Peridynamic theory of solids from the perspective of classical statistical mechanics

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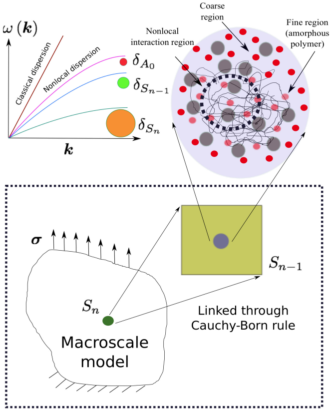
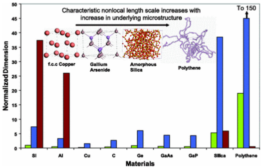
Primary motivation: Multiscale modeling



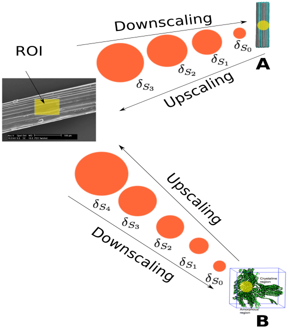


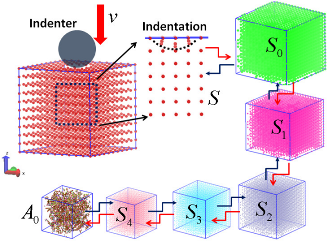
Background

- 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 Micromorpic theory → Micoscale PD system is a finitely many particle system**





R. Rahman, J. T. Foster, and A. Haque: A multiscale modeling scheme based on peridynamic theory. In: *International Journal of Computational Multiscale Engineering* (2014).

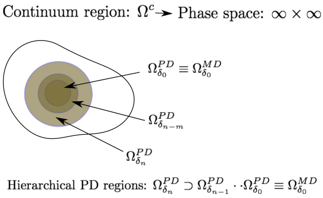
Peridynamics and Hierarchical Multiscale modeling

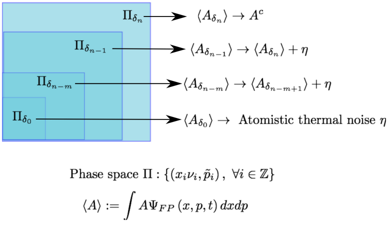
- Conventional coarse-graining schemes are typically limited to similar cutoff distances for fine and coarse scale models... similar resolution.
- In the PD based hierarchical model the cutoff distance (i.e. δ) varies among wide range of length scales: e.g. between nm to mm ....
- We do not need any multibody potential for each lengh 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**: $PD_{nano\ or\ meso} \equiv PD_{macro} + \texttt{Random noise}$..

R Rahman and JT Foster: Bridging the length scales through nonlocal hierarchical multiscale modeling scheme. In: *Computational Materials Science* 92 (2014), pp. 401–415.

Thermostat for a peridynamic system

- Shrinking down the length scale from macro to nano level $\implies$ phase-space approaches to be finite ($\mathcal{N}$ 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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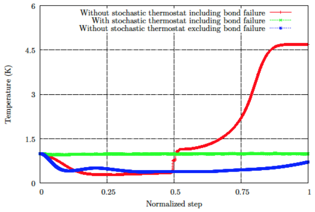
Thermostat for a peridynamic system

- 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 $T_{expected} = 1.0K$.
- Bond breakage or randomly distributed particles causes the PD model to be unstable under global thermostat.



Role of fluctuation-dissipation on termperature evolution

Few notes: Upscaling of fluctuation-dissipation

- The fluctuation-dissipation is re-defined such that $\sigma^* = 2\gamma^* \rho k_B T^*$. σ^*, γ^* 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: $\rho\gamma^*(\omega) = \frac{1}{\rho\langle \dot{u}^2 \rangle} \int_0^\infty e^{-\mathtt{i}\omega t} \langle v(t)\, v(t+\tau)\rangle dt$ $\implies$ mobility of the particles.
- At meso or nanoscales T^* provides perturbation in the system, just like "heat bath".
- Hence introduce *Dissipative Peridynamics*

Dissipative Peridynamics

$$
\begin{aligned}
\underline{\boldsymbol{T}}\left(\underline{\boldsymbol{Y}},\dot{\underline{\boldsymbol{Y}}},\Theta\right) &= \underline{\boldsymbol{T}}^{e}\left(\underline{\boldsymbol{Y}},\Theta\right)+\underline{\boldsymbol{T}}^{d}\left(\underline{\boldsymbol{Y}},\dot{\underline{\boldsymbol{Y}}},\Theta\right)+\delta\underline{\boldsymbol{T}}^{R}\left(t\right), && (1)\\
\partial_t \boldsymbol{u} &= \frac{\widetilde{\boldsymbol{p}}}{\rho}, && (2)\\
\partial_t \widetilde{\boldsymbol{p}} &= \int_{\mathcal{B}}\left\{\underline{\boldsymbol{T}}^{e}\left[\boldsymbol{x},t\right]\left\langle \boldsymbol{x}^{'}-\boldsymbol{x}\right\rangle_{PD}-\underline{\boldsymbol{T}}^{e}\left[\boldsymbol{x}^{'},t\right]\left\langle \boldsymbol{x}-\boldsymbol{x}^{'}\right\rangle_{PD}\right\}dV_{\boldsymbol{x}'}\\
&- \int_0^t dt' K\left(t'-t\right)\widetilde{\boldsymbol{p}}\left(t\right)+\widetilde{\boldsymbol{f}}_R\left(t\right). && (3)\\
& && (4)
\end{aligned}
$$

Note: Since $\boldsymbol{u}=\overline{\boldsymbol{u}}+\eta$ (η is Gaussian noise), $\boldsymbol{u}$ 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: `http://lammps.sandia.gov/doc/pair_peri.html`
- 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

1. Rahman, R., and J. T. Foster. "Bridging the length scales through nonlocal hierarchical multiscale modeling scheme." Computational Materials Science 92 (2014): 401-415.

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2. Rahman, Rezwanur, John T. Foster, and Anwarul Haque. "A multiscale modeling scheme based on peridynamic theory." International Journal for Multiscale Computational Engineering 12.3 (2014).

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3. Rahman, R., and J. T. Foster. "Peridynamic theory of solids from the perspective of classical statistical mechanics." Physica A: Statistical Mechanics and its Applications (2015).

Summary

- Things can be added: i) Multi-Physics PD moldel, 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?