Mesoscale Simulations with Microscale Tools: Peridynamics in a Molecular Dynamics Code

LAMMPS Users’ Workshop

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What is Peridynamics?

- Peridynamics is a nonlocal extension of solid mechanics that permits discontinuous solutions

Classical (Cauchy) equation of motion
- \[ \rho \ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t) \]
  - Assumes (strong form) differentiable displacement field
  - Fracture (discontinuous displacement field) treated as pathology

Peridynamic equation of motion
- \[ \rho \ddot{u}(x,t) = \int_{H} f(u' - u, x' - x) \, dV' + b(x,t) \]
  - No assumption of differentiable fields (admits fracture)
  - No obstacle to integrating nonsmooth functions
  - \( f(\cdot, \cdot) \) is “force” function; contains constitutive model
  - \( f = 0 \) for particles \( x,x' \) more than \( \delta \) apart
  (like cutoff radius in MD!)

“\textit{In peridynamics, cracks are part of the solution, not part of the problem.}”
- F. Bobaru
Prototype microelastic brittle (PMB) material model*

- \( x \equiv \text{initial position} \)
- \( y \equiv \text{current position} \)

\[
\Phi(y' - y, x' - x) = \frac{1}{2} \frac{c}{\|x' - x\|} \left( \|y' - y\| - \|x' - x\| \right)^2
\]

\[
f(y' - y, x' - x) = \nabla \Phi = \frac{c}{\|x' - x\|} \left( \|y' - y\| - \|x' - x\| \right) \frac{y' - y}{\|y' - y\|}
\]

Prototype microelastic brittle (PMB) material model

- Bond stretch

\[ s = \frac{|y' - y| - |x' - x|}{|x' - x|} \]

- Bond fails when stretch too large

\[ y(x,t) \rightarrow y'(x',t) \]

\[ x = \text{initial position} \]

\[ y = \text{current position} \]
Discretizing Peridynamics: Space

- Spatial Discretization: Approximate integral with sum*

\[
\int_{H} f(u(x', t) - u(x, t), x' - x) dV' \quad \Rightarrow \quad \sum_{p} f(u(x_p, t) - u(x_i, t), x_p - x_i) \Delta V_p
\]

Discretizing Peridynamics: Time

- Temporal Discretization:
  - Explicit central difference in time

\[ \ddot{u}(x, t) \approx \ddot{u}_i^n = \frac{u_{i}^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} \]

- Velocity-Verlet

\[ v_i^{n+1/2} = v_i^n + \left( \frac{\Delta t}{2m} \right) f_i^n \]
\[ u_i^{n+1} = u_i^n + (\Delta t) v_i^{n+1/2} \]
\[ v_i^{n+1} = v_i^{n+1/2} + \left( \frac{\Delta t}{2m} \right) f_i^{n+1} \]
Discretizing Peridynamics

- Discrete peridynamic model is *collection of particles in space*
- Peridynamic particles interact via *pair or multibody potential*
- Peridynamic particles advanced in time via *velocity-Verlet* scheme
- Does this sound familiar?
- This discretization of peridynamics has the same computational structure as molecular dynamics, so put it in an *MD* code!
- Peridynamics has sometime been called a “*continuum formulation of molecular dynamics*.”
Why Peridynamics in LAMMPS?

• Provide open source peridynamic code
  - Primary Peridynamic code (EMU) not publicly available
  - Peridynamics-in-LAMMPS is “EMU Lite”
  - Multiphysics peridynamic code (Peridigm) currently under development

• Leverage portability, fast parallel implementation of LAMMPS
  - Stand on the shoulders of LAMMPS developers*

• Provide (nonlocal) continuum mechanics simulation capability within molecular dynamics code

• Multiscale simulation
  - Atoms → peridynamics → classical mechanics

*Thanks to Steve Plimpton for lots of helpful advice, and for answering all my dumb questions!
• Added “SI” units to LAMMPS for macroscale models
  - MD: angstroms, femtoseconds, etc.
  - PD: meters, seconds, etc.
• Defined new peridynamic particle class
  - Typical MD variables for each atom: current position, velocity, force, mass
  - Additional PD particle variables: volume, stretch, initial position
• Defined new peridynamic force functions for peridynamic particles
  - Prototype microelastic brittle (PMB) model described earlier
  - Linear peridynamic solid (LPS) model; Viscoelastic model
  - LAMMPS highly extensible; easy to introduce new potentials

\[
\rho \ddot{y}_i^n = \sum_p \frac{c}{\|x_p - x_i\|} \left( \|y_p - y_i\| - \|x_p - x_i\| \right) \Delta V_p \frac{y_p - y_i}{\|y_p - y_i\|} + b_i^n
\]
Peridynamics-in-LAMMPS (PDLAMMPS)

- Use TWO LAMMPS “neighborlists”

- Neighborlist #1: Store list of bonds for all particles
  - A LAMMPS “neighborlist” computed and stored at simulation start
  - Each particle knows its bond pairs
  - Bonds computed only once at simulation start
  - Bonds broken as necessary, **never reformed**

- Neighborlist #2: **Contact resolution**
  - A standard LAMMPS “neighborlist” (recomputed as necessary)
  - Allow for contact forces (otherwise non-bonded particles don’t interact)
  - Append force to EOM

\[
f_s = \sum_j \min \left\{ 0, c_s \left( \frac{\|\mathbf{y}_j - \mathbf{y}_i\|}{2r_s} - 1 \right) \right\}
\]
Example #1
Dynamic Brittle Fracture in Glass

- Soda-lime glass plate
  - Dimensions: 3” x 1” x 0.05”
  - Density: 2.44 g/cm³
  - Elastic Modulus: 79.0 GPa

- Notch at top; apply tension

- Discretization (finest)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores

- Joint with Florin Bobaru, Youn-Doh Ha (Nebraska), & Stewart Silling (SNL)
Example #1
Dynamic Brittle Fracture in Glass

- Movie #1
  - Crack propagation

- Movie #2
  - Strain energy density

Weak Scaling

- **Dawn (LLNL):** IBM BG/P System
  - 500 teraflops; 147,456 cores

- Part of Sequoia procurement
  - 20 petaflops; 1.6 million cores

- Scalability Results (weak scaling)
  - Cube of same material as plate

<table>
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<th># Cores</th>
<th># Particles</th>
<th>Particles/Core</th>
<th>Runtime (sec)</th>
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Hard Sphere Impact on Brittle Disk*

- **Projectile**
  - Sphere (diameter 0.01 m)
  - Velocity 100 m/s
- **Target**
  - Disk: diameter 0.074 m, thickness 0.0025 m
  - Elastic modulus 14.9 GPa
  - Density 2200 kg/m³
- **Discretization**
  - Mesh spacing 0.005 m
  - 100,000 particles
  - 0.2 milliseconds

Hard Sphere Impact on Brittle Disk

- Movie #1
  - View of top monolayer

- Movie #2
  - Side view
Software

• Peridynamics-in-LAMMPS
  - Module in LAMMPS distribution: lammps.sandia.gov
  - More information & user’s guide at www.sandia.gov/~mlparks (Click on “software”)

• To use:
  - cd lammps/src
  - make yes-peri

• Papers
  - www.sandia.gov/~mlparks; mlparks@sandia.gov