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

LAMMPS Users' Workshop

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Applied Mathematics and Applications
Sandia National Laboratories

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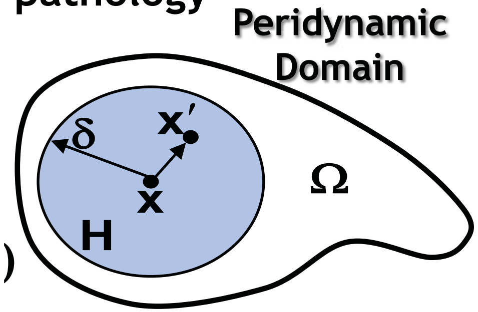
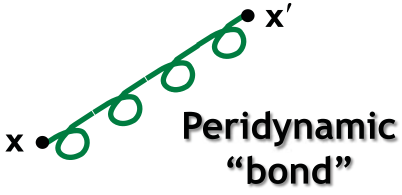
What is Peridynamics?

- Peridynamics is a nonlocal extension of solid mechanics that permits discontinuous solutions
- Classical (Cauchy) equation of motion
  - $\rho\ddot{u}(x,t) = \nabla \bullet \sigma(x,t) + b(x,t)$
  - 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(·,·) is “force” function; contains constitutive model
  - f = 0 for particles x,x’ more than δ apart (like cutoff radius in MD!)





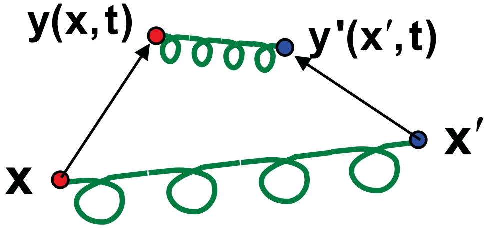
“In peridynamics, cracks are part of the solution, not part of the problem.”
- F. Bobaru

Peridynamics: Example Material Model

- Prototype microelastic brittle (PMB) material model*

$x \equiv$ initial position

$y \equiv$ current position



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

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

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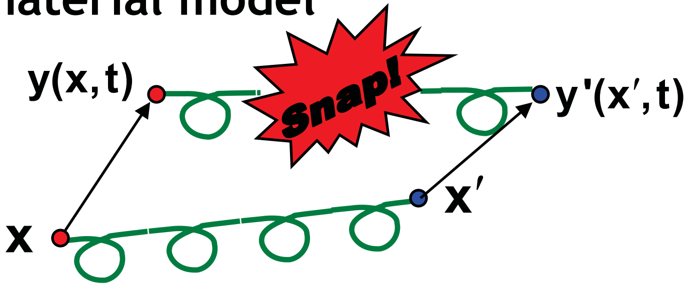
*S.A. Silling and E. Askari, *A meshfree method based on the peridynamic model of solid mechanics,* Computers and Structures, 83, pp. 1526-1535, 2005.

Peridynamics: Bond Breaking

- Prototype microelastic brittle (PMB) material model

$x \equiv$ initial position

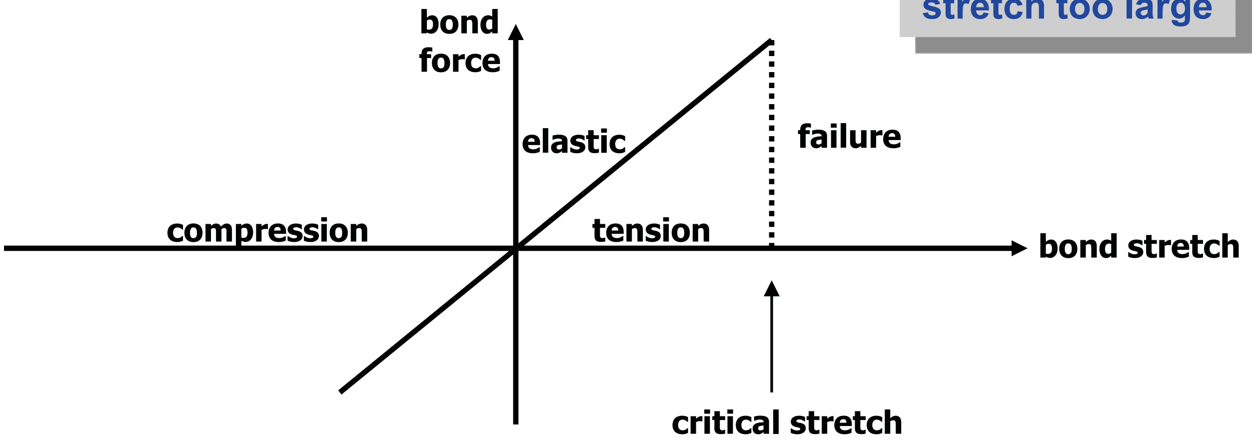
$y \equiv$ current position



- Bond stretch

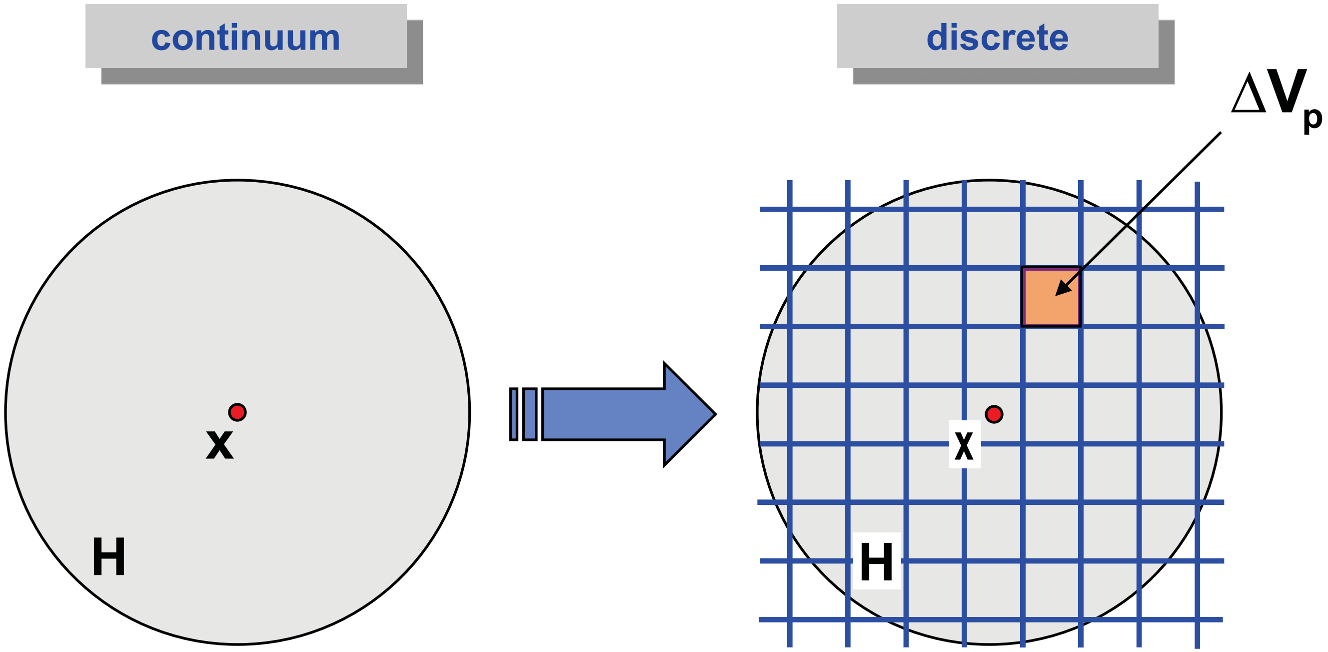
$$s = \frac{\|y' - y\| - \|x' - x\|}{\|x' - x\|}$$

Bond fails when stretch too large



Discretizing Peridynamics: Space

- Spatial Discretization: Approximate integral with sum*



$$\int_H f(u(x',t)-u(x,t),x'-x)dV' \Longrightarrow \sum_p f(u(x_p,t)-u(x_i,t),x_p-x_i)\Delta V_p$$

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[*] S.A. Silling and E. Askari, *A meshfree method based on the peridynamic model of solid mechanics,* Computers and Structures, 83, pp. 1526-1535, 2005.

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!

Peridynamics-in-LAMMPS (PDLAMMPS)

- 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; Viscoplastic model
  - LAMMPS highly extensible; easy to introduce new potentials

$$\rho \ddot{\mathbf{y}}_i^n = \underbrace{\sum_p \frac{\overset{\text{“spring constant”}}{\mathbf{c}}}{\|\mathbf{x}_p - \mathbf{x}_i\|}\left(\|\overset{\text{current positions}}{\mathbf{y}_p - \mathbf{y}_i}\| - \|\overset{\text{initial positions}}{\mathbf{x}_p - \mathbf{x}_i}\|\right)\overset{\text{volume}}{\Delta \mathbf{V}_p}\frac{\mathbf{y}_p - \mathbf{y}_i}{\|\mathbf{y}_p - \mathbf{y}_i\|}}_{\text{internal force}} + \overset{\text{body force}}{\mathbf{b}_i^n}$$

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

$$f_s = \sum_j \min\left\{0, c_s\left(\frac{\|y_j - y_i\|}{2r_s} - 1\right)\right\}$$

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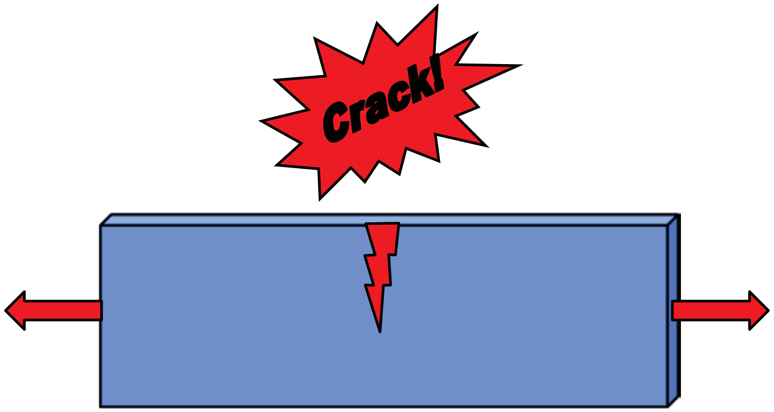
Example #1
Dynamic Brittle Fracture in Glass

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

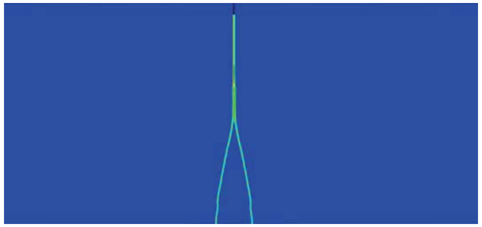


- Notch at top; apply tension

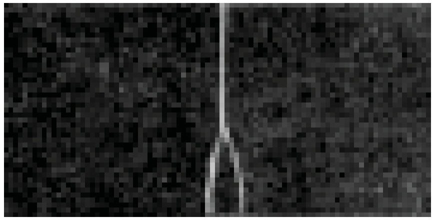
- Discretization (finest)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores

- Joint with Florin Bobaru, Youn-Doh Ha (Nebraska), & Stewart Silling (SNL)

Example #1
Dynamic Brittle Fracture in Glass



Peridynamics



Physical Experiment*

- Movie #1
  - Crack propagation

- Movie #2
  - Strain energy density

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*S F. Bowden, J. Brunton, J. Field, and A. Heyes, *Controlled fracture of brittle solids and interruption of electrical current*, Nature, 216, 42, pp.38-42, 1967.

Weak Scaling

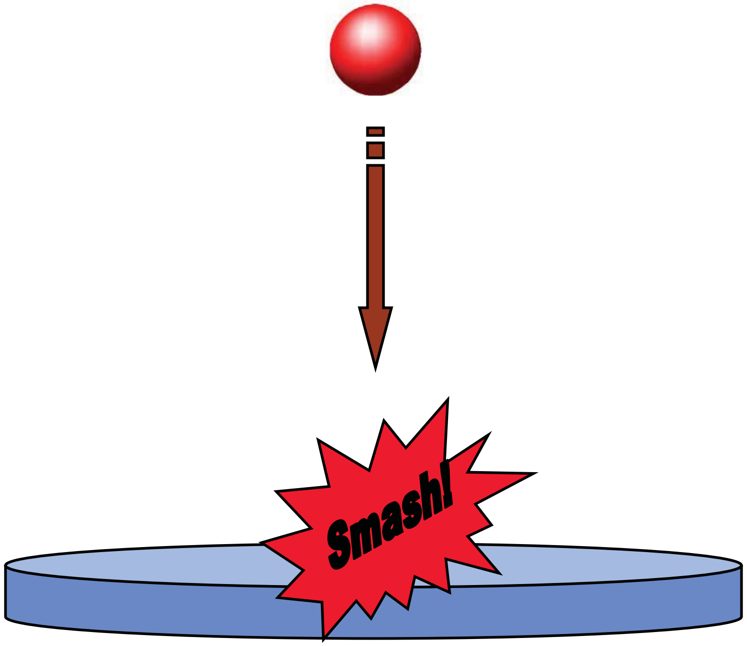
- Dawn (LLNL): IBM BG/P System
  - 500 teraflops; 147,456 cores
- Part of Sequoia procurement
  - 20 petaflops; 1.6 million cores
- Scalability Results (weak scaling)
  - Cube of same material as plate

Dawn **at LLNL**

# Cores	# Particles	Particles/Core	Runtime (sec)	T(P)/T(P=512)
512	262,144	4096	14.417	1.000
4,096	2,097,152	4096	14.708	0.980
32,768	16,777,216	4096	15.275	0.963

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/m^3
- Discretization
  - Mesh spacing 0.005 m
  - 100,000 particles
  - 0.2 milliseconds



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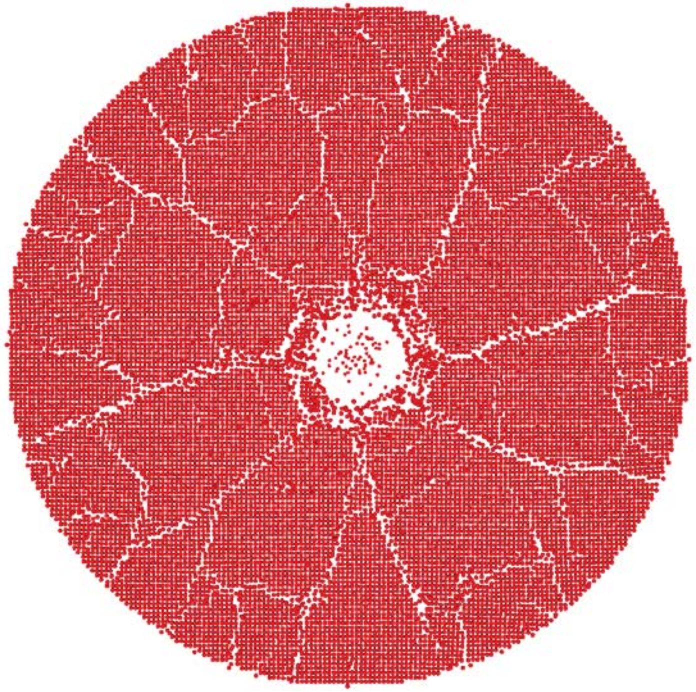
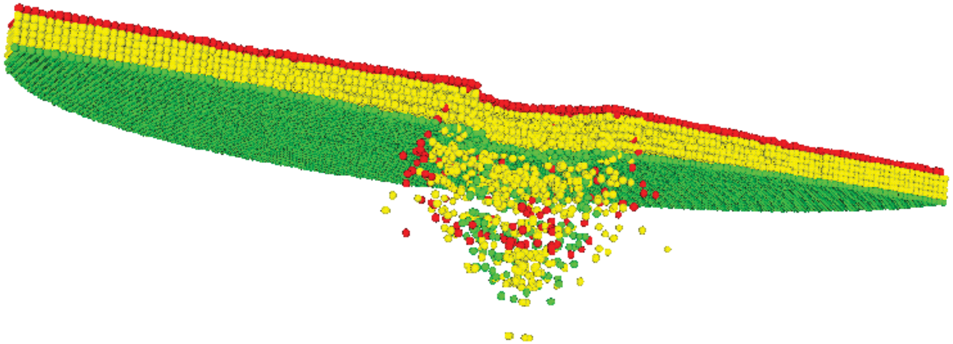
Hard Sphere Impact on Brittle Disk

- 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
  - MLP, R.B. Lehoucq, S.J. Plimpton, and S.A. Silling, *Implementing Peridynamics within a molecular dynamics code*, Computer Physics Communications 179(11) pp. 777-783, 2008.
  - MLP, P. Seleson, S.J. Plimpton, R.B. Lehoucq, and S.A. Silling, *Peridynamics with LAMMPS: A User Guide*, Sandia Tech Report SAND 2008-1035.