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

\[ \rho(x) \ddot{u}(x,t) = \int_{\Omega} \kappa(u(x',t) - u(x,t)) \nabla \cdot \mathbf{u}(x',t) \, dx' + b(x,t), \quad t \geq 0 \]

with \( \Omega \) the neighborhood of \( x \) (i.e., a spherical region of radius \( \delta \) around \( x \), where \( \delta \) is called the horizon), \( \mathbf{u} \) the displacement vector field, \( \rho \) the mass density, and \( \kappa \) 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.

Molecular dynamics

Higher-order gradient theory

? Peridynamics

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:

\[ m_i \ddot{u}_i(t) = \sum_{j \neq i} \frac{\kappa}{c^2} \left[ u_j(t) - u_i(t) \right] \quad (1) \]

Peridynamics model:

\[ \rho(x) \ddot{u}(x,t) = \int_{\Omega} \kappa(u(x',t) - u(x,t)) \nabla \cdot \mathbf{u}(x',t) \, dx' \quad (2) \]

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

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:

\[ \frac{\delta^2 u_i}{\delta t^2} = \frac{\kappa}{c^2} \left[ u_j(t) - u_i(t) \right] \quad \frac{\delta^2 u_i}{\delta t^2} = \frac{\kappa}{c^2} \left[ u_j(t) - u_i(t) \right] \]

\[ \frac{\delta^2 u_i}{\delta t^2} = \frac{\kappa}{c^2} \left[ u_j(t) - u_i(t) \right] \]

IV. Lennard-Jones Model

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

Lennard-Jones model:

\[ m_i \ddot{u}_i(t) = \sum_{j \neq i} \frac{\kappa}{c^2} \left[ u_j(t) - u_i(t) \right] \quad (1) \]

Peridynamics model:

\[ \rho(x) \ddot{u}(x,t) = \int_{\Omega} \kappa(u(x',t) - u(x,t)) \nabla \cdot \mathbf{u}(x',t) \, dx' \quad (2) \]

where \( u_i(t) \) is the position of particle \( i \) at time \( t \).

V. Embedded-Atom Model

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

\[ E_{\text{tot}} = \sum_i \phi_i(\rho_i) + \frac{1}{2} \sum_{i,j} \phi_{ij}(\rho_{ij}) \quad \text{with} \quad \rho_i = \sum_j f_i(r_{ij}), \]

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

In our work, we derive an upsampling 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 \( u(x,0) = 0(x) \) for all \( x \in \Omega \), where \( 0(x) \) 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:

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

VII. Conclusions

We have introduced the peridynamics (PD) model as an upsampling 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