SAND2012-1037P

Computational Peridynamics

Temple University

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What is Peridynamics?

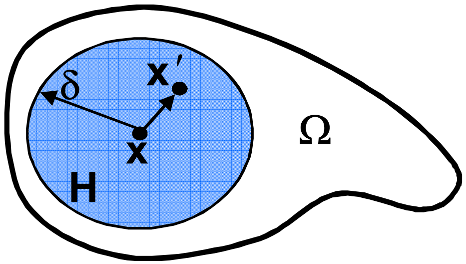
- Peridynamics is a nonlocal extension of classical solid mechanics that permits discontinuous solutions

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

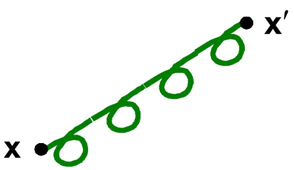
- Peridynamic equation of motion (integral, nonlocal)

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

  - 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"



Peridynamic Domain



Peridynamic "bond"

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

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

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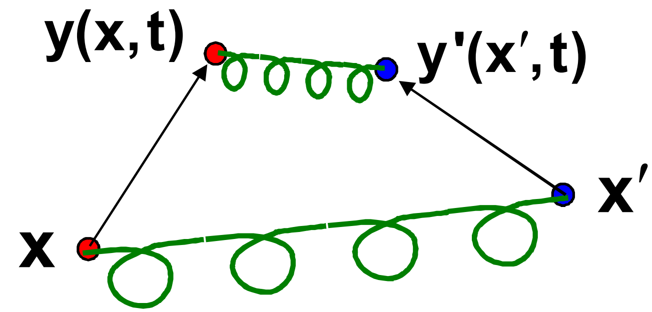
Peridynamic Material Modeling

- PROPORTIONAL MICROELASTIC BRITTLE (PMB) MATERIAL MODEL*

$x \equiv$ initial position

$y \equiv$ current position



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

Hooke's Law

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

*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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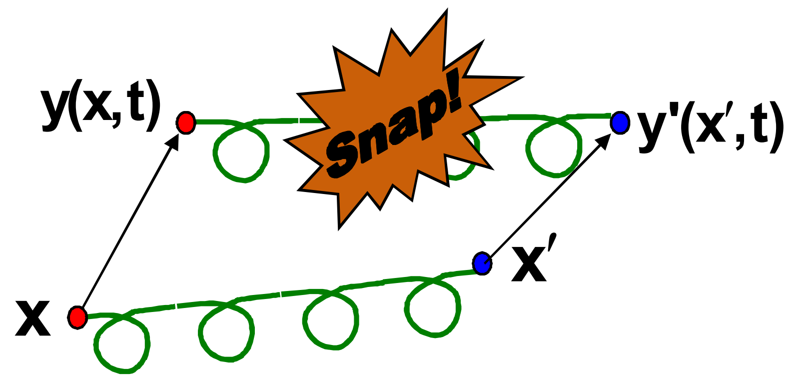
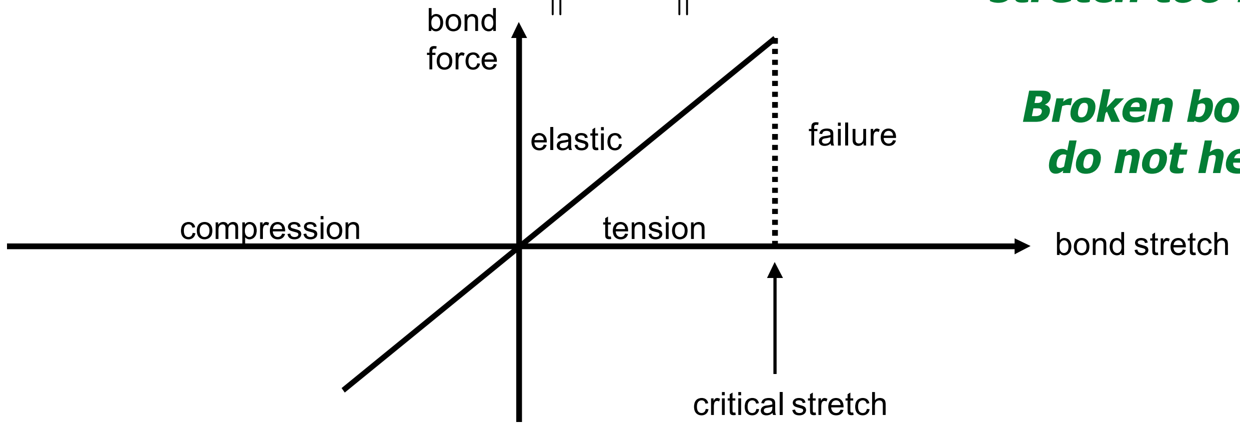


$$s = \frac{\|y' - y\| - \|x' - x\|}{\|x' - x\|}$$



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 Modeling

- Linear Peridynamic Solid (LPS)*
- Nonlocal analog to linear isotropic elastic solid
- k is bulk modulus, μ is shear modulus

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

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

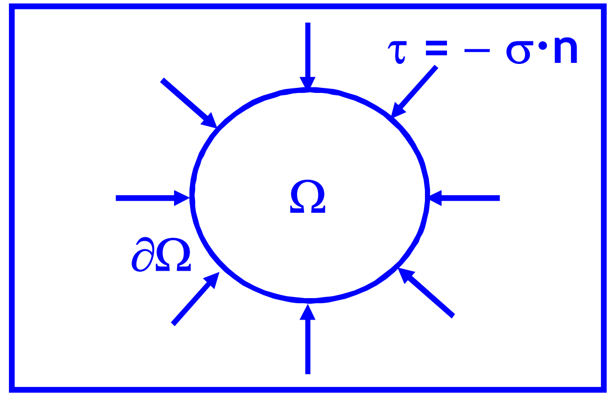
- Many other peridynamic material models available: elastic-plastic, viscoelastic, etc.

- Can wrap classical material models (existing material libraries) in peridynamic “skin”

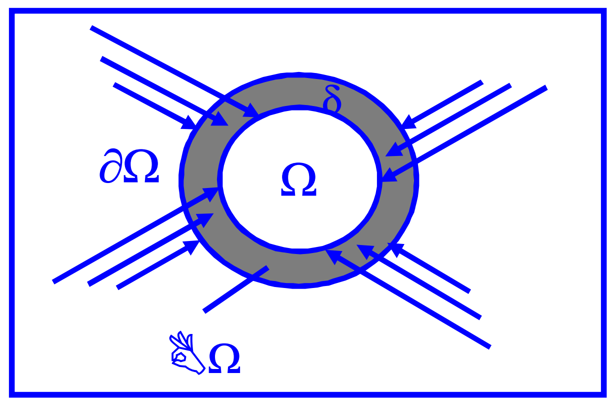
*S.A. Silling, M. Epton, O. Weckner, J. Xu, & E. Askari, Peridynamic States and Constitutive Modeling, J. Elasticity, 88, pp. 151-184, 2007.

Local vs. Nonlocal Models

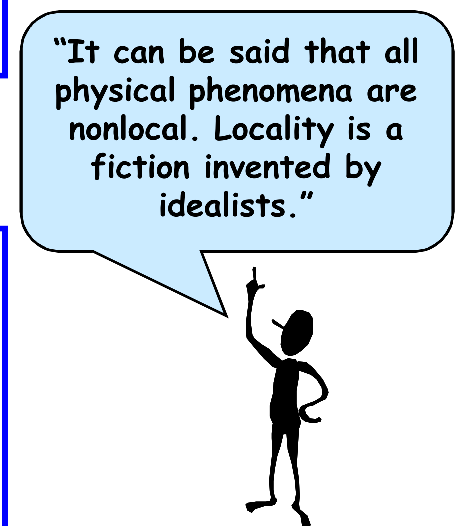
- ❑ **Local model:**
  - ❑ Contact force
  - ❑ Exterior of circle imparts force to interior via surface
  - ❑ Cauchy cut principle
- ❑ Examples:
  - ❑ Classical elasticity, etc.
  - ❑ Any PDE-based model
- ❑ **Nonlocal model:**
  - ❑ Action-at-a-distance
  - ❑ **Exterior of circle interacts directly with 👌Ω in interior of circle**
- ❑ Examples:
  - ❑ Molecular dynamics
  - ❑ Peridynamics



Local Interation



Nonlocal Interaction



A. Cemal Eringen

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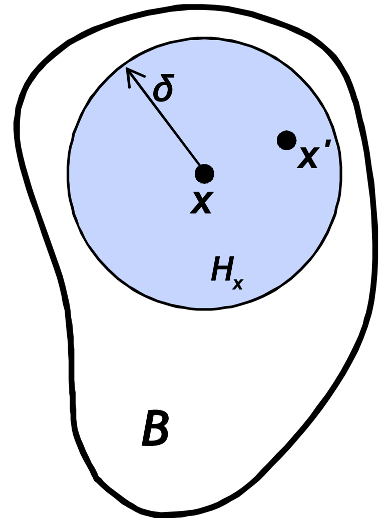
Length Scales

- What does it mean to have a length scale?
  - What does it mean to be multiscale?
- Example #1: $\ddot{u}(x) = au''(x)$
  - Equation has no length scale; same dynamics at all scales
- Example #2: $\ddot{u}(x) = au''(x) + bu''''(x)$
  - Dimensional analysis gives that sqrt(b/a) has units of length
  - Rescaling x can make first term dominant or second term dominant
  - Scaling of x changes behavior of equation
- Peridynamic horizon δ represents a *length scale*
  - Behavior (dynamics) of EOM vary with length scale
  - Exhibit desired physics on applied length scale
- Peridynamics provides desired dynamics at multiple length scales!
  - Rescaling space (equivalent to rescaling δ) provides transition from microscale to macroscale (classical) models!
- Connection between nonlocal models and higher-gradient models



Peridynamic Model (nonlocal)

$$\rho\ddot{u}(x,t) = \int_{-\delta}^{\delta} \frac{c}{|\varepsilon|}\left[u(x+\varepsilon,t) - u(x,t)\right] d\varepsilon$$

Taylor series

Higher-Gradient Model (weakly nonlocal)

$$\rho\ddot{u}(x,t) = K_a\left[\frac{d^2u}{dx^2} + \frac{\delta^2}{24}\frac{d^4u}{dx^4} + \frac{\delta^4}{1080}\frac{d^6u}{dx^6} + \dots\right]$$

lim $\delta \rightarrow 0$

Local, Scale Invariant

$$\rho\ddot{u}(x,t) = K_a\frac{d^2u}{dx^2}$$

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Relationship with Classical Theory

- Assuming u sufficiently smooth, re-write integral equation using nonlocal stress tensor ν

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

$$= \nabla \cdot \nu(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t)$$

Peridynamic stress tensor

- Nonlocal stress never needed in practice!

- If u sufficiently smooth, convergence to classical elasticity in limit as $\delta \to 0$

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

Piola-Kirchhoff stress tensor

- Peridynamics can be viewed as nonlocal extension of classical theory

*R.B Lehoucq and S.A. Silling, *Force flux and the peridynamic stress tensor,* J. Mech. Phys. Solids, 56, pp. 1566-1577, 2008.
*S.A. Silling and R..B Lehoucq, *Convergence of Peridynamics to Classical Elasticity Theory,* J. Elasticity, 93(1), pp. 13-37, 2008.

Part I
Codes and Applications

Part II
Discretizations and Numerical Methods

Part III
Peridynamic Finite Elements

Part IV
Nonlocal Substructuring

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Peridynamic Codes

- **Peridigm** (Open source, C++)
  - Developers: Parks, Littlewood, Mitchell, Silling
  - Intended as Sandia's primary open-source PD code
  - Built upon Sandia's Trilinos Project **(trilinos.sandia.gov)**
  - Massively parallel, Exodus mesh input, Multiple material blocks
  - Explicit, implicit time integration
  - State-based linear elastic, elastic-plasticity, viscoelastic models
  - DAKOTA interface for UQ/optimization/calibration, etc. **(dakota.sandia.gov)**
- **PDLAMMPS (Peridynamics-in-LAMMPS)** (Open source, C++)
  - Developers: Parks, Seleson, Plimpton, Silling, Lehoucq
  - Particular discretization of PD has computational structure of molecular dynamics (MD)
  - LAMMPS: Sandia's open-source massively parallel MD code (**lammps.sandia.gov**)
  - First open-source PD code
  - More info & user guide: **www.sandia.gov/~mlparks**
- **Peridynamics in Sierra/SolidMechanics** (C++)
  - Developer: Littlewood
  - Sandia engineering analysis code
- **EMU** (F90)
  - Developer: Silling (**www.sandia.gov/emu/emu.htm**)
  - Research code

Peridynamics via Agile Components

Peridigm

Software Quality Tools

- Mailing Lists
- Version Control
- Build System
- Testing (CTest)
- Project Management
- Issue Tracking
- Wiki

DAKOTA

- UQ
- Optimization
- Error Estimation
- Calibration

ParaView

- Visualization

Visualization Toolkit

- Service Tools

Trilinos

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)

Solver Tools

- Iterative Solvers (Belos)
- Direct Solvers (Amesos)
- Nonlinear Solvers (NOX)
- Eigensolvers (Anasazi)
- Preconditioners (IFPack)
- Multilevel (ML)

Peridynamics-in-LAMMPS (PDLAMMPS)

- **Goals**
  - First open source peridynamic code (distributed with LAMMPS; lammps.sandia.gov)
  - Provide (nonlocal) continuum mechanics simulation capability within MD code
  - Leverage portability, fast parallel implementation of LAMMPS (Stand on the shoulders of LAMMPS developers)
- **Capability**
  - Prototype microelastic brittle (PMB), Linear peridynamic solid (LPS) models
  - Viscoplastic model
  - General boundary conditions
  - Material inhomogenity
  - LAMMPS highly extensible; easy to introduce new potentials and features
  - More information & user's guide at www.sandia.gov/~mlparks (Click on "software")
- **Papers**
  - M.L. Parks, P. Seleson, S.J. Plimpton, R.B. Lehoucq, and S.A. Silling, *Peridynamics with LAMMPS: A User Guide*, Sandia Tech Report SAND 2010-5549.
  - M.L. Parks, 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.

- ***A personal observation…***
  - Time from starting implementation to running first experiment: Two weeks
  - Time for same using XFEM, other approaches: ????
  - Conclusion: Peridynamics is an expedient approach for fracture modeling

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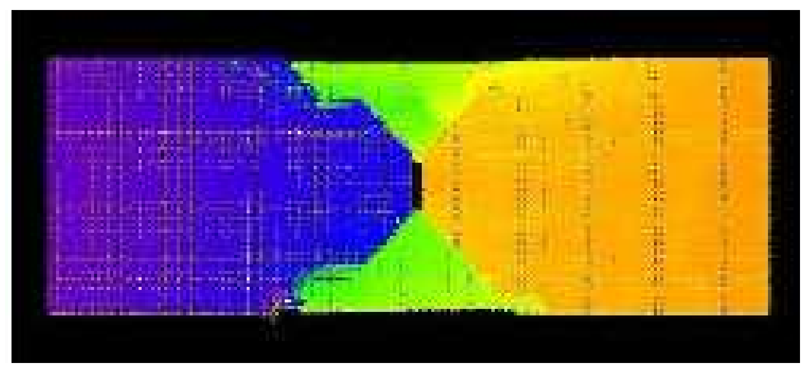
Simulation performed with EMU Fortran 90 code (Silling)

Some Applications…

- Splitting and fracture mode changes in fiber-reinforced composites*
- Fiber orientation between plies strongly influences crack growth

Typical crack growth in notched laminate (photo courtesy Boeing)



Peridynamic Model

* E. Askari, F. Bobaru, R.B. Lehoucq, M.L. Parks, S.A. Silling, O.Weckner, Peridynamics for multiscale materials modeling, in SciDAC 2008, Seattle, Washington, vol. 125 of Journal of Physics: Conference Series, (012078) 2008.

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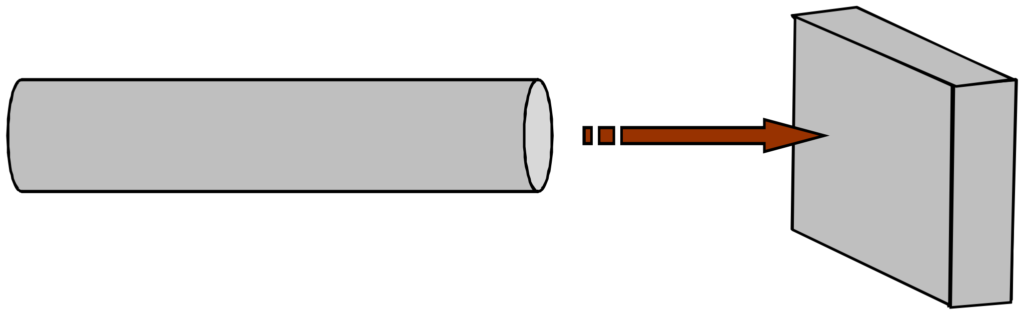
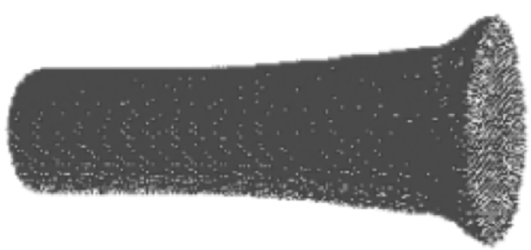
Simulation performed with EMU Fortran 90 code (Silling)

Some Applications…

- Taylor impact test of 6061-T6 aluminum*



Experiment



Peridynamic Model*

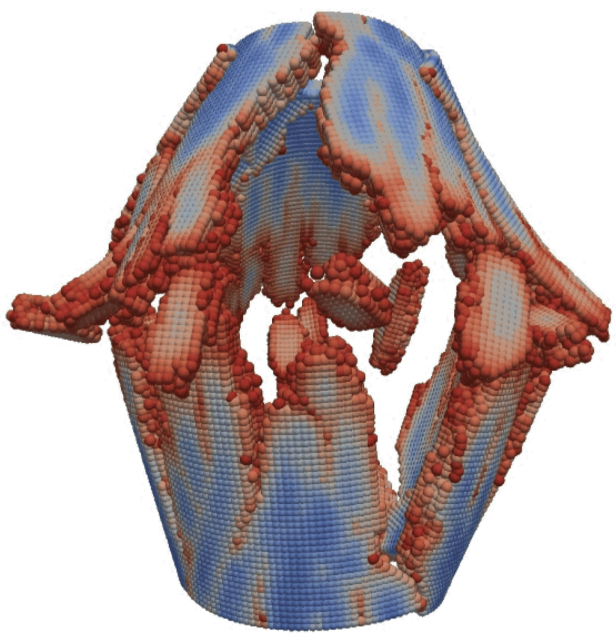
* J. Foster, S.A. Silling, W.W. Chen, Viscoplasticity Using Peridynamics, Sandia National Laboratories Technical Report SAND2008-7835, 2008.

Simulation performed with Peridigm

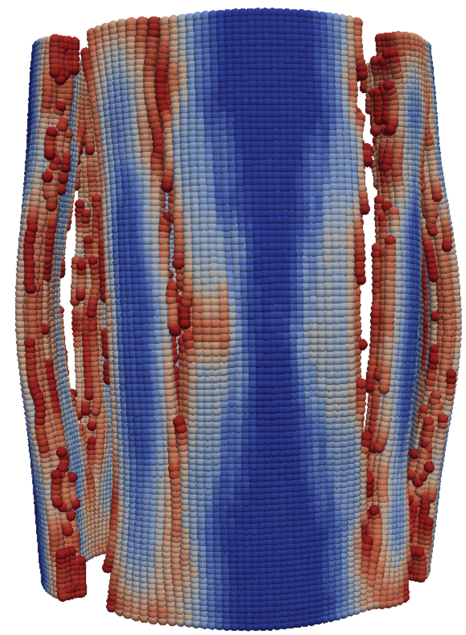
Some Applications…

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

Before



After (brittle failure)



After (ductile failure)

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

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Simulation performed with Peridigm

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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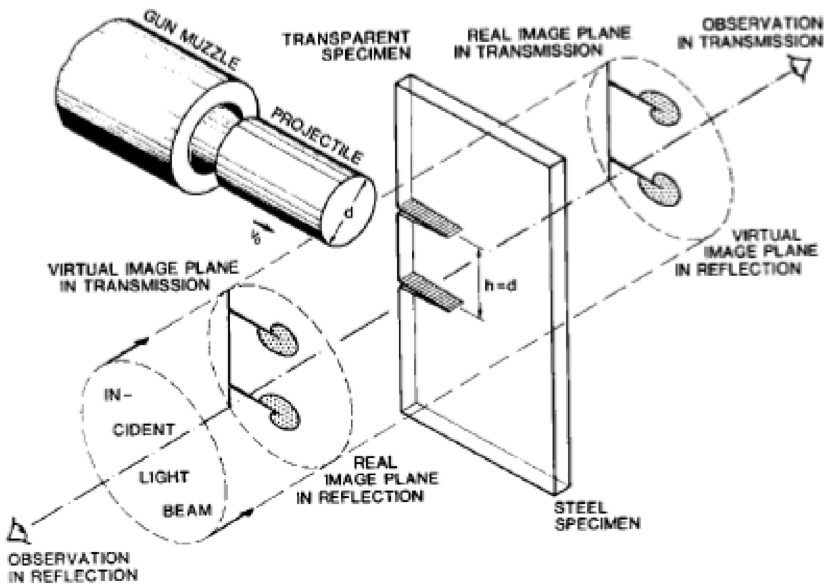
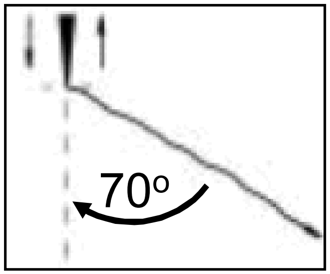
Simulation performed with EMU Fortran 90 code (Silling)

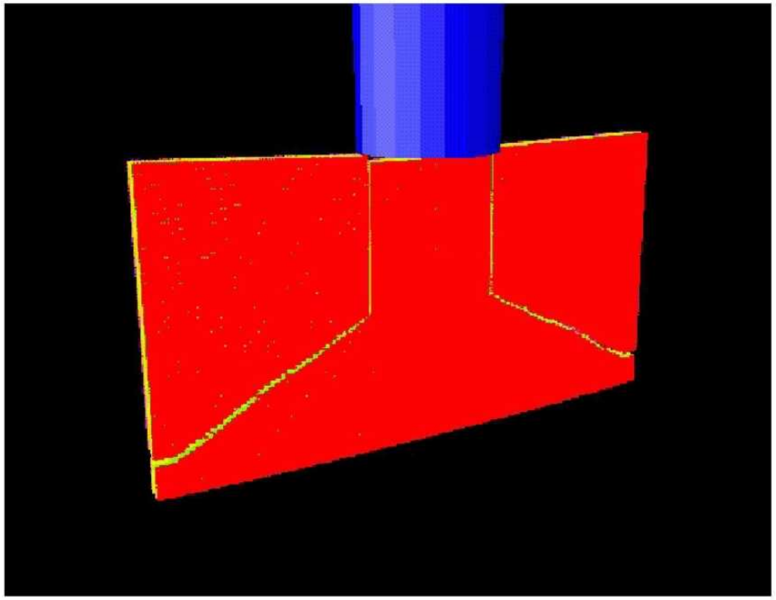
Some Applications…

- ❑ **Dynamic fracture in steel (Kalthoff & Winkler, 1988)**
- ❑ **Mode-II loading at notch tips results in mode-I cracks at 70º angle**
- ❑ **Peridynamic model reproduces the 70º crack angle***



Experimental Results





Peridynamic Model

* S. A. Silling, Dynamic fracture modeling with a meshfree peridynamic code, in Computational Fluid and Solid Mechanics 2003, K.J. Bathe, ed., Elsevier, pp. 641-644.

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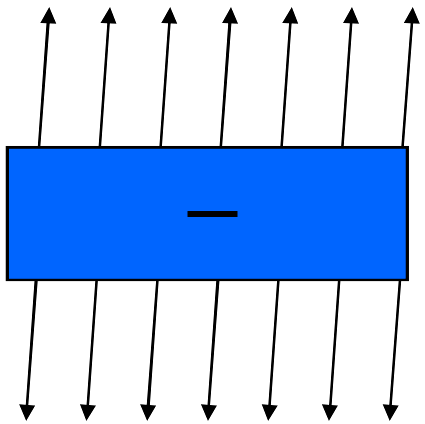
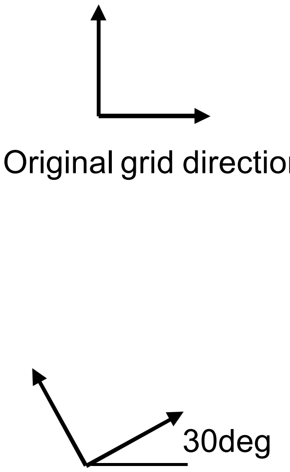
Simulation performed with EMU Fortran 90 code (Silling)

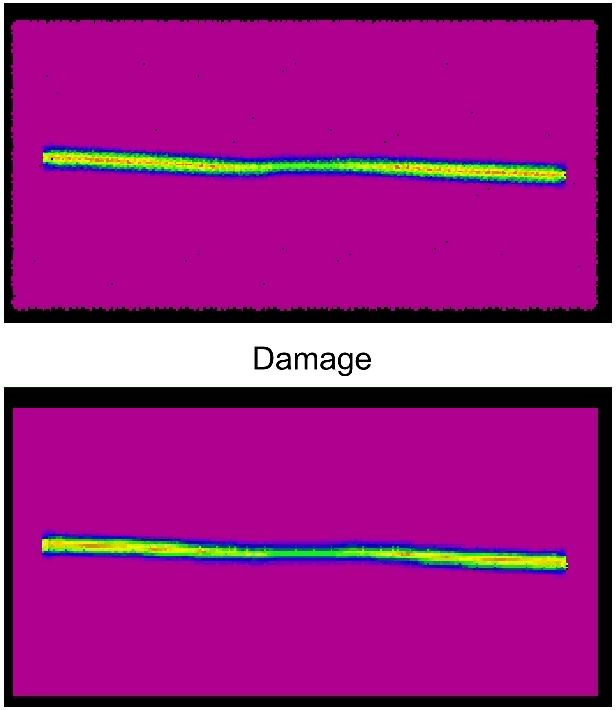
Some Applications…

- Discrete peridynamic model exhibits mesh-independent crack growth
- Plate with a pre-existing defect is subjected to prescribed boundary velocities
- Crack growth direction depends continuously on loading direction

$$\dot{\varepsilon} = (0.25\text{s}^{-1}) \begin{bmatrix} 0 & 0.1 \\ 0 & 1 \end{bmatrix}$$


(Mostly) Mode-I loading
(with a little Mode-II)



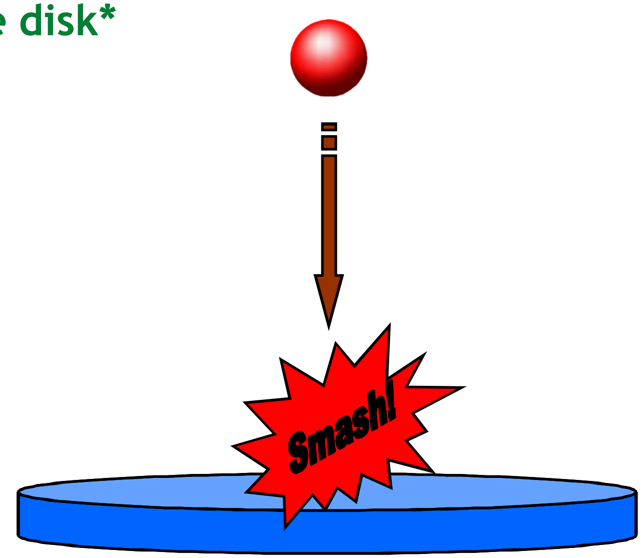

Damage

- Nonlocal network of bonds in many directions allows cracks to grow in any direction.

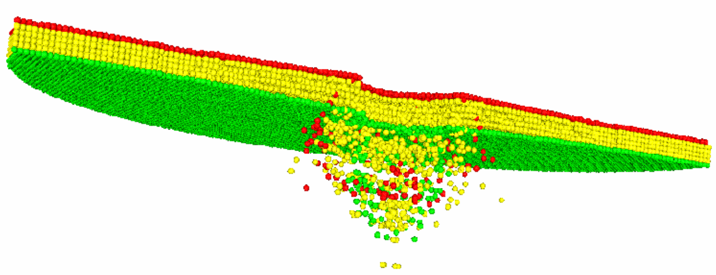
Simulation performed with PDLAMMPS code (Parks)

Some Applications…

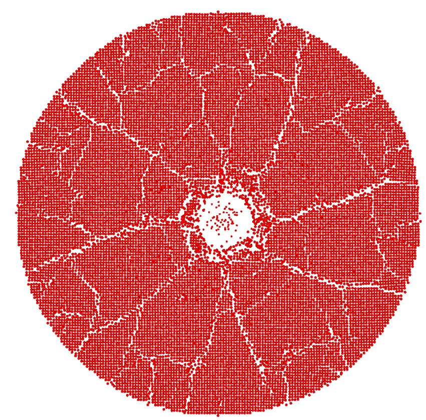
- **Example Simulation:** Hard sphere impact on brittle disk*
- Spherical Projectile
  - Diameter: 0.01 m
  - Velocity: 100 m/s
- Target Disk
  - Diameter: 0.074 m,
  - Thickness: 0.0025 m
  - Elastic modulus: 14.9 Gpa
  - Density: 2200 kg/m^3
- Discretization
  - Mesh spacing: 0.005 m
  - 100,000 particles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



Results



Side View



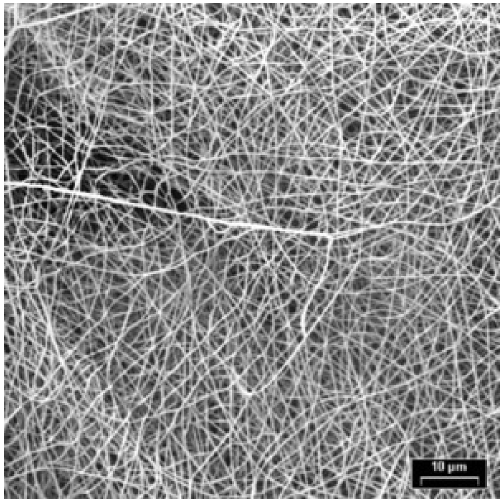
Top Monolayer

*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.

Simulation performed with PDLAMMPS code (Parks)

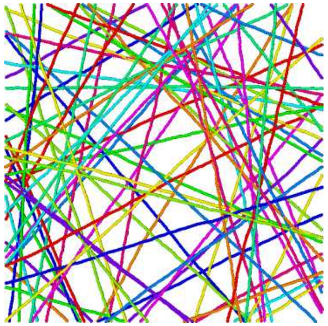
Some Applications…

- **Example Simulation:** **Failure of Nanofiber Network***
- **Nanofiber networks**
  - Large surface area to volume ratio
  - High axial strength and extreme flexibility
  - Used in composites, protective clothing, catalysis, electronics, chemical warfare defense
- **Numerical Model**
  - 400 nm x 400 nm x 10 nm
  - Biaxial strain induces failure
  - PD PMB material model (augmented for van der Walls forces)
- **Findings****
  - van der Walls important for strength and toughness
  - Heterogeneity in bonds strength increases toughness, ductility

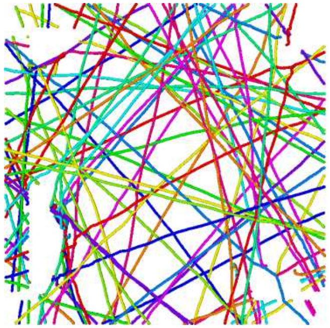


Nanofiber Network
(http://www.me.wpi.edu/MTE/current_projects.htm)

Results



t=0; 0% strain



t=30 ns; 17.6% strain

t=50 ns; 29.4% strain

* E. Askari, F. Bobaru, R.B. Lehoucq, M.L. Parks, S.A. Silling, and O. Weckner, Peridynamics for multiscale materials modeling, in SciDAC 2008, Seattle, Washington, July 13-17, 2008, vol. 125 of Journal of Physics: Conference Series, (012078) 2008.
** F. Bobaru, Influence of van der Waals forces on increasing the strength and toughness in dynamic fracture of nanofiber networks: a peridynamic approach, Modelling Simul. Mater. Sci. Eng., 15 (2007), pp. 397-417.

Simulation performed with PDLAMMPS code (Parks)

Some Applications…

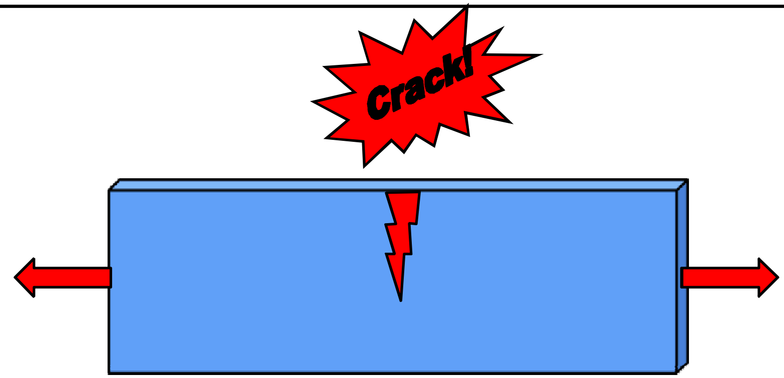
- **Example simulation:** Dynamic brittle fracture in glass
  - Joint with Florin Bobaru, Youn-Doh Ha (Nebraska), & Stewart Silling (SNL)

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

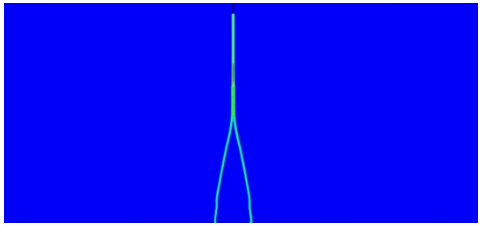
- Discretization (finest)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)

Setup

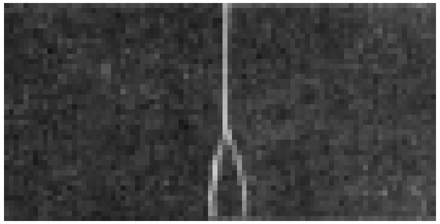
- Glass microscope slide
- Dimensions: 3” x 1” x 0.05”
- Notch at top, pull on ends



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.

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Simulation performed with PDLAMMPS code (Parks)

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

# 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

Part I
Codes and Applications

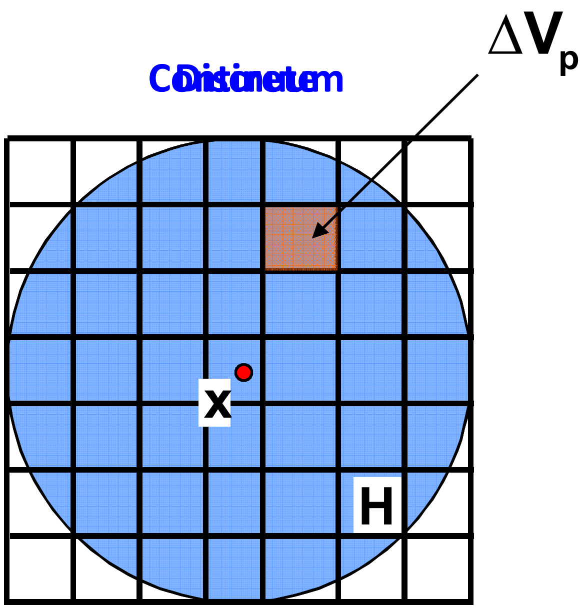
Part II
Discretizations and Numerical Methods

Part III
Peridynamic Finite Elements

Part IV
Nonlocal Substructuring

Discretizing Peridynamics

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



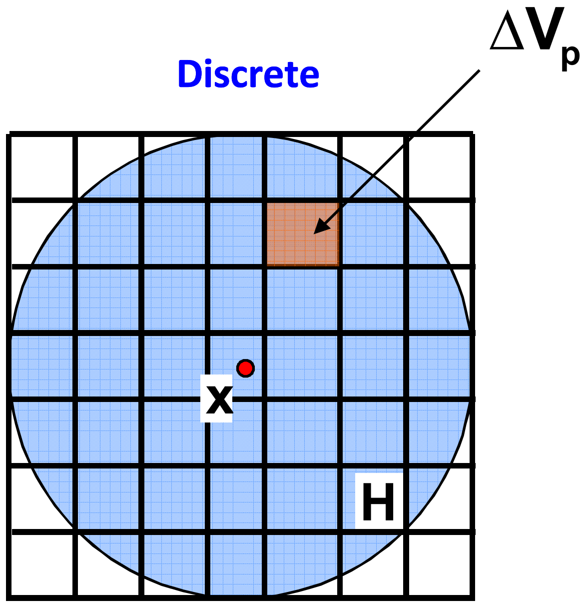
$$\int_H f(u(x',t) - u(x,t), x' - x)\, dV'$$

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

*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.

Discretizing Peridynamics

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



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

- **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

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

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

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

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Discretizing Peridynamics

- **Spatial Discretization**
  - Approximate integral with sum*
  - Midpoint quadrature
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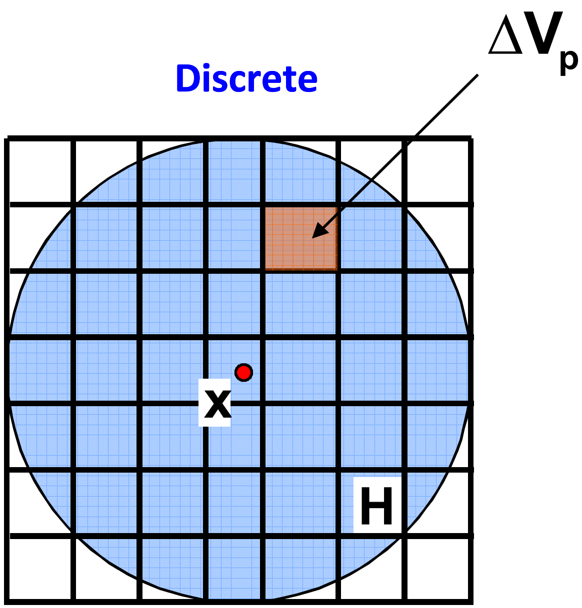

$$\sum_p f(u(x_p,t) - u(x_i,t), x_p - x_i)\Delta V_p$$

- **Temporal Discretization**
  - Explicit central difference in time

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

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

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

- **This approach is sometimes called the "EMU" numerical method (Silling)**

EMU

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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

- **This approach is simple but expedient. What more can we do?**

- **Temporal discretization**
  - Implicit time integration (Newmark-beta method, etc.)

- **Spatial discretization (strong form)**
  - Midpoint quadrature (EMU method)
  - Gauss quadrature*

- **Spatial discretization (weak form)**
  - Nonlocal Galerkin finite elements (1D)*
    - Nonlocal integration-by-parts*
    - Nonlocal mass & stiffness matrices, force vector*

- **Let's explore Peridynamic finite elements…**

*E. Emmrich and O. Weckner, *The peridynamic equation and its spatial discretization*, *Math. Model. Anal.*, 12(1), pp. 17-27, 2007.

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Nonlocal Substructuring

*B. Aksoylu and M.L. Parks, *Variational Theory and Domain Decomposition for Nonlocal Problems*. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

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Why is Conditioning Important?

- **What is the condition number of a matrix?**

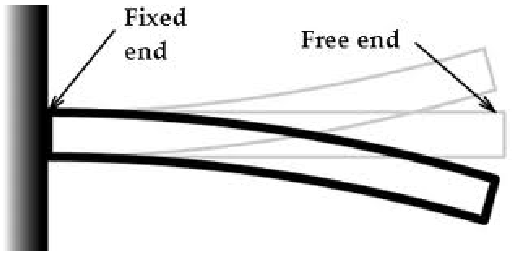
$$\kappa(A) = \|A\| \cdot \|A^{-1}\|$$

- **Why do we care?**
  - Condition number dictate convergence rates of linear solvers
  - Condition numbers dictate the accuracy of computed solution
  - Rule of thumb:
    If $\kappa(A) = 10^{16-d}$, then computed solution has d digits of accuracy.

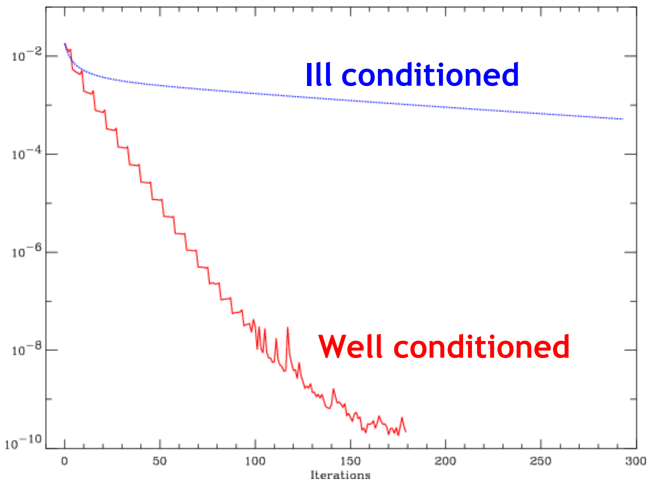
    If $\kappa(A) = 10^{16}$, expect zero digits of accuracy!

- Old saying: ***"You get the answer you deserve…"***

- **Driving motivation for effective preconditioners**



Cantilevered beam



Convergence curves for optimal Krylov methods

Why is Conditioning Important?

- **Why do I care about condition numbers of peridynamic models?**
  - First step towards scalable preconditioners
  - First step towards effective utilization of leadership class supercomputers for peridynamic simulations
- **New component in nonlocal modeling is peridynamic horizon δ**
  - How does δ affect the conditioning?
  - Develop preconditioners/solvers optimized for nonlocal models at extreme scales
- **DOE current computing platforms**
  - Jaguar (ORNL)
  - 2.595 petaflops (~2.5 quadrillion calculations per second)
  - 224,162 cores

- **US Department of Energy future computing platforms**
  - Exaflop machines by 2018

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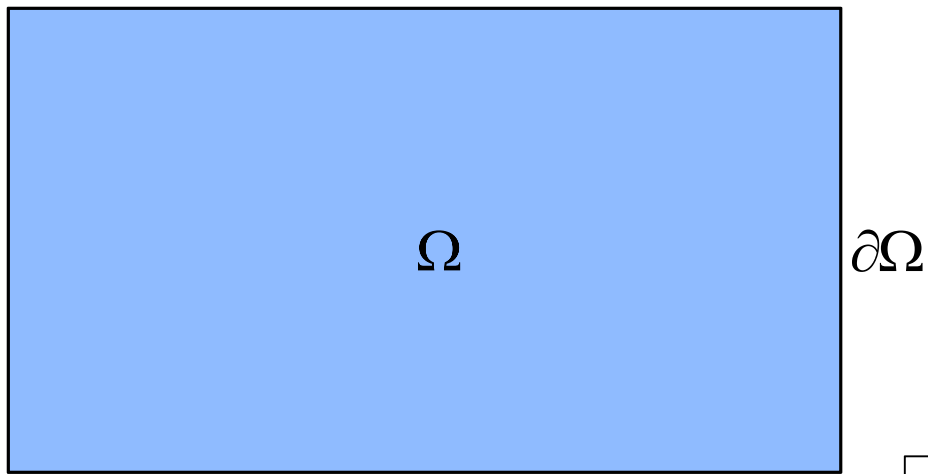
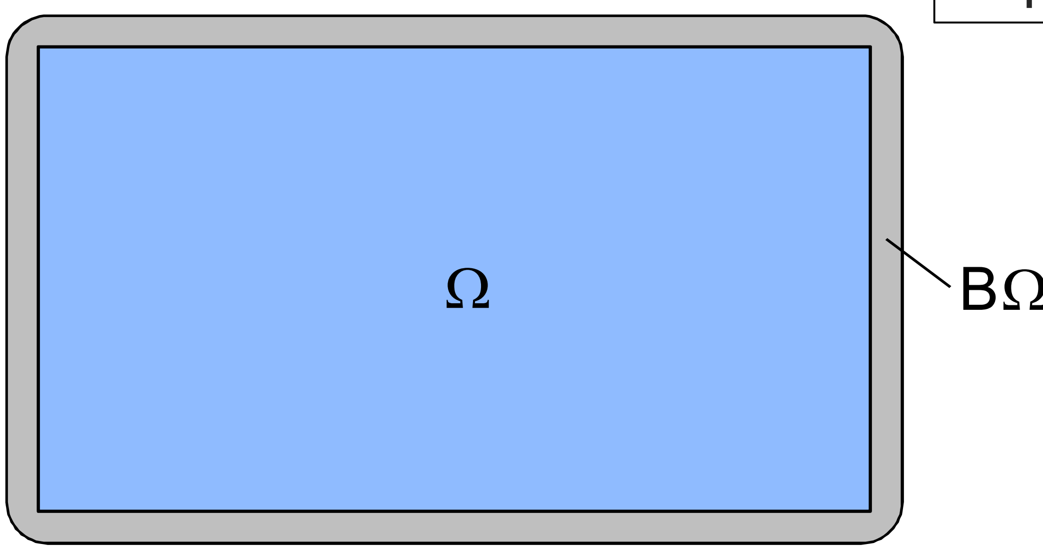
Nonlocal Boundaries

- Classical domain and boundary: $\bar{\Omega} = \Omega \cup \partial\Omega$



∂Ω interacts with all points in 👌Ω

- Nonlocal domain and boundary: $\bar{\bar{\Omega}} = \Omega \cup \mathrm{B}\Omega$



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Nonlocal Weak Form

- ❑ EMU/PDLAMMPS discretize strong form of equation (like finite differences)
- ❑ What about nonlocal finite elements?
- ❑ Prototype operator

$$L\{u\}(x) = -\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right]dx'$$

$$C(x,x') = C(x',x)$$

$$C(x,x') = 0 \text{ if } \|x - x'\| > \delta$$

- ❑ Need nonlocal weak form* → Multiply by test function and "integrate by parts"

$$a(u,v) = -\int_{\bar{\bar{\Omega}}}\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right]v(x)dx'dx$$

$$= \frac{1}{2}\int_{\bar{\bar{\Omega}}}\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right]\left[v(x') - v(x)\right]dx'dx$$

- ❑ Compare with local Poisson operator

$$-\nabla^2 u(x) \quad \longrightarrow \quad \frac{1}{2}\int \nabla u \cdot \nabla v \, dx$$

*E. Emmrich and O. Weckner, *The peridynamic equation and its spatial discretization*, *Math. Model. Anal.*, 12(1), pp. 17-27, 2007.

Nonlocal Quadrature

- Review: Local Quadrature
  - One integral required
  - Compute products of ***gradients*** of shape functions and apply Gauss quadrature
  - Gradient ***drops*** polynomial order (lower order quadrature scheme required)

$$a(u,v) = \frac{1}{2}\int \nabla u \cdot \nabla v \, dx$$

- Nonlocal Quadrature
  - Two integrals required
  - Compute products of differences of shape functions and integrate
  - No gradient → higher polynomial order (higher order quadrature needed)
  - Nonlocality generates substantially more work over each element
  - Discontinuous integrands a challenge for quadrature routines (more later…)

$$a(u,v) = -\int_{\bar{\bar{\Omega}}}\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right] v(x)\,dx'dx$$

$$= \frac{1}{2}\int_{\bar{\bar{\Omega}}}\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right]\left[v(x') - v(x)\right]dx'dx$$

  - Integration by parts is standard in local (classical) FEM.

Spectral Equivalence

- For simplicity, assume

$$C(x,x') = \chi_\delta(x - x') \equiv \begin{cases} 1 & \text{if } \|x - x'\| \le \delta \\ 0 & \text{otherwise} \end{cases}$$

"Canonical" Kernel Function

- Principal Theorem*

$$\lambda_1(\bar{\bar{\Omega}})\delta^{d+2} \le \frac{a(u,u)}{\|u\|_{L_2(\bar{\bar{\Omega}})}} \le \lambda_2(\bar{\bar{\Omega}})\delta^{d} \qquad u \in L_{2,0}(\bar{\bar{\Omega}})$$

- Let K be a finite element discretization of a(u,u). Then,

$$\kappa(K) \sim \mathcal{O}(\delta^{-2})$$

- This is not tight!
  - Consider lim $\delta \to 0$. Cond # estimate $\to \infty$, true $\kappa(K) \to h^{-2}$.
  - Condition number not mesh independent (bound is mesh independent).
  - In practice, observe **very** weak mesh dependence.
  - Bound descriptive when $h < \delta$.
  - Alternative approach: Zhou & Du†
- Dominant length scale in nonlocal model set by δ.
  - Contrast with local model, where length scaled introduced by h

*B. Aksoylu and M.L. Parks, *Variational Theory and Domain Decomposition for Nonlocal Problems*. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

† K. Zhou, Q. Du, Mathematical and numerical analysis of linear peridynamic models with nonlocal boundary conditions, SIAM J. Num. Anal., 48(5), pp. 1759—1780, 2010.

† Q. Du and K. Zhou. Mathematical analysis for the peridynamic nonlocal continuum theory. Mathematical Modelling and Numerical Analysis, 2010. doi:10.1051/m2an/2010040.

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Nonlocal Weak Form – 1D

- Let $\Omega = (0,1)$, $\partial\Omega = [-\delta,0]\cup[1, \delta]$.
- $u=0$ on $\partial\Omega$
- Let $C(x,x') = \begin{cases} 1 & \text{if } \|x - x'\| \le \delta \\ 0 & \text{otherwise} \end{cases}$
- Weak form becomes

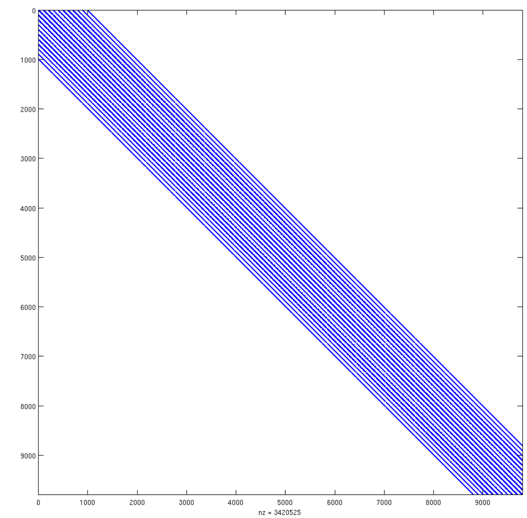
$$a(u,v) = -\int_{-\delta}^{\delta}\int_{x-\delta}^{x+\delta}[u(x') - u(x)]v(x)dx'dx$$

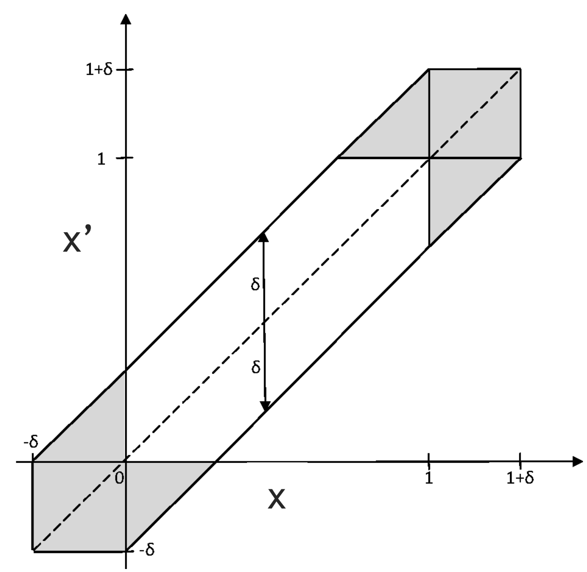
- Numerical Study
  - PW constant and PW linear SFs
  - Hold δ constant, vary h
  - Hold h constant, vary δ

Stiffness Matrix Sparsity Pattern

2D Model

(10,000 unknowns, 3.4M nnz)





Integration Domain in (x,x')

(grey = outside Ω)

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Nonlocal Finite Elements and Conditioning – 1D

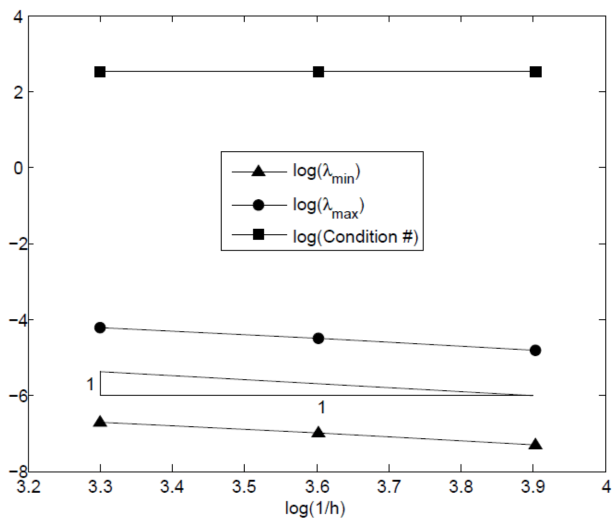
- Observations: $\kappa(K) \sim O(\delta^{-2})$, only weak h-dependence

(a) Constant δ, vary h.

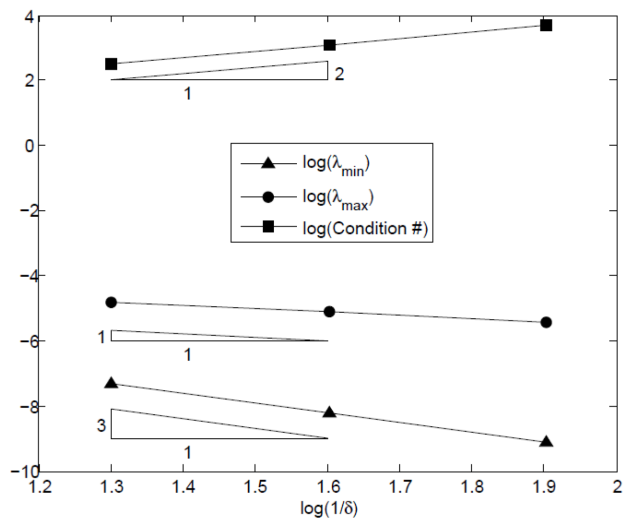
$1/h$	$1/\delta$	Piecewise Constant Shape Functions $\lambda_{\min}$	Piecewise Constant Shape Functions $\lambda_{\max}$	Piecewise Constant Shape Functions Condition #	Piecewise Linear Shape Functions $\lambda_{\min}$	Piecewise Linear Shape Functions $\lambda_{\max}$	Piecewise Linear Shape Functions Condition #
2000	20	1.94E-07	6.07E-05	3.13E+02	1.94E-07	6.07E-05	3.13E+02
4000	20	9.69E-08	3.04E-05	3.13E+02	9.69E-08	3.04E-05	3.14E+02
8000	20	4.84E-08	1.52E-05	3.14E+02	4.84E-08	1.52E-05	3.14E+02

(b) Constant h, vary δ.

$1/h$	$1/\delta$	Piecewise Constant Shape Functions $\lambda_{\min}$	Piecewise Constant Shape Functions $\lambda_{\max}$	Piecewise Constant Shape Functions Condition #	Piecewise Linear Shape Functions $\lambda_{\min}$	Piecewise Linear Shape Functions $\lambda_{\max}$	Piecewise Linear Shape Functions Condition #
8000	20	4.84E-08	1.52E-05	3.15E+02	4.84E-08	1.52E-05	3.14E+02
8000	40	6.24E-09	7.61E-06	1.22E+03	6.24E-09	7.60E-06	1.22E+03
8000	80	7.92E-10	3.80E-06	4.80E+03	7.91E-10	3.80E-06	4.80E+03



(a) Constant δ, vary h.



(b) Constant h, vary δ.

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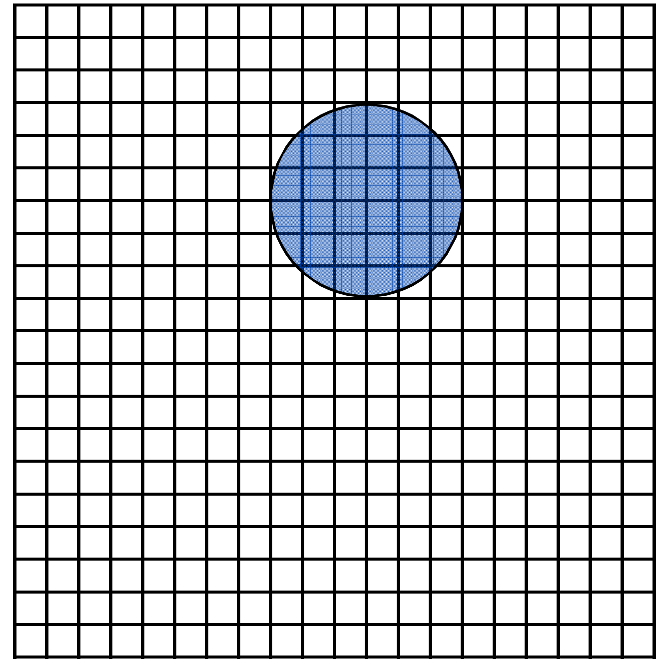
Nonlocal Weak Form – 2D

- Let $\Omega = (0,1)\times(0,1)$, $\partial\Omega = [-\delta,0]\cup[1, \delta]$.
- $u=0$ on $\partial\Omega$
- Let $C(x,x') = \begin{cases} 1 & \text{if } \|x - x'\| \leq \delta \\ 0 & \text{otherwise} \end{cases}$

- Weak form requires quadruple quadrature

- Integrand discontinuous!
  - Gauss quadrature not accurate
  - Adaptive quadrature (expensive)
  - Break up integral into many separate integrals where integrand continuous over each subregion



- Numerical Study
  - PW constant SFs
  - Hold δ constant, vary h
  - Hold h constant, vary δ

Nonlocal Finite Elements and Conditioning – 2D

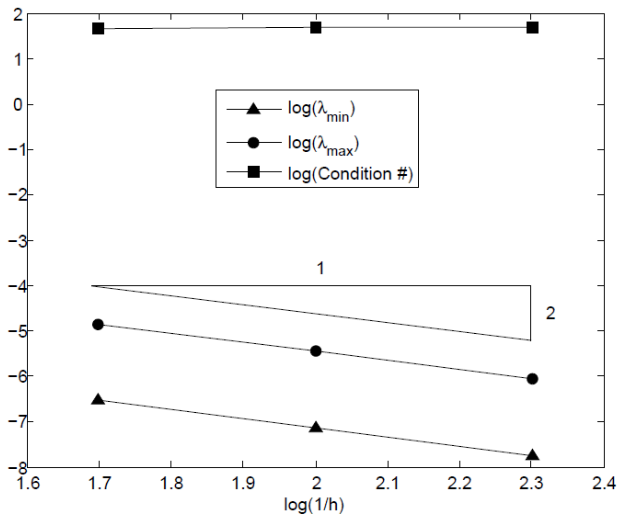
- Observations: $\kappa(K) \sim O(\delta^{-2})$, only weak h-dependence

(a) Constant δ, vary h.

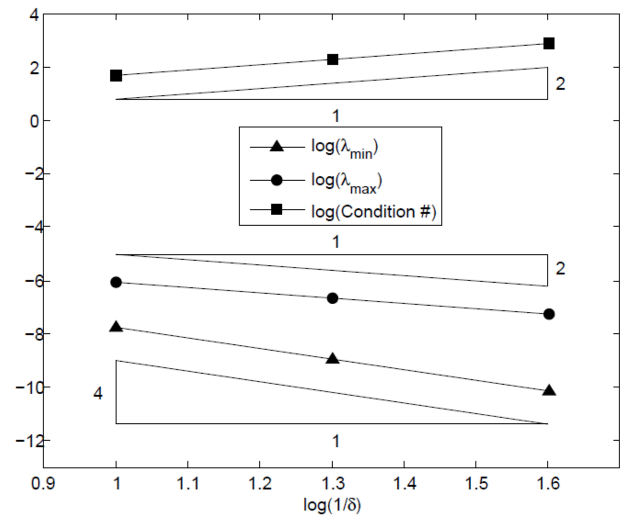
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
50	10	2.95E-07	1.40E-05	4.77E+01
100	10	7.11E-08	3.54E-06	4.97E+01
200	10	1.75E-08	8.86E-07	5.05E+01

(b) Constant h, vary δ.

$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
200	10	1.75E-08	8.86E-07	5.05E+01
200	20	1.17E-09	2.22E-07	1.90E+02
200	40	7.63E-11	5.50E-08	7.21E+02



(a) Constant δ, vary h.



(b) Constant h, vary δ.

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[*]B. Aksoylu and M.L. Parks, *Variational Theory and Domain Decomposition for Nonlocal Problems*. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

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Why is Domain Decomposition (DD) Important?

- DD is the mathematical and computational technology allowing us to map our problems onto parallel computers
- Cut problem into pieces, assign each piece to a core.

- Example: $-\nabla^2 u(x)=f(x)$

  - Standard DD approach: $\kappa \approx (Hh)^{-1}$
  - h = mesh size, H = subdomain size
  - As # cores increases, H decreases, κ increases!
  - **Not scalable!**

- Ideal preconditioner
  - $\kappa \approx O(1)$

- Scalable preconditioner (weak scalability)
  - $\kappa \approx O((1+\log(H/h))^2)$

- **Nonlocal domain decomposition theory is critical path to effective utilization of leadership class supercomputers for peridynamic modeling and simulation.**

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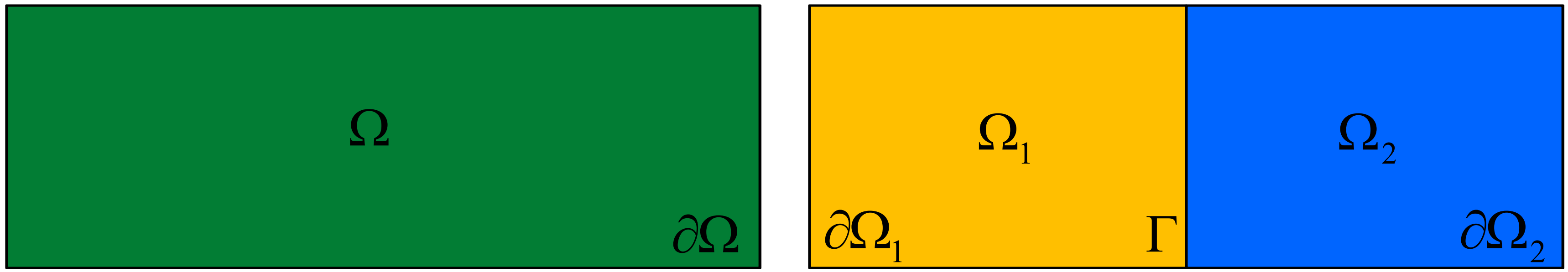
Review: Classical Substructuring

- One, two domain strong formulations



$$-\nabla^2 u(x) = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{on } \partial\Omega$$

$$-\nabla^2 u_1(x) = f \quad \text{in } \Omega_1 \qquad -\nabla^2 u_2(x) = f \quad \text{in } \Omega_2$$
$$u_1 = 0 \quad \text{on } \partial\Omega_1 \qquad u_2 = 0 \quad \text{on } \partial\Omega_2$$

One domain and two domain formulations equivalent

(assuming f sufficiently regular)

$$u_1 = u_2 \quad \text{on } \Gamma$$
$$\frac{\partial u_1}{\partial n} = -\frac{\partial u_2}{\partial n} \quad \text{on } \Gamma$$

Transmission Conditions

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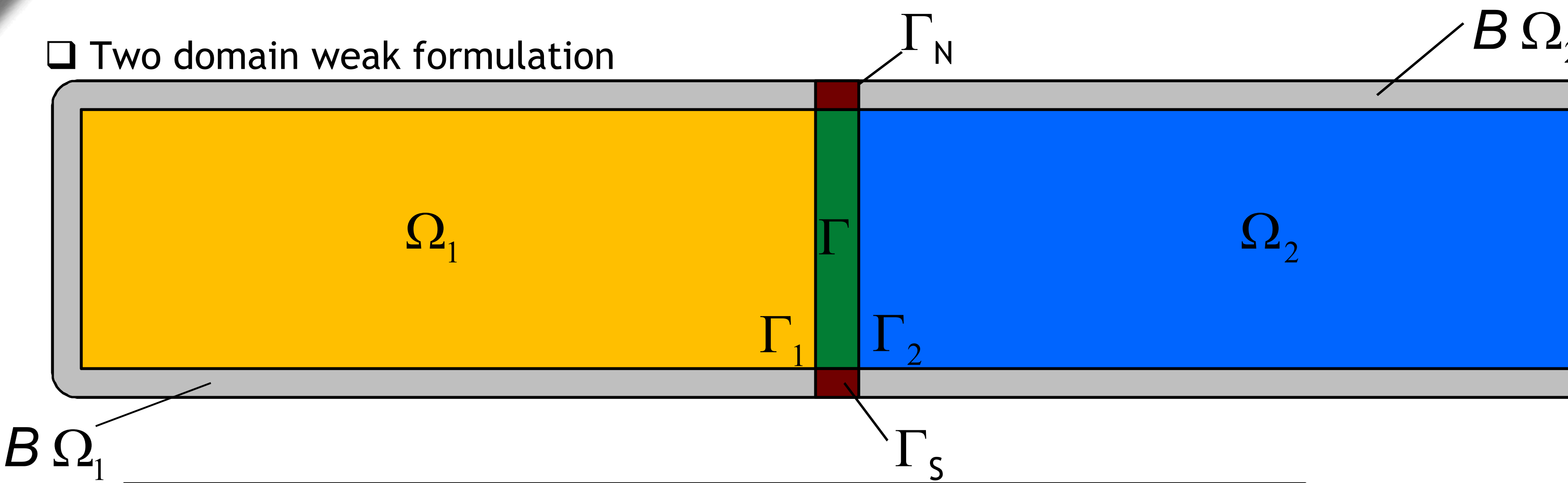
Nonlocal Domain Decomposition

- Two domain weak formulation



$$a_{\Omega^{(i)}}\left(u^{(i)}, v_i\right) = \left(f, v_i\right)_{\Omega_i} \qquad \forall v_i \in V^{(i),0},\ \ i=1,2$$

$$u^{(1)} = u^{(2)} \quad \text{on } \overline{\Gamma}$$

$$\sum_{i=1,2} a_{\Omega^{(i)}}\left(u^{(i)}, R^{(i)}\mu\right) = (u,\mu)_{\Gamma} + \sum_{i=1,2} a_{\Omega^{(i)}}\left(u^{(i)}, R^{(i)}\mu\right)_{\Omega_i} \qquad \forall \mu \in \Lambda\Gamma$$

Transmission Conditions

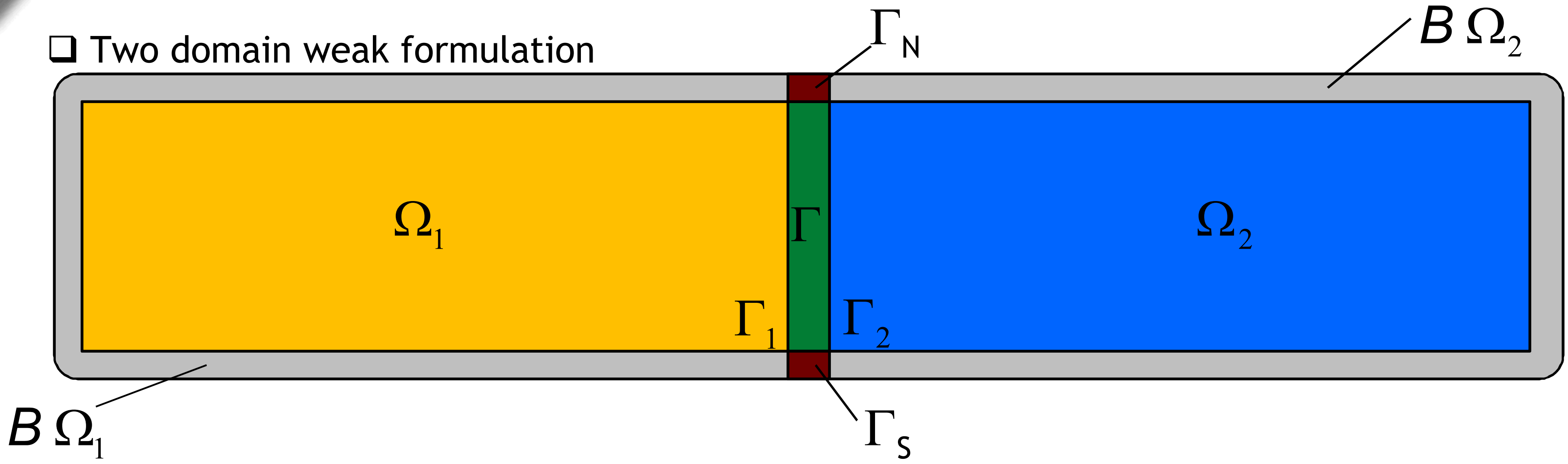
$$a_{\Omega^{(i)}}\left(u^{(i)}, v_i\right) = a_{\Omega_i}\left(u^{(i)}, v_i\right) + a_{\Gamma}(u,v)$$

$$a_{\Omega_i}(u,v) = -\int_{\Omega_i}\left\{\int_{\Omega^{(i)}\cup B\Omega^{(i)}} \chi_\delta(x-x')\left[u(x')-u(x)\right]dx\right\}v(x)dx'$$

$$a_{\Gamma}(u,v) = -\int_{\Gamma}\left\{\int_{\overline{\overline{\Omega}}} \chi_\delta(x-x')\left[u(x')-u(x)\right]dx\right\}v(x)dx'$$

Nonlocal Domain Decomposition

- ❑ Two domain weak formulation



- ❑ **Differences from classical (local) DD**
  - ❑ Interface region is volumetric (of width δ) to decompose domains
  - ❑ Flux balance transmission condition also contains governing equation for interface region

Nonlocal Domain Decomposition

- Linear algebraic representation unchanged (interpretation different)
- Stiffness matrix takes familiar block arrowhead form

$$Ku = \begin{bmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_\Gamma \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_\Gamma \end{bmatrix}$$

- Schur complement

$$S_\Gamma u_\Gamma = \tilde{f} \qquad S_\Gamma = S^{(1)} + S^{(2)}$$

$$S^{(i)} = K_{\Gamma\Gamma}^{(i)} - K_{\Gamma i}\left(K_{ii}\right)^{-1} K_{i\Gamma} \qquad i=1,2$$

$$\tilde{f} = f_\Gamma - K_{\Gamma 1}\left(K_{11}\right)^{-1} f_1 - K_{\Gamma 2}\left(K_{22}\right)^{-1} f_2$$

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1D Problem

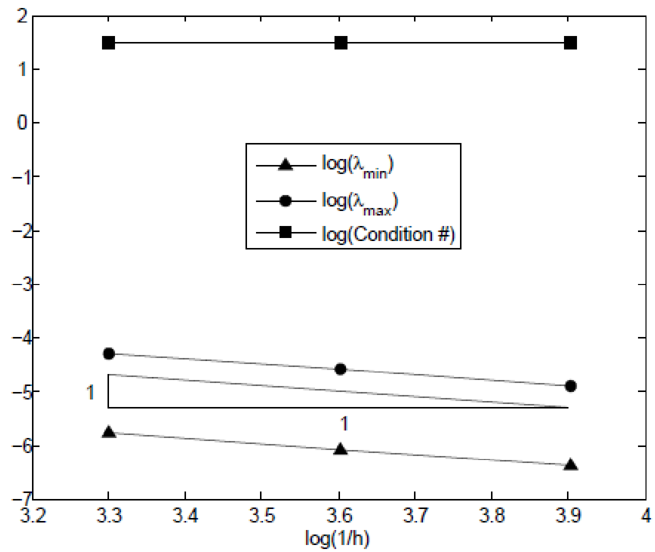
- Observations: $\kappa(S) \sim O(\delta^{-1})$, only weak h-dependence

(a) Fixed δ, vary h.

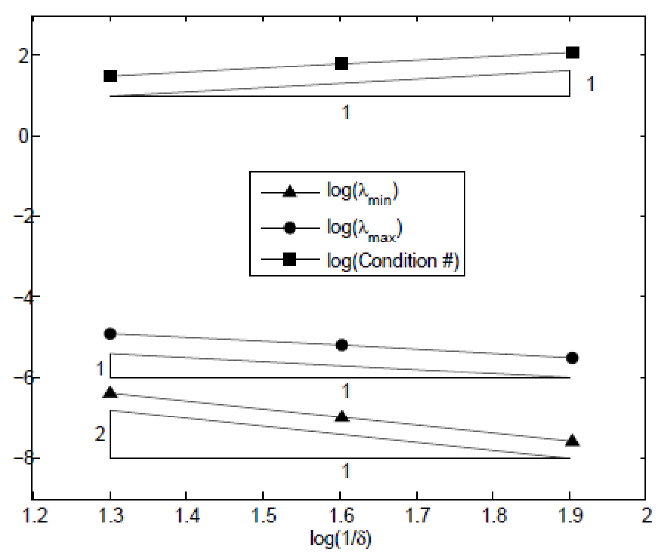
$1/h$	$1/\delta$	Piecewise Constant Shape Functions $\lambda_{\min}$	$\lambda_{\max}$	Condition #	Piecewise Linear Shape Functions $\lambda_{\min}$	$\lambda_{\max}$	Condition #
2000	20	1.64E-06	5.01E-05	3.06E+01	1.63E-06	4.97E-05	3.04E+01
4000	20	8.21E-07	2.50E-05	3.05E+01	8.21E-07	2.49E-05	3.03E+01
8000	20	4.12E-07	1.25E-05	3.04E+01	4.12E-07	1.25E-05	3.03E+01

(b) Fixed h, vary δ.

$1/h$	$1/\delta$	Piecewise Constant Shape Functions $\lambda_{\min}$	$\lambda_{\max}$	Condition #	Piecewise Linear Shape Functions $\lambda_{\min}$	$\lambda_{\max}$	Condition #
8000	20	4.12E-07	1.25E-05	3.04E+01	4.12E-07	1.25E-05	3.03E+01
8000	40	1.03E-07	6.26E-06	6.07E+01	1.03E-07	6.23E-06	6.04E+01
8000	80	2.57E-08	3.13E-06	1.22E+02	2.57E-08	3.11E-06	1.21E+02



(a) Constant δ, vary h.



(b) Constant h, vary δ.

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2D Problem

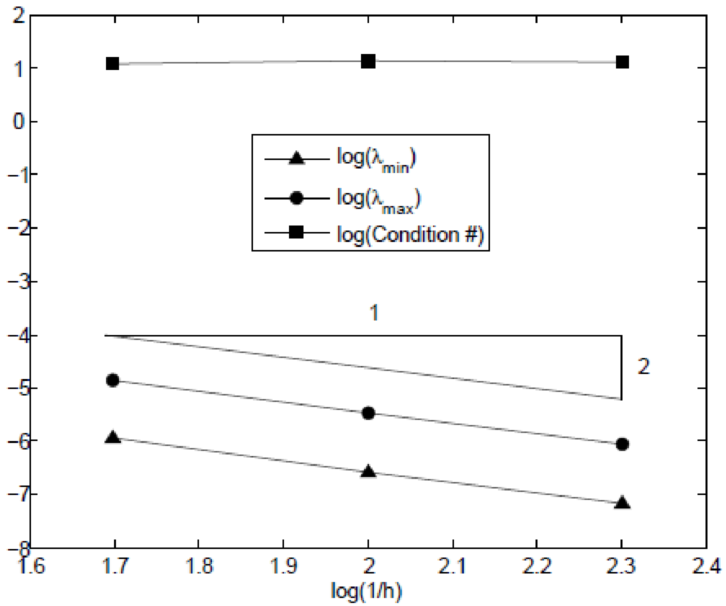
- Observations: $\kappa(S) \sim O(\delta^{-1})$, only weak h-dependence

(a) Constant δ, vary h.

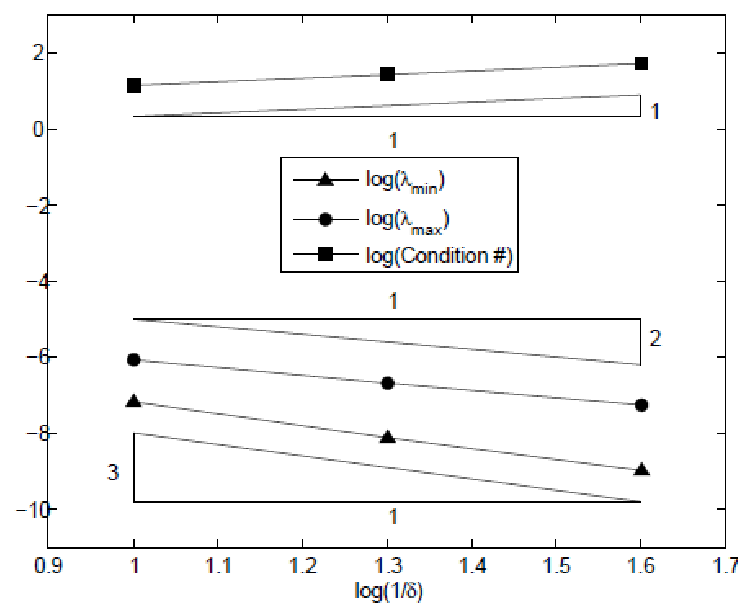
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
50	10	1.14E-06	1.38E-05	1.21E+01
100	10	2.57E-07	3.48E-06	1.36E+01
200	10	6.61E-08	8.70E-07	1.32E+01

(b) Constant h, vary δ.

$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
200	10	6.61E-08	8.70E-07	1.32E+01
200	20	7.87E-09	2.18E-07	2.77E+01
200	40	1.09E-09	4.51E-08	4.96E+01



(a) Constant δ, vary h.



(b) Constant h, vary δ.

Summary

- **Review of peridynamics; Relationship with classical theory**

- **Codes & Applications**
  - Peridigm PDLAMMPS, Peridynamics in Sierra/Solid Mechanics EMU
  - Fracture, fragmentation, failure

- **Discretizations & Numerical Methods**
  - Particle-like discretization of strong form

- **Peridynamic Finite Elements**
  - Nonlocal weak forms
  - Conditioning results

- **Peridynamic Domain Decomposition**
  - Nonlocal Schur Complement
  - Conditioning results

- **Codes, Papers: www.sandia.gov/~mlparks, mlparks@sandia.gov**

- **Thank you!**

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