and temperature like term, respectively, responsible for the random kicks.
- In Fourier space: $\rho \gamma^* (\omega) = \frac{1}{\rho \langle u^2 \rangle} \int_0^\infty e^{-i \omega t} \langle v(t) v(t + \tau) \rangle dt$ \implies mobility of the particles.
- At meso or nanoscales $T^*$ provides perturbation in the system, just like “heat bath”.
- Hence introduce Dissipative Peridynamics
Dissipative Peridynamics

\[ T(\mathbf{Y}, \dot{\mathbf{Y}}, \Theta) = T^e(\mathbf{Y}, \Theta) + T^d(\mathbf{Y}, \dot{\mathbf{Y}}, \Theta) + \delta T^R(t), \] (1)

\[ \partial_t u = \frac{\bar{p}}{\rho}, \] (2)

\[ \partial_t \tilde{p} = \int_B \left\{ T^e[x, t] \langle x' - x \rangle_{PD} - T^e[x', t] \langle x - x' \rangle_{PD} \right\} dV_{x'} - \int_0^t dt' K(t' - t) \tilde{p}(t) + \tilde{f}_R(t). \] (3)

Note: Since \( u = \bar{u} + \eta \) (\( \eta \) is Gaussian noise), \( u \) can not be pertaining to classical elasticity model. i.e. We need nonlocal model to incorporate Langevin dynamics.
LAMMPS and Peridynamics: PDLAMMPS

- To use PDLAMMPS: make yes − peri then build LAMMPS.
- For multiscale modeling link LAMMPS library with your C++ code and invoke LAMMPS functionalities, e.g. `lmp → input () → one (.....)` or access other atomstic info.
- Use Python wrapper for LAMMPS and invoke LAMMPS commands in your Python code.
- LAMMPS + PDLAMMPS can be called from you umbrella code (C++, Python or Fortran....).
LAMMPS and Peridynamics: PDLAMMPS

- Linear elastic solid (pair_style: peri/lps), Elastic-plastic solid (pair_style: peri/eps) and Visco-elastic solid (pair_style: peri/ves)
- Compute: Plasticity was added in PDLAMMPS.
- PDLAMMPS documentation:
- To construct/access the neighborhood vector: FixPeriNeig : FixClass. Currently built once.
- Particle attributes: AtomVecPeri : AtomVecClass.
- For your new PD material model: PairPeri_foo : Pair, add constitutive model in the method: PairPeri_foo :: compute().
- LAMMPS functionality for Langevin dynamics was easily integrated with the PDLAMMPS through LAMMPS input script. EASY !!!!, e.g. pairstyle : peri/lps + fix nve + fix Langevin.
Relevant publications


Summary

- Things can be added: i) Multi-Physics PD model, ii) Diffusion model, iii) Introduce implicit schemes (e.g. Trilinos, PTESc etc ...) for PDLAMMPS etc.

- Incorporate Fractional Langevin Dynamics in the LAMMPS in order to use with the PD model.

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Questions?