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Computational Peridynamics

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What is Peridynamics?

- **Peridynamics is a nonlocal extension of classical mechanics that permits discontinuous solutions (cracks)**
- Classical (Cauchy) equation of motion

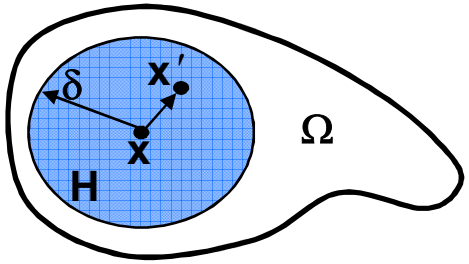
$$\rho\ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t) \qquad \sigma = g(\nabla u)$$

  - Assumes (strong form) differentiable displacement field
  - Fracture (discontinuous displacement field) treated as pathology
- Peridynamic equation of motion

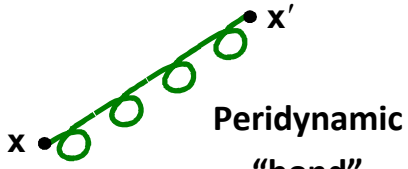
$$\rho\ddot{u}(x,t) = \int_H f(u(x'),u(x),x',x)dV' + b(x,t)$$

  - **Replace PDEs with integral equations**
  - No assumption of differentiable fields (admits fracture)
  - Use same equations everywhere (even at cracks!)
  - f(·, ·) is "force" function; contains constitutive model
  - f = 0 for particles x,x' more than δ apart (like cutoff radius in MD!)
  - PD is "continuum form of molecular dynamics"
  - In $\delta \rightarrow 0$ limit, recover classical elasticity
- Impact
  - Nonlocality → Multiple length scales
  - Larger solution space (resolve dynamic fracture patterns)
  - Simpler, more expedient mathematical and computational model

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



Peridynamic Domain



Peridynamic "bond"

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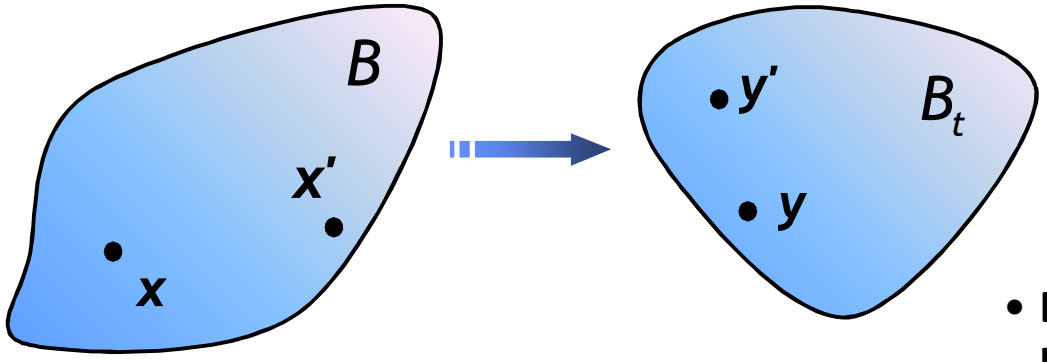
Deformation

Undeformed Body **Deformed Body**



$$y = x + u, \quad y' = x' + u'$$
$$x, x' \in B \quad y, y' \in B_t$$

$$y' - y = x' - x + u' - u$$
$$= (I + \nabla u)(x' - x) + O(\| x' - x \|^2)$$

- **Deformation gradient is a local linear approximation of true deformation**
- **Classical theory uses this approximation**
- **Nonlocality allows use of *true* deformation**

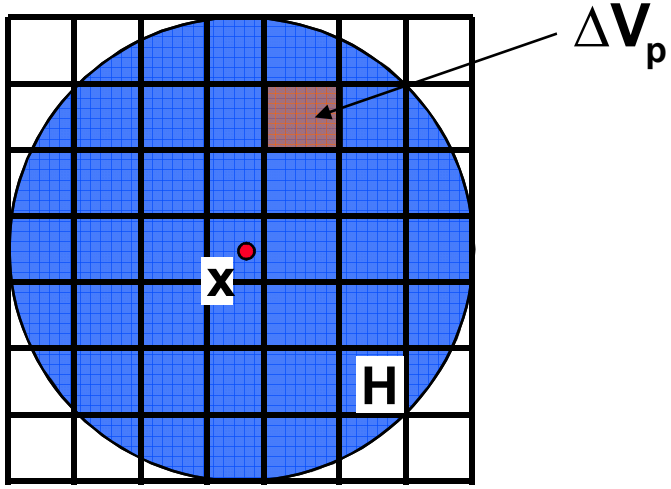
Classical Equation of Motion

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{b}$$
$$\boldsymbol{\sigma} = \mathbf{g}(\nabla \mathbf{u})$$

"It can be said that all physical phenomena are nonlocal. Locality is a fiction invented by idealists."
- A. Cemal Eringen

Discretizing Peridynamics

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



$$\sum_{p \in H} f(u(x_p', t), u(x, t), x_p' - x) \Delta V_p$$

- **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 approach sometimes called the "EMU" numerical method…**

EMU

*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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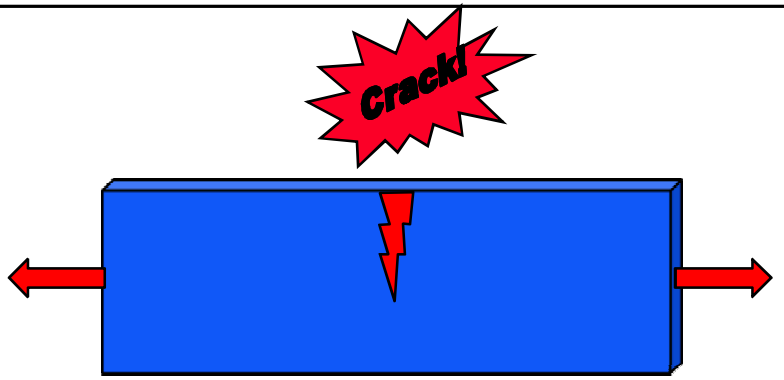
Peridynamics-in-LAMMPS (PDLAMMPS)

- This discretization of peridyamics has same computational structure as molecular dynamics, so put it into a molecular dynamics code (LAMMPS)!
- Goals:
  - Provide open source peridynamic code (distributed with LAMMPS)
  - Leverage portability, fast parallel implementation of LAMMPS
- Example simulation: dynamic brittle fracture in glass
  - Joint with Florin Bobaru, Youn-Doh Ha (Nebraska), & Stewart Silling (SNL)

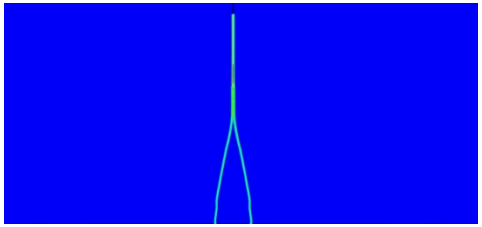
Setup

Fracture in Glass

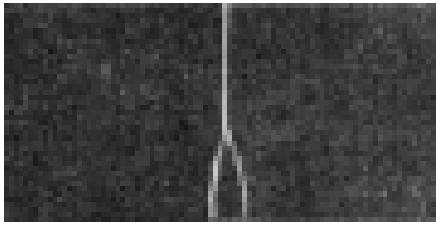
- Glass microscope slide
- Dimensions: 3”x1”x0.05”
- Notch at top, pull on ends



Results



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.

Peridynamics-in-LAMMPS (PDLAMMPS)

- 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

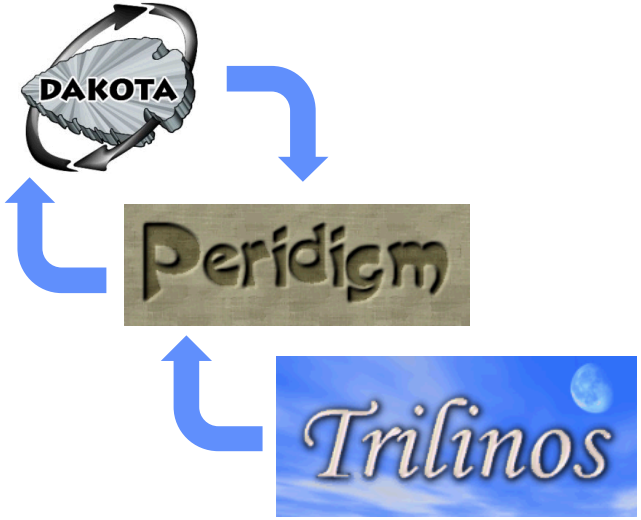
Weak Scaling Results

# 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

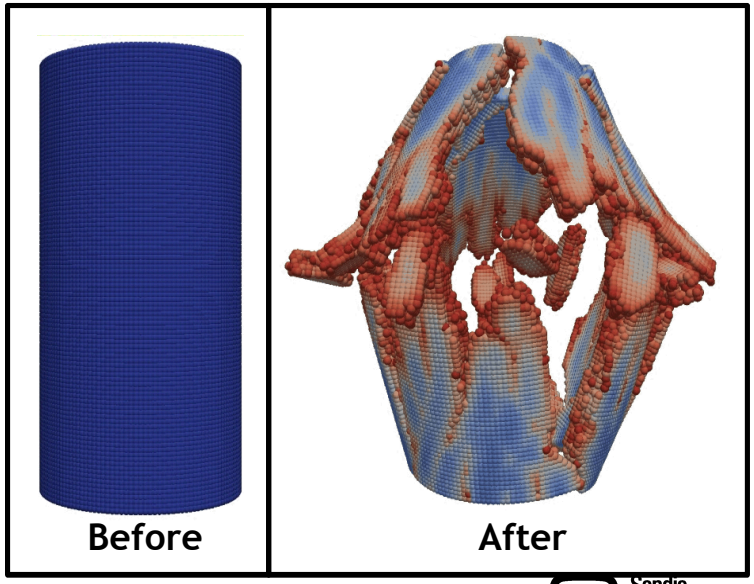
- PDLAMMPS is a “feature lite” peridynamic code…
- Towards multiphysics peridynamics with Peridigm…

Multiphysics Peridynamics via Agile Components

- Agile components: World-class algorithms delivered as reusable libraries
  - Full range of independent yet interoperable software components
  - Interfaces and capabilities
  - Choose capabilities a-la-carte (toolkit, not monolithic framework)
  - Software quality tools and practices
- Enable rapid development of new production codes



- Trilinos: Software framework providing parallelization tools, analysis tools, solver tools, interfaces, etc.
- DAKOTA: Toolkit for optimization, error estimation, uncertainty quantification
- Peridigm:
  - Multi-physics
  - Scalable
  - Optimization-enabled
  - Born-in UQ



Fragmenting Brittle Cylinder
(color indicates damage)

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Multiphysics Peridynamics via Agile Components

Peridigm

Software Quality Tools

Mailing Lists

Version Control

Build System

Testing (CTest)

Project Management

Issue Tracking

Wiki

UQ

Optimization

Error Estimation

Calibration

Visualization

Service Tools

Parallelization Tools

Data Structures (Epetra)

Load Balancing (Zoltan)

Analysis Tools

UQ (Stokhos)

Optimization (MOOCHO)

Services

Interfaces (Thyra)

Tools (Teuchos, TriUtils)

Field Manager (Phalanx)

DAKOTA Interface (TriKota)

Model Evaluator(EpetraExt)

Solver Tools

Iterative Solvers (Belos)

Direct Solvers (Amesos)

Nonlinear Solvers (NOX)

Eigensolvers (Anasazi)

Preconditioners (IFPack)

Multilevel (ML)

Time Integration (Rythmos)

Missing

Explicit 2nd Order Time Integration

Neighborhood Search

Stateful Model Evaluator

Current & Ongoing Research

- Peridigm (CSRF)
  - Well designed, maintainable, extensible, production quality peridynamic code
- Peridynamics-in-LAMMPS (discussions with ExxonMobil Research)
- Continuing work with Boeing (787), ORICA (bench blasting), ARL (fragmenting munitions), ExxonMobil (driven fracture in shale)
- Advanced discretization & solver techniques
  - Peridynamic (nonlocal) finite element methods
  - Peridynamic (nonlocal) domain decomposition methods
- Coupling peridynamics and classical mechanics
  - PD/classical FEM interactions through contact; move towards coupling
- Recent multiscale peridynamic LDRD ending -- recognized with SNL ERA
  - Statistical mechanics foundation of peridynamics (Sears, Lehoucq)
  - Upscaling molecular dynamics to peridynamics (Parks)
  - Peridynamic energy equation (Silling, Lehoucq)
- ASCR proposal (pending funding) to extend mathematical foundations
  - Identified nonlocal mathematics as fruitful research area (everything is new!)
  - Support nonlocal finite element research (above)