SAND2012-2142P

Computational Peridynamics

NAVAIR visit to SNL

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SAND2012-????

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What is Peridynamics?

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

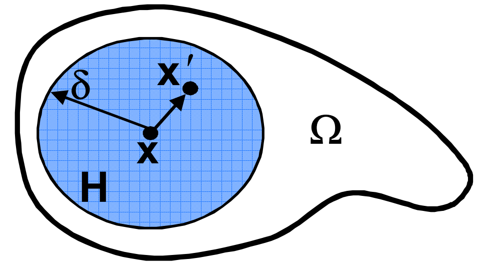
- Peridynamic equation of motion (integral, nonlocal)

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

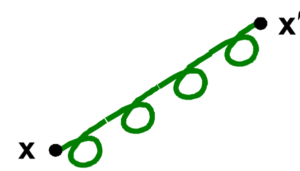
  - Replace PDEs with integral equations
  - No obstacle to integrating nonsmooth functions (fracture)
  - Utilize same equation everywhere; cracks not "special"
  - When bonds stretch too much, they break
  - f(·, ·) is "force" function; contains constitutive model
  - f = 0 for particles x,x' more than δ apart
    (analogous to cutoff radius in molecular dynamics!)
  - Peridynamics is "continuum form of molecular dynamics"

- Impact
  - Nonlocality
  - Larger solution space (fracture)
  - Length scales (multiscale material model)

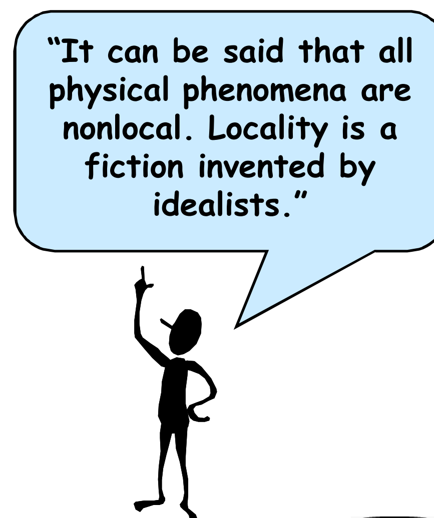
- Ancestors
  - Kröner, Eringen, Edelen, Kunin, Rogula, etc.



Peridynamic Domain



Peridynamic "bond"



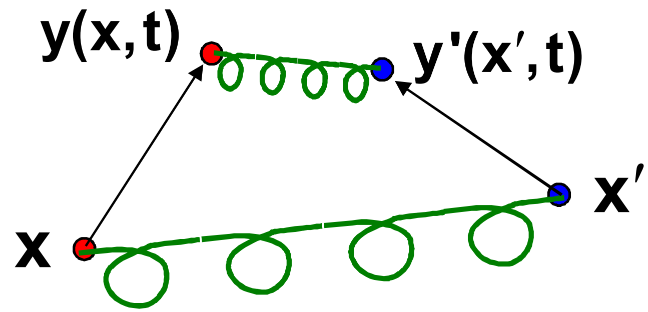
A. Cemal Eringen

Peridynamic Material Models

- Proportional microelastic brittle (PMB) material model*

$x \equiv$ initial position

$y \equiv$ current position



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

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

*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.

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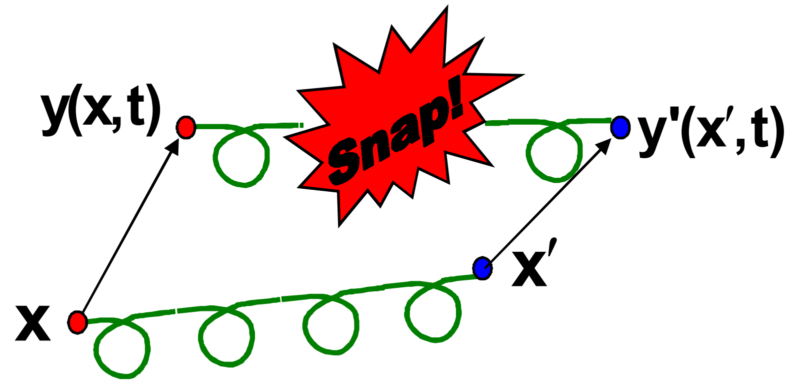
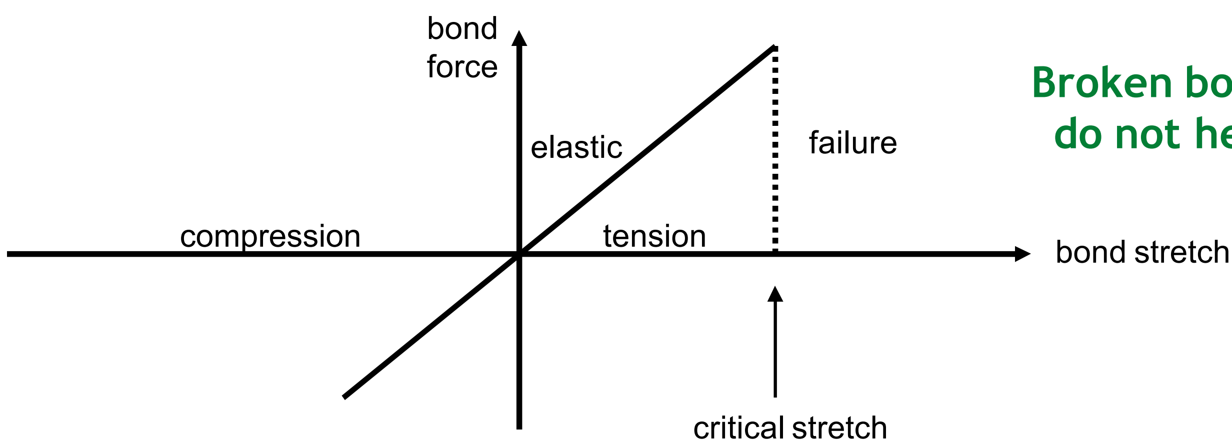


$$s = \frac{\|y' - y\| - \|x' - x\|}{\|x' - x\|}$$

Bond fails when stretch too large

Broken bonds do not heal



*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.

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Peridynamic Material Models

- Linear Peridynamic Solid (LPS)*
- Nonlocal analog to isotropic linear elastic solid

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t) = \int_H \left(\mathbf{T}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle - \mathbf{T}[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

$$\mathbf{T}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle = \left(\frac{3k\theta}{m} \underline{\omega}\,\underline{\mathbf{x}} + \frac{15\mu}{m} \underline{\omega}\,\mathbf{e}^{d} \right) \frac{\mathbf{x}' - \mathbf{x}}{\left\| \mathbf{x}' - \mathbf{x} \right\|}$$

- k is bulk modulus, μ is shear modulus

- LPS arises from multibody potential (similar to embedded-atom model)

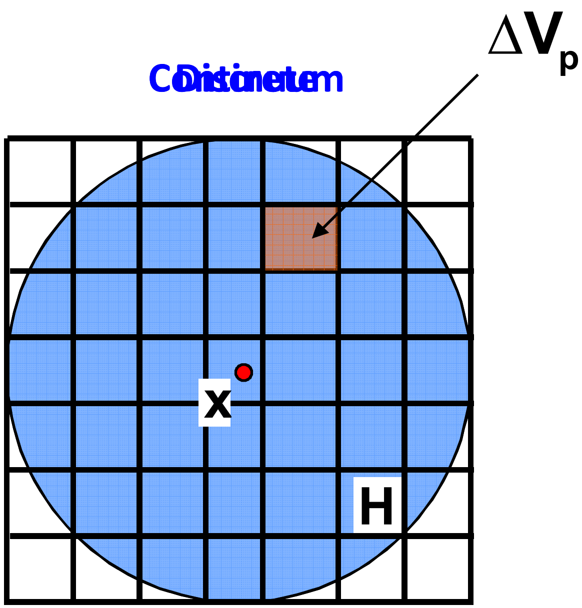
- History:
  - Pair potentials produce Poisson ratio ν = ¼ (All bonds independent)
  - EAM is pair potential + density-dependent term (general Poisson ratio)

- Many other material models available: elastic-plastic, viscoelastic, etc.
- Can wrap classical material models in peridynamic "skin"

*S.A. Silling, M. Epton, O. Weckner, J. Xu, & E. Askari, *Peridynamic States and Constitutive Modeling, J. Elasticity*, 88, pp. 151-184, 2007.

Discretizing Peridynamics

- Spatial Discretization
  - Approximate integral with sum*
  - Midpoint quadrature
  - Piecewise constant approximation



$$\int_H f(u(x',t) - u(x,t), x' - x)\, dV'$$

$$\sum_p f(u(x_p,t) - u(x_i,t), x_p - x_i)\, \Delta V_p$$

*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.

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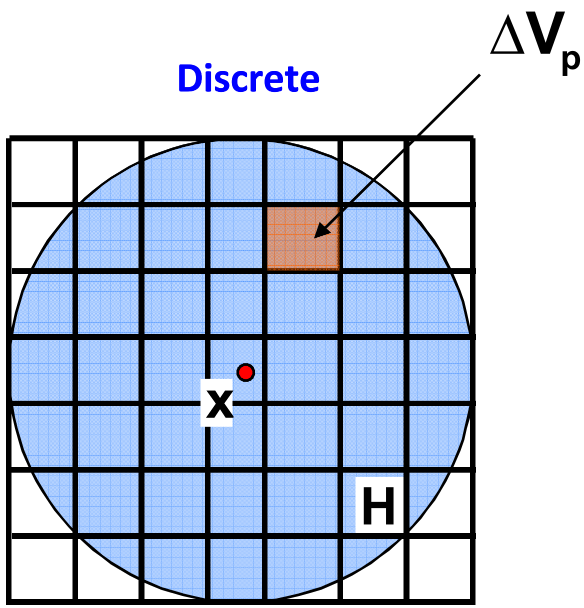

$$\sum_{p} f(u(x_p,t)-u(x_i,t),x_p-x_i)\Delta V_p$$

- 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

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

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

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

- This discretization has same computational structure as molecular dynamics!

(Discrete collection of particles in space interacting via pair or multibody potentials)

*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.

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Sandia Peridynamic Codes

- Peridigm (C++)
  - Developers: Parks, Littlewood, Mitchell, Silling
  - Primary Sandia open-source PD code
  - Built upon Sandia's Trilinos Project, algorithms and enabling technologies for the solution of large-scale, complex multi-physics engineering and scientific problems. (trilinos.sandia.gov)
  - Notable features: Massively parallel, Exodus mesh input/output multiple material blocks, explicit, implicit time integration State-based elastic-plastic, viscoelastic models, DAKOTA interface for UQ/optimization/calibration, etc.
- Peridynamics in Sierra/SolidMechanics (C++)
  - Developer: Littlewood
  - Primary Sandia engineering analysis code
- PDLAMMPS (Peridynamics-in-LAMMPS) (C++)
  - Developers: Parks, Seleson, Plimpton, Silling, Lehoucq
  - LAMMPS: Sandia's open-source massively parallel MD code (lammps.sandia.gov)
  - First open-source PD code
- EMU (F90)
  - Developer: Silling (www.sandia.gov/emu/emu.htm)
  - Research code

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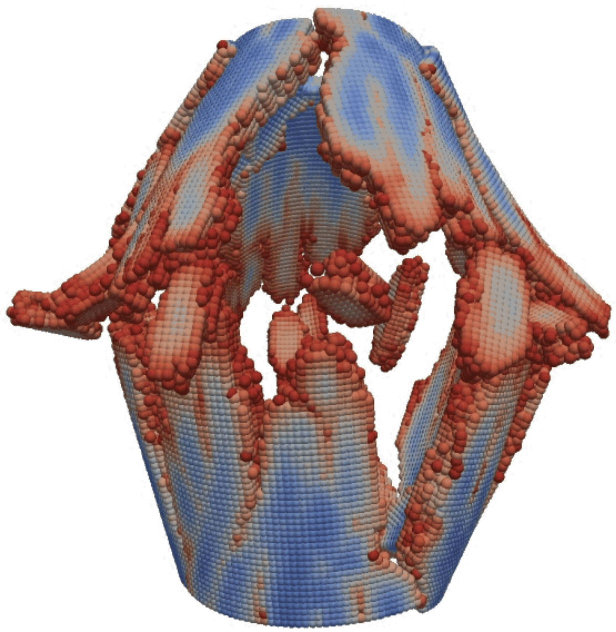
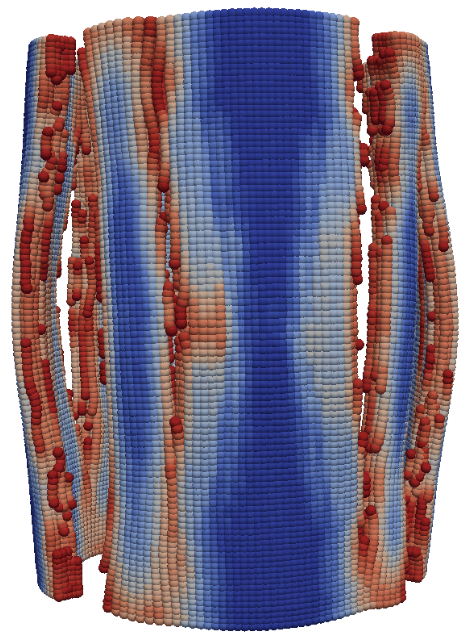
Fracture & Failure Modeling

- **Fragmenting Brittle Cylinder**
  - Motivated by tube fragmentation experiments of Winter (1979), Vogler (2003)*

Before



After
(brittle model)



After
(plastic model)

Color indicates damage

* D. Grady, Fragmentation of Rings And Shells: The Legacy of N.F. Mott, Springer, 2006.

Some Applications…

- ❑ **Fragmenting metal ring**
  - ❑ Motivated by ring fragmentation experiments of Grady & Benson*
  - ❑ Note regions of necking and failure
  - ❑ Utilized new peridynamic plasticity model**

* D. Grady, D. Benson, Fragmentation of metal rings by electromagnetic loading, Experimental Mechanics, 23(4), pp. 393-400, 1983

** J. Mitchell, A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics, SAND2011-3166, 2011.

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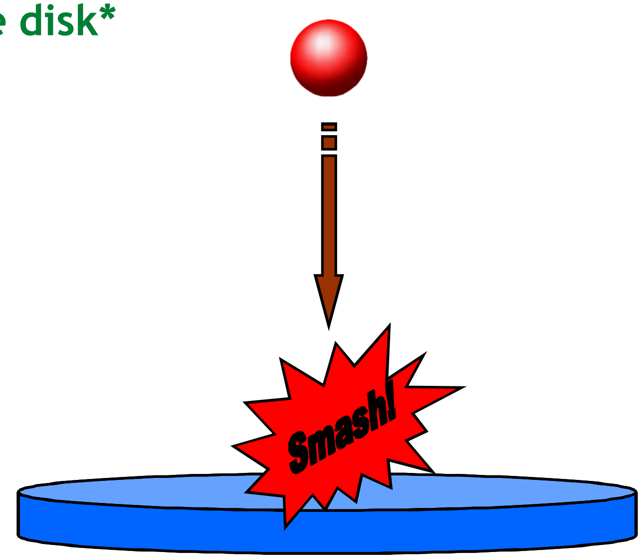
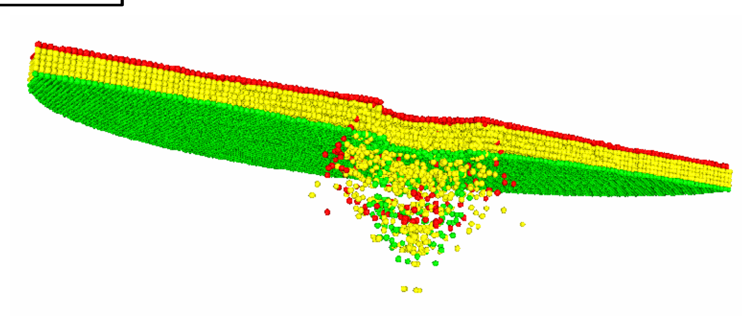
Some Applications…

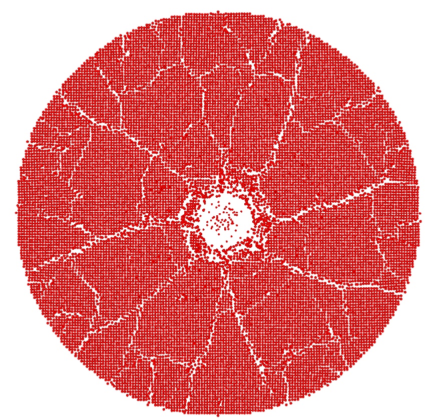
- **Example Simulation:** Hard sphere impact on brittle disk*
- Spherical Projectile
  - Diameter: 0.01 m
  - Velocity: 100 m/s
- Target Disk
  - Diameter: 0.074 m,
  - Thickness: 0.0025 m
  - Elastic modulus: 14.9 Gpa
  - Density: 2200 kg/m^3
- Discretization
  - Mesh spacing: 0.005 m
  - 100,000 particles
  - Simulation time: 0.2 milliseconds



Results



Side View



Top Monolayer

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

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Some Applications…

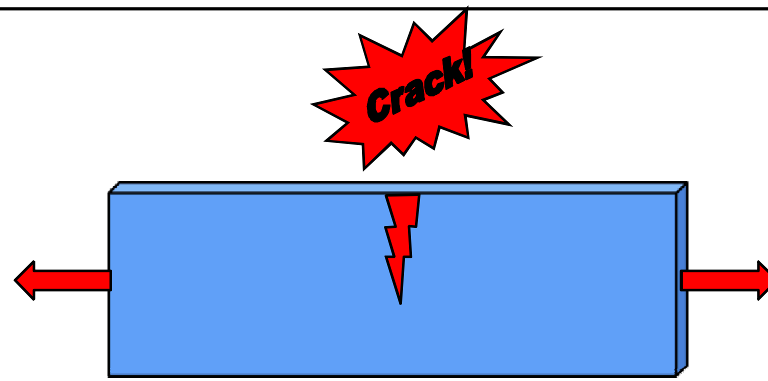
- **Example simulation: Dynamic brittle fracture in glass**
  - Joint with Florin Bobaru, Youn-Doh Ha (Nebraska), & Stewart Silling (SNL)

- **Soda-lime glass plate (microscope slide)**
  - Dimensions: 3” x 1” x 0.05”
  - Density: 2.44 g/cm3
  - Elastic Modulus: 79.0 Gpa

- **Discretization (finest)**
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)

Setup

- Glass microscope slide
- Dimensions: 3” x 1” x 0.05”
- Notch at top, pull on ends



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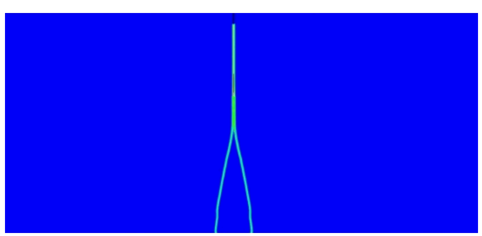
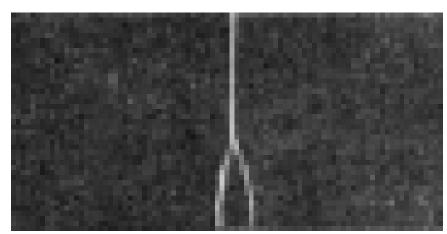


Peridynamics



Physical Experiment*

Strain Energy Density

*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.

Some Applications…

- Dawn (LLNL): IBM BG/P System
  - 500 teraflops; 147,456 cores
- Part of Sequoia procurement
  - 20 petaflops; 1.6 million cores
- Discretization (finest)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores
- Largest peridynamic simulations in history

***Dawn* at LLNL**

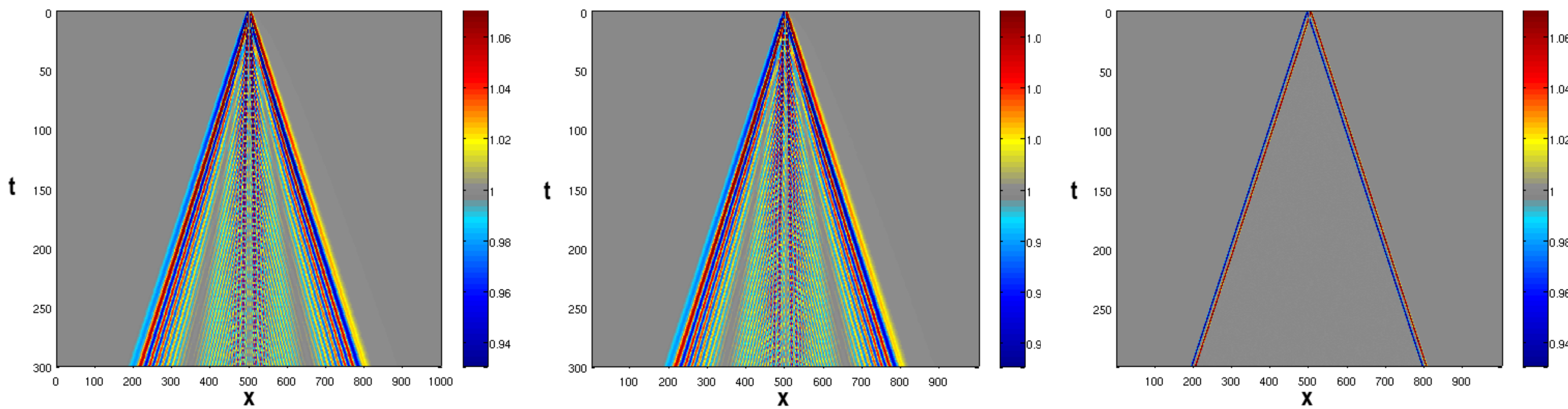
Weak Scaling Results (PDLAMMPS)

# 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

Some Applications…

- ❑ Goal: Cast upscaling of molecular dynamics as continuum peridynamic model
- ❑ Why: Approximate MD modeling fidelity at greatly reduced cost
  - ❑ MD has fixed lattice - This fixes computational costs
  - ❑ Peridynamics is continuum model - Can discretize on any mesh I want
- ❑ Example: 1D Nonlocal Mass/Spring Network*

“MD” Model | Peridynamic Model | Classical (Local) Model



- ❑ Peridynamic model captures behavior at multiple length scales; Local model doesn’t!
- ❑ Peridynamic model incurred only 20% the computational cost of MD model*
  - ❑ Peridynamic spatial discretization much more coarse than MD
  - ❑ Nonlocality allows larger CFL-compliant timestep
- ❑ Research topic: Model stress corrosion cracking with PD (mechanics, failure) and MD/ReaxFF (chemistry)

*P. Seleson, M.L. Parks, M. Gunzburger, and R.B. Lehoucq, Peridynamics as an Upscaling of Molecular Dynamics, Multiscale Modeling and Simulation, 8(1), pp. 204-227, 2009

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Summary

- What is peridynamics?
- Peridynamic Material Models
- Discretizations
- Codes
- Applications
- Multiscale modeling
- Papers, codes
  - www.sandia.gov/~mlparks; mlparks@sandia.gov