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

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Michael Parks

Applied Mathematics and Applications
Sandia National Laboratories

Steven Plimpton
Scalable Algorithms

Richard Lehoucq
Applied Mathematics and Applications

Stewart Silling
Multiscale Dynamic Materials Modeling

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Overview

- **Why Peridynamics in Molecular Dynamics?**
- **Peridynamic Model (Continuum Mechanical Model)**
  - **Prototype microelastic brittle model**
- **Discretizing Peridynamics**
- **Peridynamics in a Molecular Dynamics Code (PDLAMMPS)**
- **Computational Example**
- **Conclusions**

Motivation: Why PD in MD?

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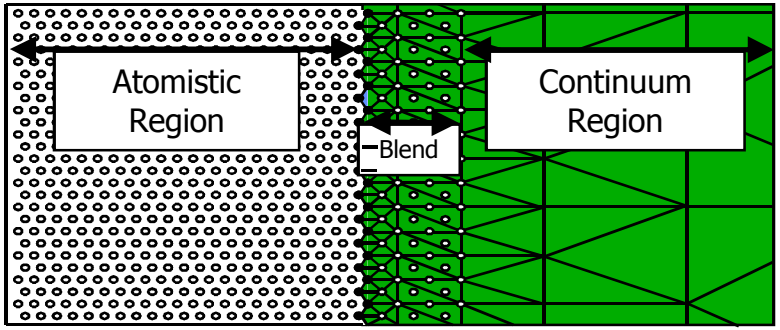
Why PD in MD?

- **Provide open source peridynamic code**
  - **Primary PD code (EMU) not publicly available**
- **Provide continuum mechanics simulation capability within molecular dynamics code**
- **Atomistic-to-Continuum (AtC) Coupling**
  - **Use MD where needed, continuum elsewhere**
  - **Link molecular dynamics + continuum mechanics (finite element) codes**



Why PD in MD?

- **Atomistic-to-Continuum (AtC) Coupling***
  - **Link molecular dynamics + continuum mechanics (finite element) codes**
  - **Significant software issues in coupling monolithic codes**

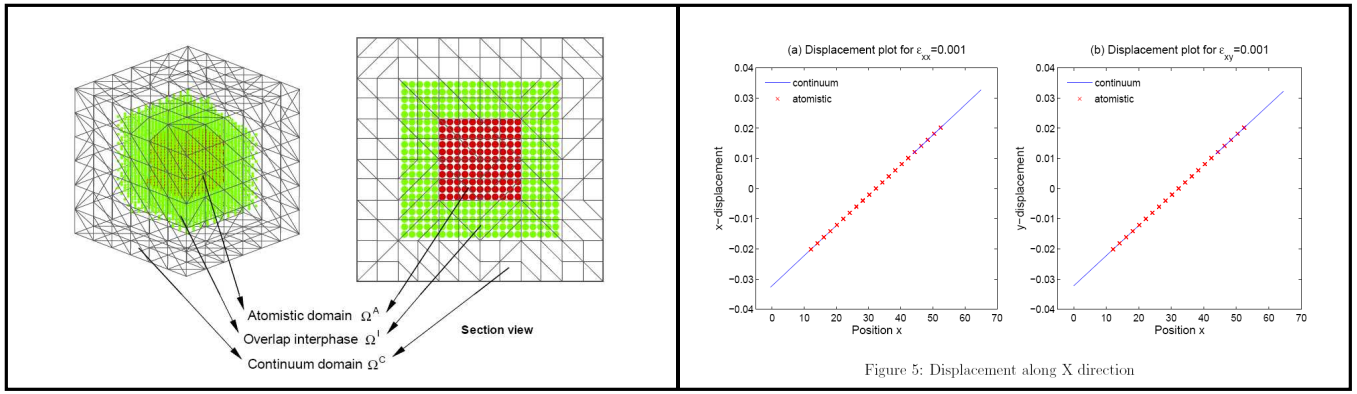


Figure 5: Displacement along X direction

  - **PD within MD code allows MD and continuum mechanics in single code**

•*M.L. P, P.B. Bochev, and R.B. Lehoucq. Connecting Atomistic-to-Continuum Coupling and Domain Decomposition. Multiscale Modeling and Simulation, 7, pp.362-380, 2008.*

•*S. Badia, M.L. P, P.B. Bochev, M. Gunzburger, and R.B. Lehoucq On Atomistic-to-Continuum (AtC) Coupling by Blending. Accepted for publication in Multiscale Modeling and Simulation, 7, pp.381-406, 2008.*

•*S. Badia, P.B. Bochev, J. Fish, M. Gunzburger, R.B. Lehoucq, M.A. Nuggehally, M.L. Parks. A Force-Based Blending Model for Atomistic-to-Continuum Coupling. International Journal for Multiscale Computational Engineering, 5, pp.387-406, 2007.*

•*J. Fish, M.A. Nuggehally, M.S. Shephard, C.R. Picu, S. Badia, M.L. Parks, and M. Gunzburger. Concurrent AtC coupling based on a blend of the continuum stress and the atomistic force. Computer Methods in Applied Mechanics and Engineering, 196, pp.4548-4560, 2007.*

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Peridynamics

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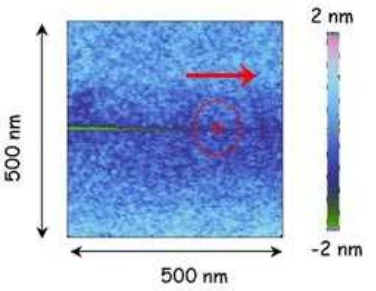
Peridynamics: Motivation

- **Reformulate mathematical model of solid mechanics so that equations hold everywhere (even at discontinuities)**
- **Classical elasticity assumes that the displacement field is continuously differentiable at every point**
  - $\mathbf{u(x',t) = u(x,t) + \nabla_x u(x,t)(x' - x) + O(\|x' - x\|^2)}$
  - **Higher-order gradient theories improve approximation; assume additional derivatives of displacement field**
- **Displacement field discontinuous (derivatives undefined) on crack tips, crack surfaces, etc.**



AFM picture of crack tip*

- **Integral-based models (Peridynamics) sidestep issue**
  - **No obstacle to integrating nonsmooth functions**

•"Glass behaves like a metal", Belle Dumé, PhysicsWeb, 28 February, 2003. (F Célarié et al. 2003 Phys. Rev. Lett. 90 075504) *http://physicsweb.org/articles/news/7/2/15*

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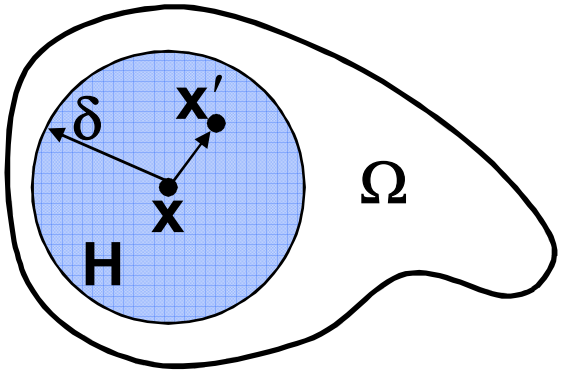
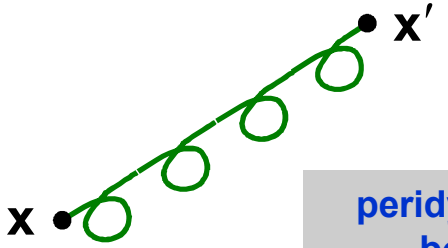
Peridynamics: Equation of Motion

- **Peridynamic Equation of Motion (Integral)**

$$\rho\ddot{u}(x,t) = \int_H f(u(x',t) - u(x,t), x' - x)\,dV' + b(x,t)$$





peridynamic bond

- **f(·,·) is pairwise force function**
- **All material-specific properties embedded in f(·,·)**
- **f = 0 for particles x,x′ more than δ apart**
- **u need not be differentiable ("rough" displacements; fracture)**
- **More general PD state theory available**

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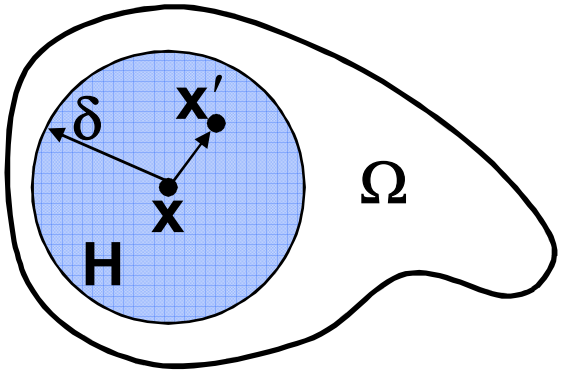
Peridynamics: Equation of Motion

- **Peridynamic Equation of Motion (Integral)**

$$\rho\ddot{u}(x,t) = \int_H f(u(x',t) - u(x,t), x' - x)dV' + b(x,t)$$



Peridynamic stress tensor*

$$\rho\ddot{u} = \nabla \cdot \upsilon(x) + b$$

- **Cauchy Equation of Motion (PDE)**

$$\rho\ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t)$$
$$\sigma(x,t) = g(\nabla u(x,t))$$

*S.A. Silling and R.B. Lehoucq, *Force Flux and the Peridynamic Stress Tensor,* Journal of Mechanics and Physics of Solids, 56, pp.1566-1577, 2008.

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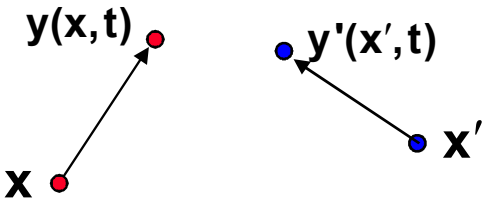
Peridynamics: Force Function

- **Prototype microelastic brittle (PMB) material model**

x ≡ initial position

y ≡ 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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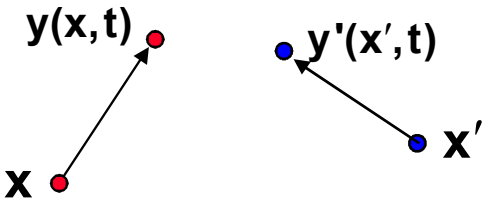
Peridynamics: Bond Breaking

- **Prototype microelastic brittle (PMB) material model**

x ≡ initial position

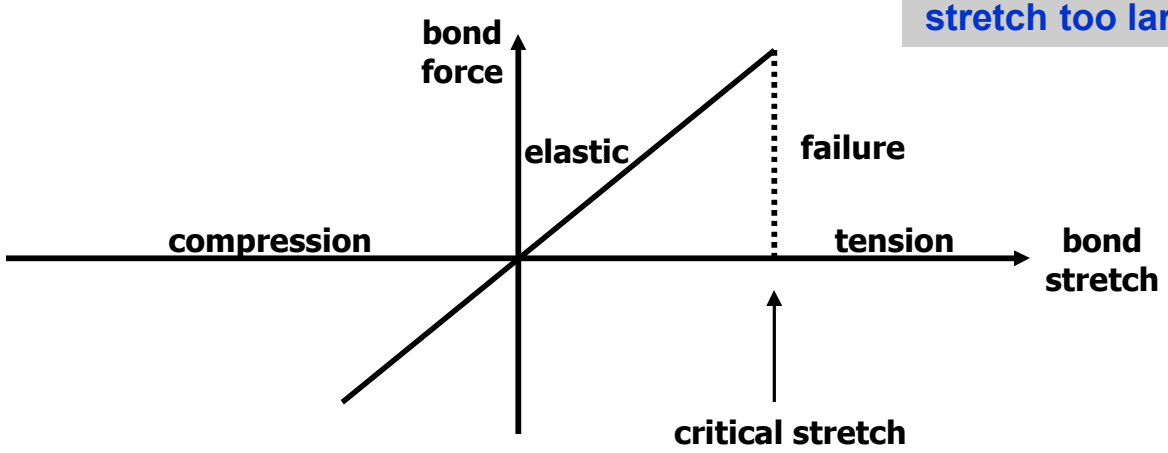
y ≡ current position



- **Bond stretch**

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

Bond fails when stretch too large



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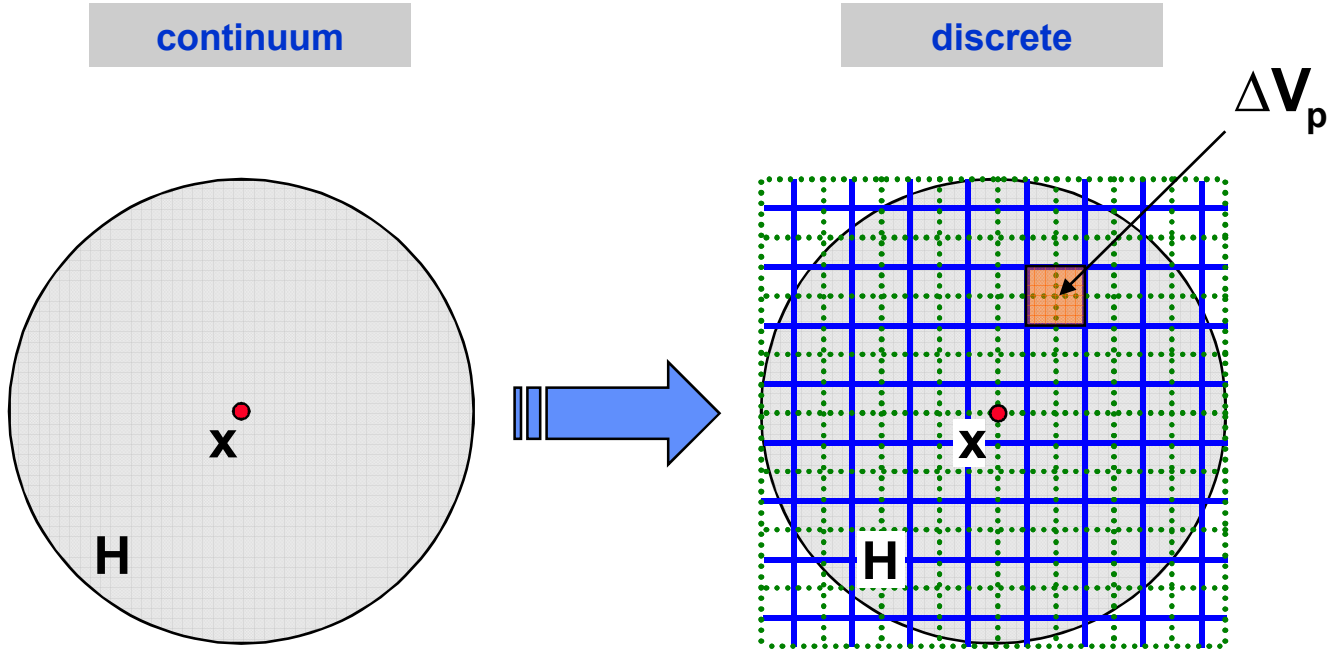
Discretizing Peridynamics

Discrete Peridynamic Equation of Motion

- **Spatial Discretization: Approximate sum with integral**



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

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Discrete Peridynamic Equation of Motion

- **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**

$$v_i^{n+1/2} = v_i^n + \left(\frac{\Delta t}{2m}\right) f_i^n$$

$$u_i^{n+1} = u_i^n + (\Delta t)\, v_i^{n+1/2}$$

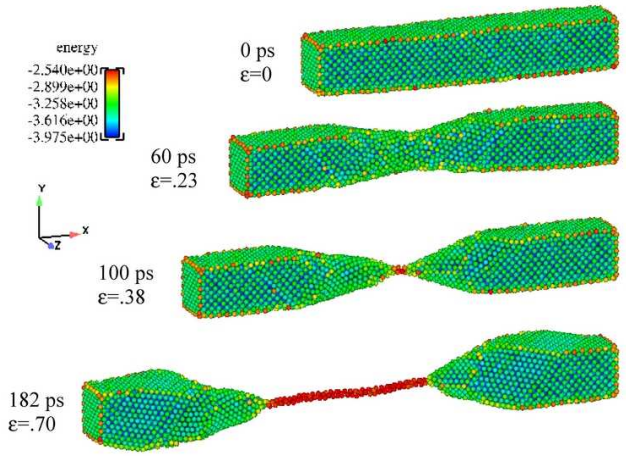
$$v_i^{n+1} = v_i^{n+1/2} + \left(\frac{\Delta t}{2m}\right) f_i^{n+1}$$

Discrete Peridynamic Equation of Motion

- Discrete Peridynamic model is collection of particles in space
- Peridynamic particles interact via pair potential
  - Peridynamic state theory more general
- Peridynamic particles advanced in time via velocity-Verlet scheme
- To the molecular dynamicists in the audience:
  - Does computational structure of discrete PD model sound familiar?

Classical Molecular Dynamics

- **Classical MD model is collection of particles in space**
- **MD particles can interact via pair potential**
- **MD particles can be advanced in time via velocity-Verlet scheme**
- **Practical limitations to MD length/time scales**



Au nanowire formation and extension*

Length ~ 16 nm

Time ~ 200 ps

Timestep = 0.001 ps

*H.S. Park and J.A. Zimmerman, *Modeling inelasticity and failure in gold nanowires*, Phys Rev B, 72, 054106 (2005).

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Peridynamics within a Molecular Dynamics Code

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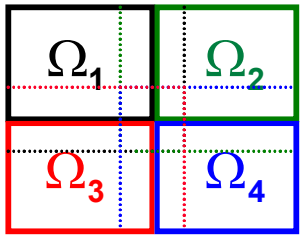
Peridynamics-in-LAMMPS (PDLAMMPS)

- Utilized LAMMPS (Sandia's open source MD package)
  - Large-scale Atomic/Molecular Massively Parallel Simulator
  - Open source, massively parallel, general purpose MD simulator
  - Many interatomic potentials for bio/polymers, solid state materials, etc.
  - Demonstrated scalability on Top500 computers (BlueGene/L, Red Storm)
  - Leverage MPI framework for particle model

- MPI: spatial data decomposition + ghosting



- Added "SI" units to LAMMPS for macroscale simulations
  - MD: angstroms, femtoseconds, etc.
  - PD: meters, seconds, etc.

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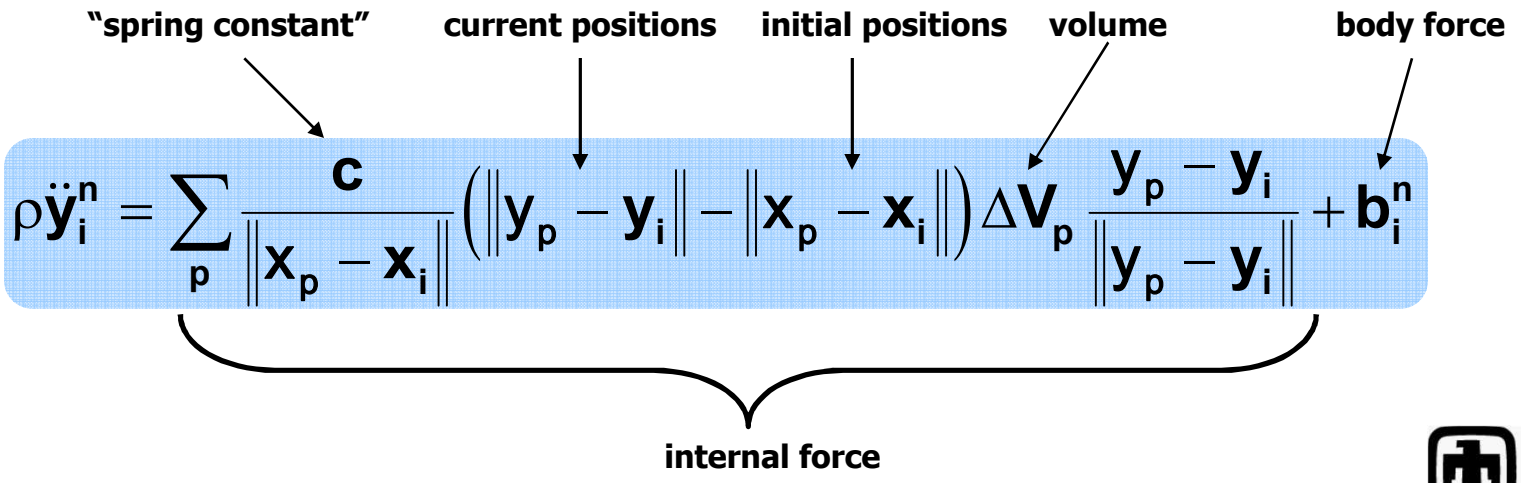
Peridynamics-in-LAMMPS (PDLAMMPS)

- Defined new peridynamic particle class
  - Typical MD variables for each atom: current position, velocity, force, mass
  - Additional PD particle variables: volume, critical stretch, initial position

- Defined new peridynamic pairwise force function for PD particles
  - Prototype microelastic brittle model described earlier
  - LAMMPS highly extensible; easy to introduce new potentials



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Peridynamics-in-LAMMPS (PDLAMMPS)

- Defined list of bonds for all particles
  - Each particle knows its bond pairs
  - Bonds computed only once before simulation start
  - Bonds broken as necessary

- Verlet list used for short-range interactions
  - Allow for contact forces
  - Nonbonded particles otherwise noninteracting
  - 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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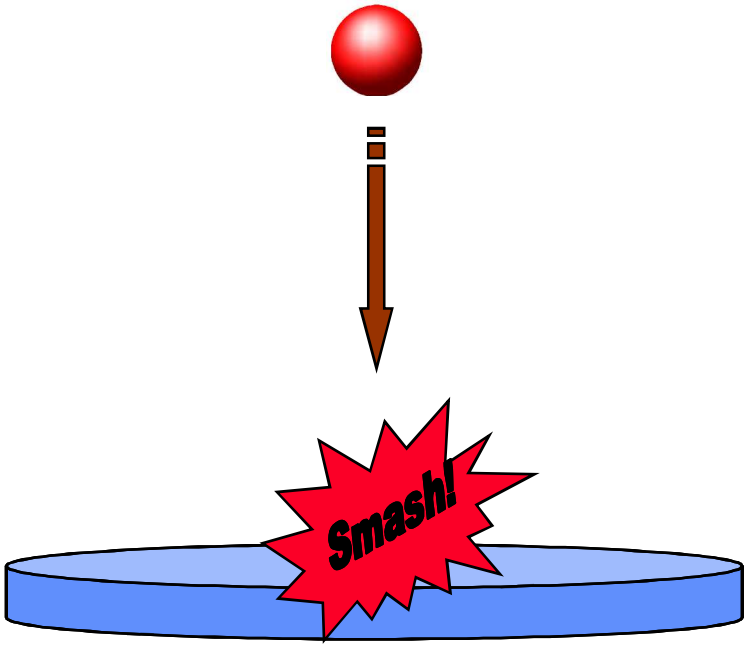
Computational Example

Hard Sphere Impact on Brittle Disk*

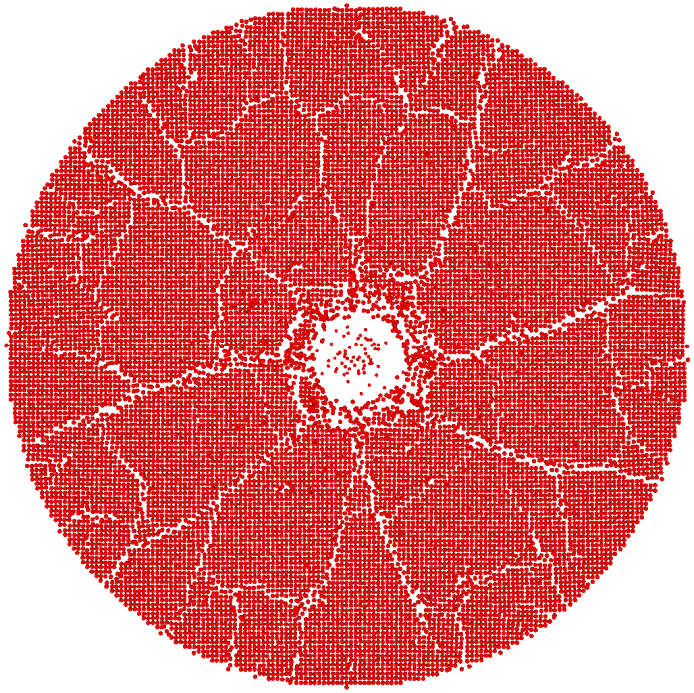
- **Projectile**
  - **Sphere (diameter 0.01 m)**
  - **Velocity 100 m/s**
- **Target**
  - **Disk: diameter 0.074 m, thickness 0.0025 m**
  - **Elastic modulus 14.9 GPa**
  - **Density 2200 kg/m^3**
- **Discretization**
  - **Mesh spacing 0.005 m**
  - **100,000 particles**
  - **Timestep 1 $\times$ 10^{-9} s**
  - **200,000 timesteps**



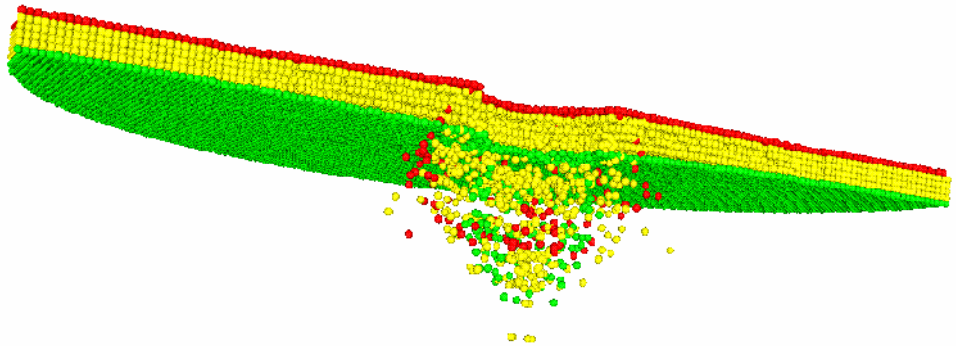
*S.A. Silling and E. Askari, *A meshfree method based on the peridynamic model of solid mechanics,* Computers and Structures, 83, pp. 1526-1535, 2005.

Hard Sphere Impact on Brittle Disk

- **Movie #1** [redacted]
  - View of top monolayer



- **Movie #2** [redacted]
  - Side view



Hard Sphere Impact on Brittle Disk

- **Scalability Results (hard scaling)**
  - **2.3 cm^3 cube of same material as disk (~100,000 particles)**
  - **Compare with equivalent Lennard-Jones simulation**

Number of Processors	LJ (sec)	LJ Speedup	PD (sec)	PD Speedup
1	4053.0	1.0	17302.6	1.0
2	2157.9	1.9	9028.4	1.9
4	1133.3	3.6	4673.6	3.7
8	587.6	6.9	2413.4	7.2
16	317.7	12.8	1327.9	13.0
32	172.4	23.5	714.6	24.2
64	94.0	43.1	380.2	45.4

Summary

- **Why PD in MD?**
  - **Continuum mechanics within MD**
  - **Atomistic-to-continuum coupling**
- **Peridynamic Model**
  - **Prototype microelastic brittle model**
  - **Easy to add other material models**
  - **PD state theory coming this fall**
- **Discretizing Peridynamics**
- **Peridynamics in a Molecular Dynamics Code (PDLAMMPS)**
- **Computational Example**

Software

- **EMU**
  - **Limited release; Ask Stewart Silling**
  - **(www.sandia.gov/emu/emu.htm)**

- **PDLAMMPS**
  - **Publicly available for download**
  - **(lammps.sandia.gov)**
  - **Use the "peri" package**

- **Papers**
  - **www.sandia.gov/~mlparks**
  - **MLP, S.J. Plimpton, R.B. Lehoucq, and S.A. Silling, *Peridynamics with LAMMPS: A User Guide*, Sandia Tech Report SAND 2008-1035.**
  - **MLP, S.J. Plimpton, R.B. Lehoucq, and S.A. Silling, *Implementing peridynamics within a molecular dynamics code*, Submitted to CPC, 2008.**

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