Peridynamics as an Upscaling of Molecular Dynamics

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Abstract

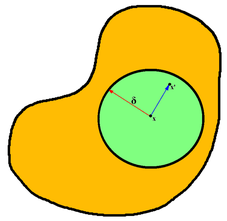
The nonlocal continuum mechanics theory *peridynamics* [1] is based on an integral formulation, in contrast to the classical theory of elasticity. We focus on the nonlocality of the peridynamics model and show how peridynamics preserves dispersion effects inherent to nonlocal molecular dynamics models.

I. The Peridynamics Model

The peridynamics (PD) equation of motion [1] is

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}_\mathbf{x}} \boldsymbol{\kappa}(\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t),\mathbf{x}'-\mathbf{x})\mathrm{d}V_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t), \quad t \geq 0$$

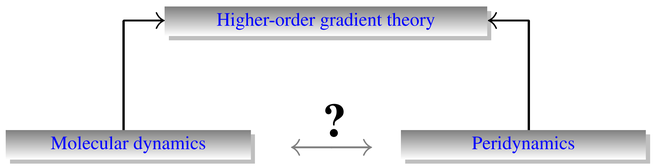
with $\mathcal{H}_\mathbf{x}$ the neighborhood of $\mathbf{x}$ (i.e., a spherical region of radius δ around $\mathbf{x}$, where δ is called the *horizon*), $\mathbf{u}$ the displacement vector field, $\mathbf{b}$ the body force, ρ the mass density, and $\boldsymbol{\kappa}$ a pairwise force density function per volume.



Note the similarity of PD with molecular dynamics (MD).

II. Upscaling to Peridynamics

We cast peridynamics as an upscaling of molecular dynamics [2]. Our goal is to have a PD continuum model that preserves the same dynamics as the original MD model. We show the correspondence between the models through higher-order gradient continuum formulations.



III. Nonlocal Linear Springs Model

We show that the higher-order gradient continuum model obtained for a 1-D nonlocal linear chain of atoms matches the peridynamics model and, in contrast, is not consistent with a local springs model.

Nonlocal MD model:

$$m_i\ddot{u}_i(t) = \sum_{\substack{j=-N \\ j\neq 0}}^{N} \frac{K}{|ja|}\left[u_{i+j}(t)-u_i(t)\right] \quad (1)$$

Peridynamics model:

$$\rho(x)\ddot{u}(x,t) = \int_{-\delta}^{\delta} \frac{c}{|\ell|}(u(x+\ell,t)-u(x,t))d\ell \quad (2)$$

$$\frac{d^2u}{dt^2} = \frac{K_a}{\rho}\left[\frac{d^2u}{dx^2} + \frac{\delta^2}{24}\frac{d^4u}{dx^4} + \frac{\delta^4}{1080}\frac{d^6u}{dx^6} + \dots\right].$$

Equations (1) and (2) are consistent under the assumptions of $N \gg 1$ and $Na = \delta$, using the relations $c = 2K_a/\delta^2$ and $K = \frac{2K_a}{N(N+1)}$.

Local MD model:

The local MD model is given by Eq. (1) with $N = 1$. It produces a higher-order gradient continuum model with different coefficients

$$\frac{d^2u}{dt^2} = \frac{K_a}{\rho}\left[\frac{d^2u}{dx^2} + \frac{a^2}{12}\frac{d^4u}{dx^4} + \frac{a^4}{360}\frac{d^6u}{dx^6} + \dots\right].$$

IV. Lennard-Jones Model

We present an upscaling of molecular dynamics for a nonlinear 1-D Lennard-Jones potential.

Lennard-Jones model:

$$m_i\ddot{y}_i(t) = \sum_{\substack{j=-N \\ j\neq 0}}^{N} -24\epsilon\left[2\left(\frac{\sigma^{12}}{(y_{i+j}(t)-y_i(t))^{13}}\right) - \left(\frac{\sigma^{6}}{(y_{i+j}(t)-y_i(t))^{7}}\right)\right],$$

with $y_i(t)$ the position of particle i at time t.

Peridynamics model:

$$\rho(x)\ddot{y}(x,t) = \int_{-\infty}^{\infty} \sum_{\substack{j=-N \\ j\neq 0}}^{N} -24\,\bar{\epsilon}\left[\left(\frac{\sigma^{12}}{(y(x+\varepsilon,t)-y(x,t))^{13}}\right) - \left(\frac{\sigma^{6}}{(y(x+\varepsilon,t)-y(x,t))^{7}}\right)\right]\Delta\left(\varepsilon - j\frac{\sigma}{C}\right)d\varepsilon,$$

with $y(x,t)$ the current position, at time t, of a particle that was at x in the reference configuration; $\bar{\epsilon}$ and C are model parameters, σ represents the model length scale, and $\Delta(x)$ is the Dirac delta function.

V. Embedded-Atom Model

We extend our work to multibody potentials and apply the upscaling of molecular dynamics for the embedded-atom model. The general form of the model is

$$E_{\text{tot}} = \sum_i F_i(\rho_{h,i}) + \frac{1}{2}\sum_i \sum_{j(\neq i)} \phi_{ij}(r_{ij}) \quad \text{with} \quad \rho_{h,i} = \sum_{j(\neq i)} f_j(r_{ij}),$$

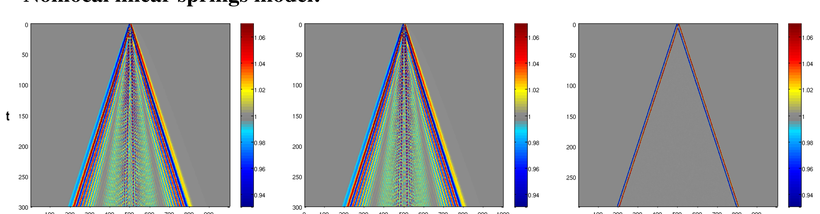
where E_{tot} is the total energy of the system, ϕ_{ij} is a core-core pairwise repulsive potential between atoms i and j separated by a distance r_{ij}, $F_i(\rho_{h,i})$ is the requested energy to embed atom i into the host electron density $\rho_{h,i}$, and f_j is the contribution to the electron density by the atom j. The equation of motion is obtained by the relation $m_i\ddot{\mathbf{y}}_i = -\nabla_i E_{\text{tot}}$. We implement analytical expressions for F_i, ϕ_{ij}, and f_j given at [3].

In our work, we derive an upscaling of the embedded-atom model, though the explicit expressions are too long for the present poster.

VI. Numerical Experiments

We present simulation results of a one-dimensional chain of atoms for the different models, i.e., nonlocal linear springs, Lennard-Jones and embedded-atom. Following [4], we choose our domain to be $\Omega = [0, 1000]$. The initial displacement profile is defined by $u(x,0) = p(x)$ for all $x \in \Omega$, where $p(x)$ is a smooth 21th-order polynomial. The plots below show the concentration (color gradient) evolution on time (y-axis from top to bottom). The x-axis represents the reference configuration.

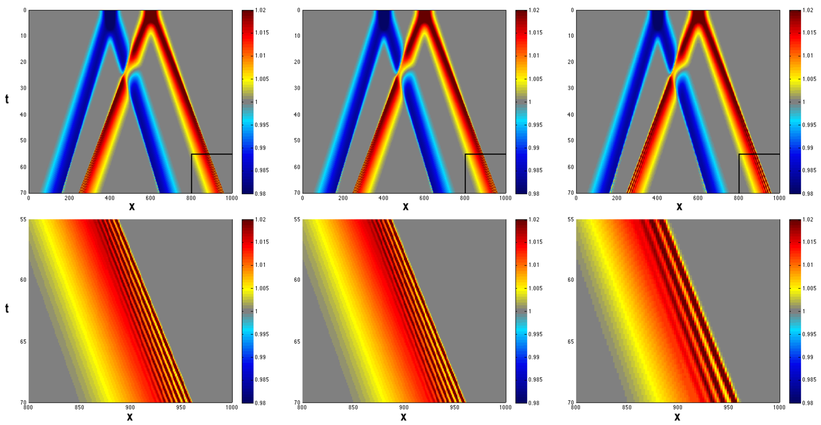
Nonlocal linear springs model:



MD: $N_x = 4,001$; $N = 20$ PD: $N_x = 2,001$; $N = 10$ CM: $N_x = 200,001$; $N = 20$

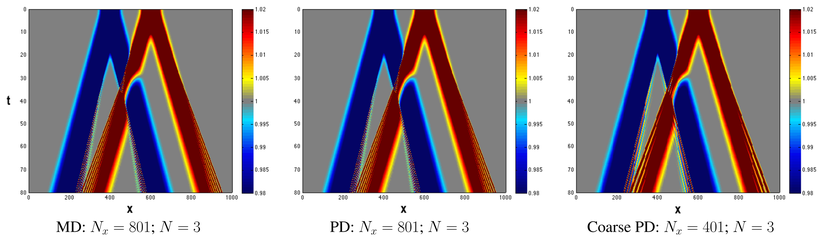
The numerical dispersion appearing in MD is preserved for the case of the PD solution, in contrast to the classical mechanics (CM) wave equation.

Lennard-Jones model:



MD: $N_x = 1,001$; $N = 3$ PD: $N_x = 1,001$; $N = 3$ Coarse PD: $N_x = 501$; $N = 3$

Embedded-atom model:



MD: $N_x = 801$; $N = 3$ PD: $N_x = 801$; $N = 3$ Coarse PD: $N_x = 401$; $N = 3$

In the above numerical simulations, we take the MD simulation results as our exact solution and compare the PD simulations with the MD results. The PD simulations reproduce dispersion effects appearing in MD, when preserving the length scale of the system. In the case of the nonlocal linear springs model, the length scale is determined by the horizon of the interaction, whereas in the Lennard-Jones (L-J) and embedded-atom (EAM) models, it is determined by the inter-particle distance (this can be observed in the higher-order gradient PDEs, although due to the limitation of space, those corresponding to L-J and EAM are omitted in this poster).

VII. Conclusions

We have introduced the peridynamics (PD) model as an upscaling of molecular dynamics (MD). We have shown that the higher-order gradient PDEs obtained from MD and PD are consistent to leading order. In particular, we have presented numerical experiments showing that dispersion effects appearing in MD simulations are recovered in PD simulations, in contrast to the classical continuum mechanics where the dispersion effects disappear.

References

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