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Computational Peridynamics

Non-standard Methods and Tools for Computational Modeling
SIAM Conference on Computational Science & Engineering

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Michael Parks

Computing Research Center
Sandia National Laboratories
Albuquerque, New Mexico

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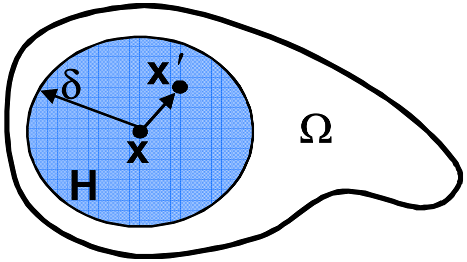
What is Peridynamics?

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

- □ Peridynamics is a nonlocal extension of classical solid mechanics that permits discontinuous solutions
- □ Peridynamic equation of motion (integral, nonlocal)

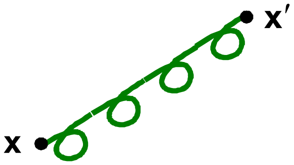
$$\rho\ddot{\mathbf{u}}(\mathbf{x},t)=\int_{\mathbf{H}}\mathbf{f}(\mathbf{u}'-\mathbf{u},\mathbf{x}'-\mathbf{x})d\mathbf{V}'+\mathbf{b}(\mathbf{x},t)$$

  - □ Replace PDEs with integral equations
  - □ Utilize same equation everywhere; nothing “special” about cracks
  - □ No assumption of differentiable fields (admits fracture)
  - □ When bonds stretch too much, they break
  - □ 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!)
  - □ PD is “continuum form of molecular dynamics”



Peridynamic Domain

- □ Impact
  - □ Larger solution space (fracture)
  - □ Account for material behavior at small & large length scales (multiscale material model)



Peridynamic “bond”

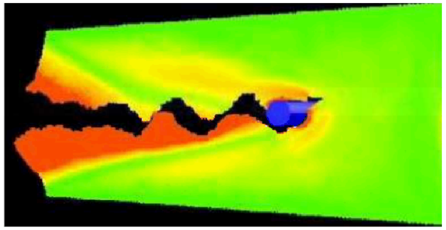
- □ Ancestors
  - □ Kröner, Eringen, Edelen, Kunin, Rogula, etc.
- □ Foreshadowing
  - □ Algorithms and numerical methods for nonlocal models are fundamentally different (and generally more expensive!) than local (classical) models.

Part I

Codes and Applications

Peridynamic Codes…

- ❑ EMU (Silling) (F90)
  - ❑ First Peridynamic code
  - ❑ Research code
  - ❑ EMU has many features, but export controlled…



Instability in slow tearing of elastic membrane* (EMU)

- ❑ PDLAMMPS (Peridynamics-in-LAMMPS) (Parks) (C++)
  - ❑ Discretize PD with same computational structure as MD
  - ❑ Core set of features, massively parallel
- ❑ Peridigm (Parks, Littlewood, Mitchell) (C++)
  - ❑ Production peridynamic code
  - ❑ Multiphysics
  - ❑ Component-based
  - ❑ Massively parallel
  - ❑ UQ/Optimization/Calibration, etc.
- ❑ Peridynamics in SIERRA/SM (Littlewood)
  - ❑ Utilizes Sandia's LAME material library

Fragmentation of metal ring (Peridigm)

*S.A. Silling and F. Bobaru, "Peridynamic modeling of membranes and fibers", International Journal of Non-Linear Mechanics, 40(2-3): 395-409 (2005).

Peridynamics-in-LAMMPS (PDLAMMPS)

- **Goals**
  - Provide 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, microplastic models
  - 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

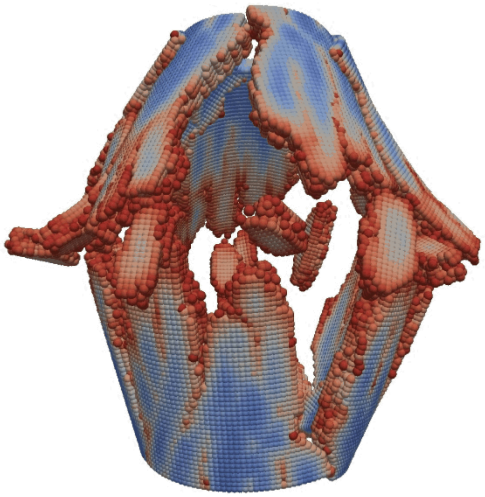
Multiphysics Peridynamics via Agile Components

- ❑ **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
- ❑ **Rapid production strategic goals**
  - ❑ Enable rapid development of new production codes; Reduce redundancy
- ❑ **Prototype application: Peridigm**
  - ❑ Particle-based, not mesh based (like FEM)
  - ❑ Multi-physics
  - ❑ Scalable
  - ❑ Optimization-enabled
  - ❑ Born-in UQ
  - ❑ Interface with SIERRA mechanics
- ❑ **Collaborators:**
  - ❑ Dave Littlewood (1444)
  - ❑ Stewart Silling (1444)
  - ❑ John Mitchell (1444)
  - ❑ John Aidun (PM,1425)

Peridigm

Peridigm Planned FY11 Development

- Exodus reader (CUBIT)
- Multiple material blocks
- Implicit time integration
- Plasticity model
- Viscoelastic model
- UQ, calibration, etc. (DAKOTA)



Fragmenting Brittle Cylinder (Peridigm)

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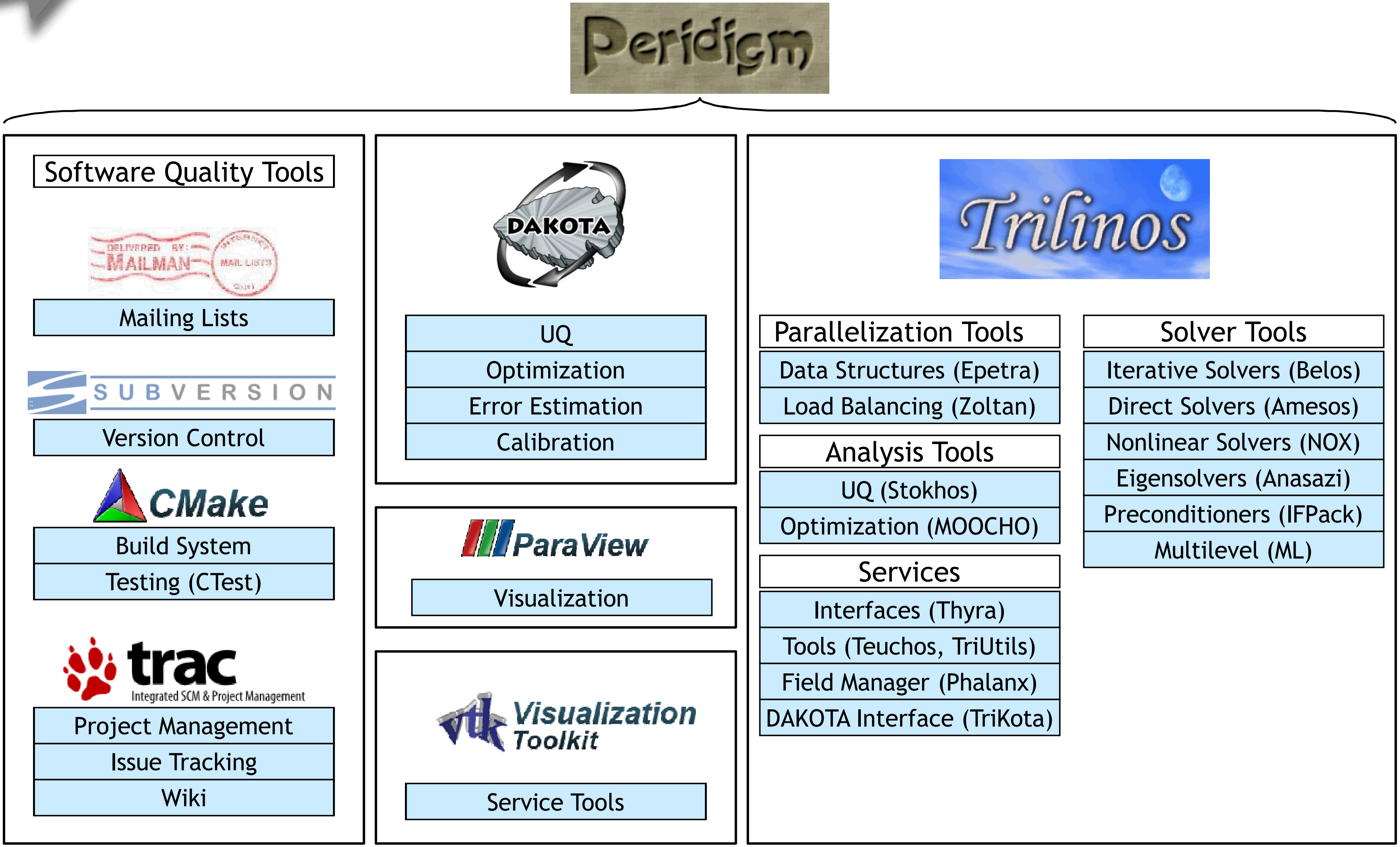
Multiphysics Peridynamics via Agile Components



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)

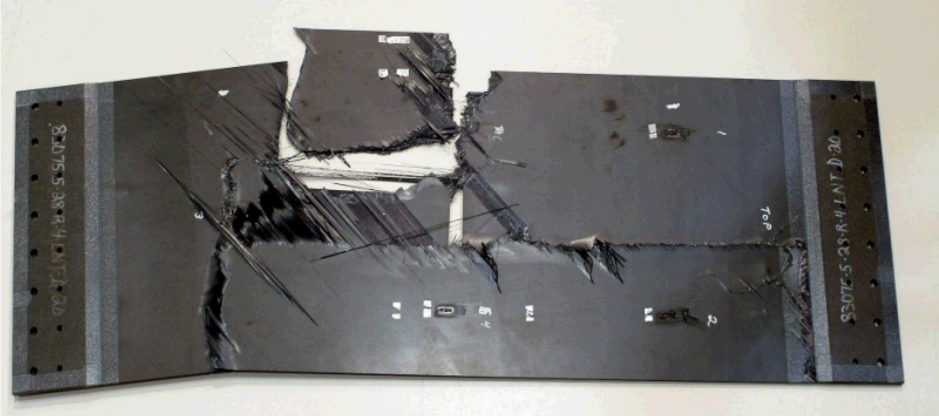
Solver Tools

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

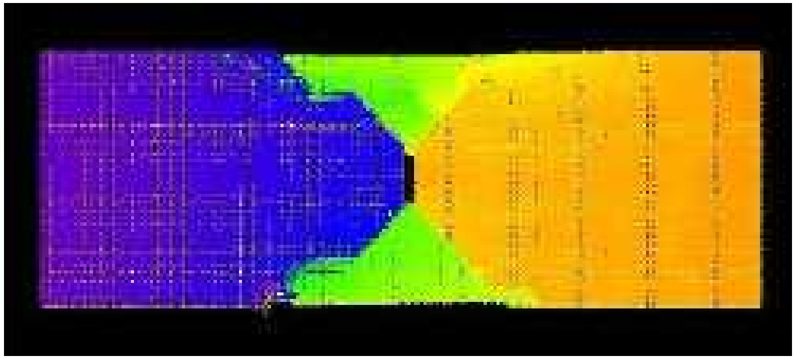
Simulation performed with EMU (Silling)

Some Applications…

- ❑ **Example Simulation:** Failure of composite laminate*
    - ❑ 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

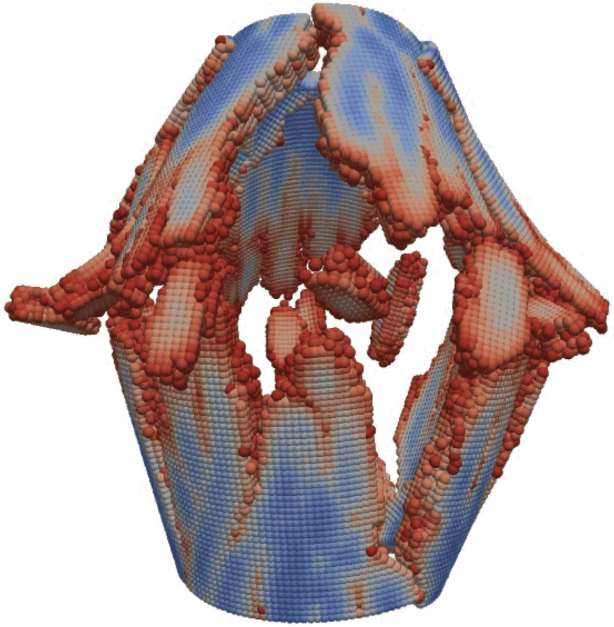
* E. Askari, F. Bobaru, R.B. Lehoucq, M.L. Parks, S.A. Silling, O.Weckner, Peridynamics for multiscale materials modeling, in SciDAC 2008, Seattle, Washington, vol. 125 of Journal of Physics: Conference Series, (012078) 2008.

Simulation performed with Peridigm (P,L,M)

Some Applications…

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

Before



After

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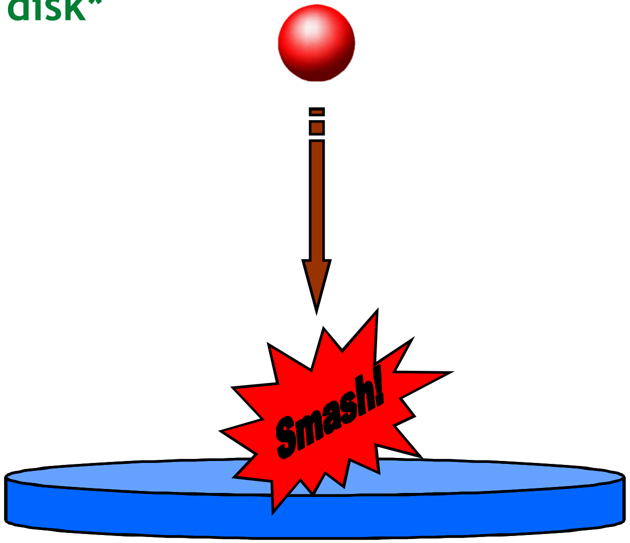
* D. Grady, Fragmentation of Rings And Shells: The Legacy of N.F. Mott, Springer, 2006.

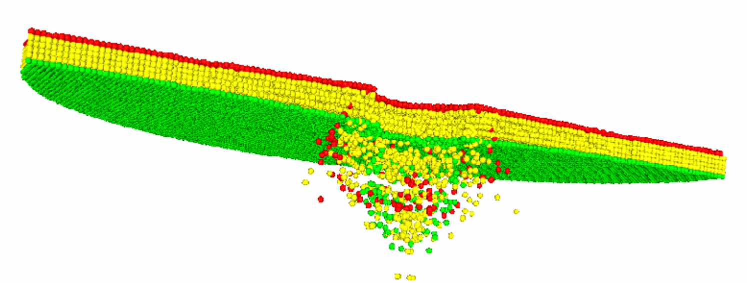
Simulation performed with PDLAMMPS (Parks)

Some Applications…

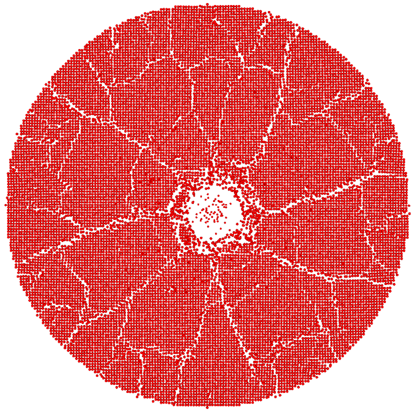
- ❑ **Example Simulation:** Hard sphere impact on brittle disk*
- ❑ Spherical Projectile
  - ❑ Diameter: 0.01 m
  - ❑ Velocity: 100 m/s
- ❑ Target Disk
  - ❑ Diameter: 0.074 m,
  - ❑ Thickness: 0.0025 m
  - ❑ Elastic modulus: 14.9 Gpa
  - ❑ Density: 2200 kg/m^3
- ❑ Discretization
  - ❑ Mesh spacing: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

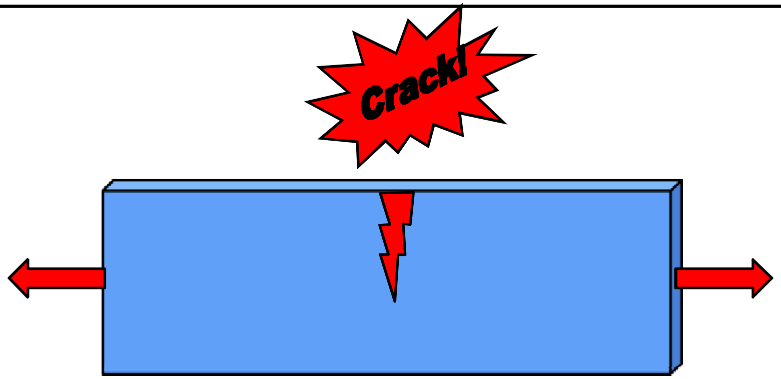
- ❑ Dimensions: 3” x 1” x 0.05”
- ❑ Density: 2.44 g/cm3
- ❑ Elastic Modulus: 79.0 Gpa

❑ Discretization (finest)

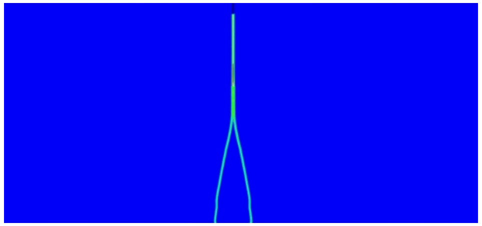
- ❑ Mesh spacing: 35 microns
- ❑ Approx. 82 million particles
- ❑ Time: 50 microseconds (20k timesteps)

Setup

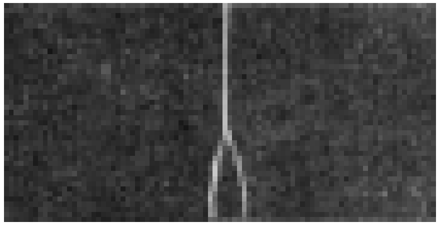
- ❑ Glass microscope slide
- ❑ Dimensions: 3” x 1” x 0.05”
- ❑ Notch at top, pull on ends



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.

Simulation performed with PDLAMMPS (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

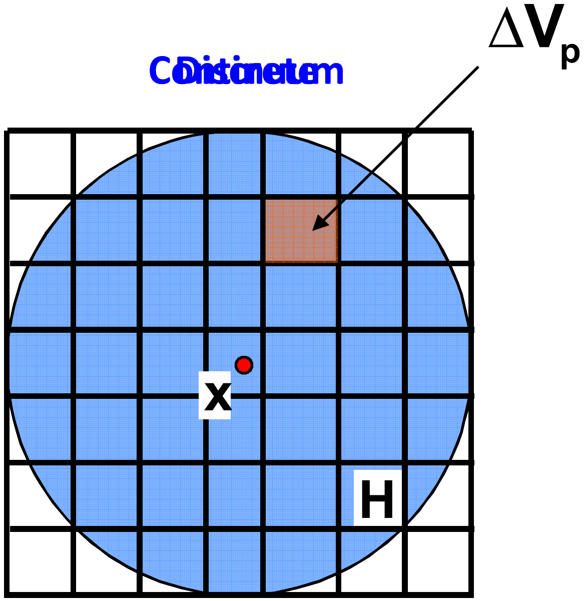
# Cores	# Particles	Particles/Core	Runtime (sec)	T(P)/T(P=512)
512	262,144	4096	14.417	1.000
4,096	2,097,152	4096	14.708	0.980
32,768	16,777,216	4096	15.275	0.963

Part II

Discretizations and Numerical Methods

Discretizing Peridynamics

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



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

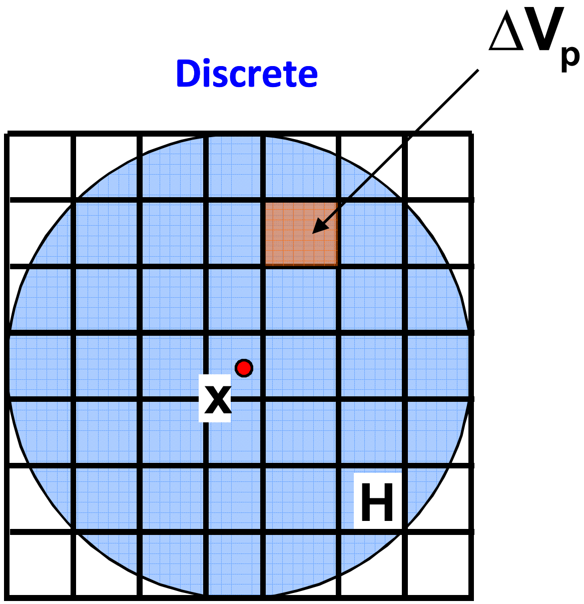
$$\sum_p f(u(x_p,t)-u(x,t),x_p-x)\,\Delta V_p$$

[*] 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

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

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

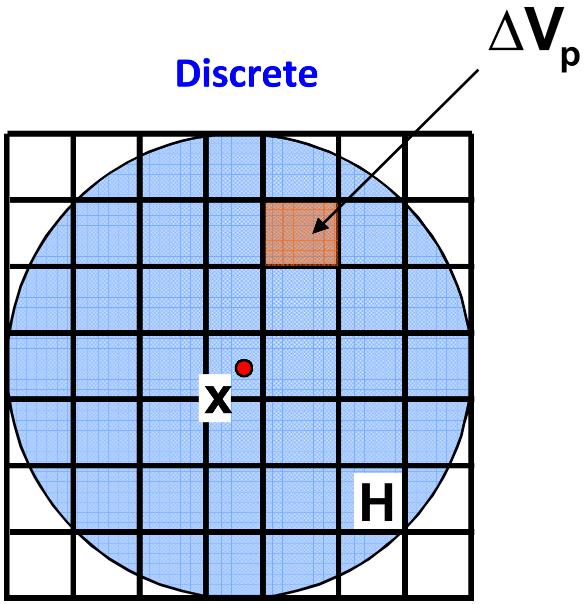
$$v_i^{n+1} = v_i^{n+1/2} + \left(\frac{\Delta t}{2m}\right) f_i^{n+1}$$

*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



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

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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)**

*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.

Part III

Peridynamic Finite Elements*

[*] B. Aksoylu and M.L. Parks, *Variational Theory and Domain Decomposition for Nonlocal Problems*. Applied Mathematics and Computation. To Appear. 2011.

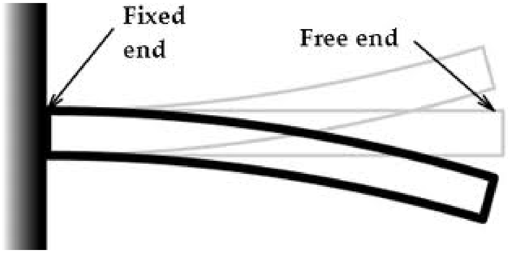
Why is Conditioning Important?

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

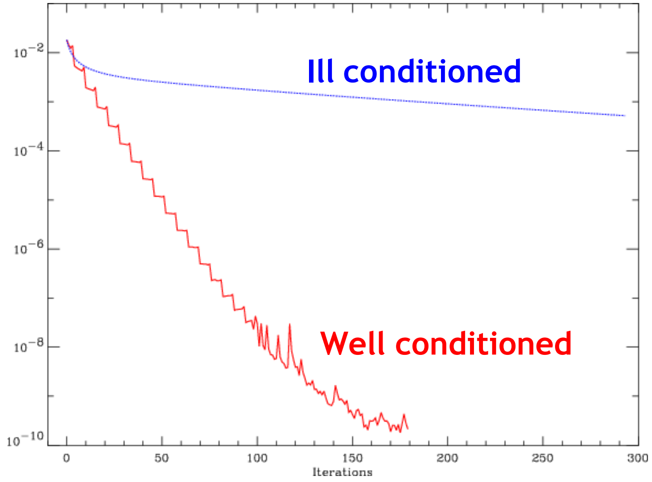
$$\kappa(A) = \|A\| \cdot \|A^{-1}\|$$

- □ **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

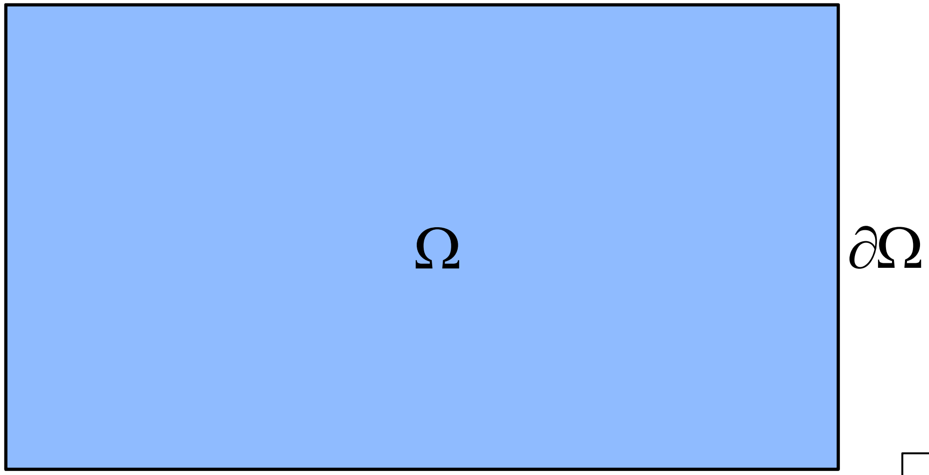
Why is Conditioning Important?

- ❑ **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

- ❑ **DOE future computing platforms**
  - ❑ **Exaflop machines by 2018**

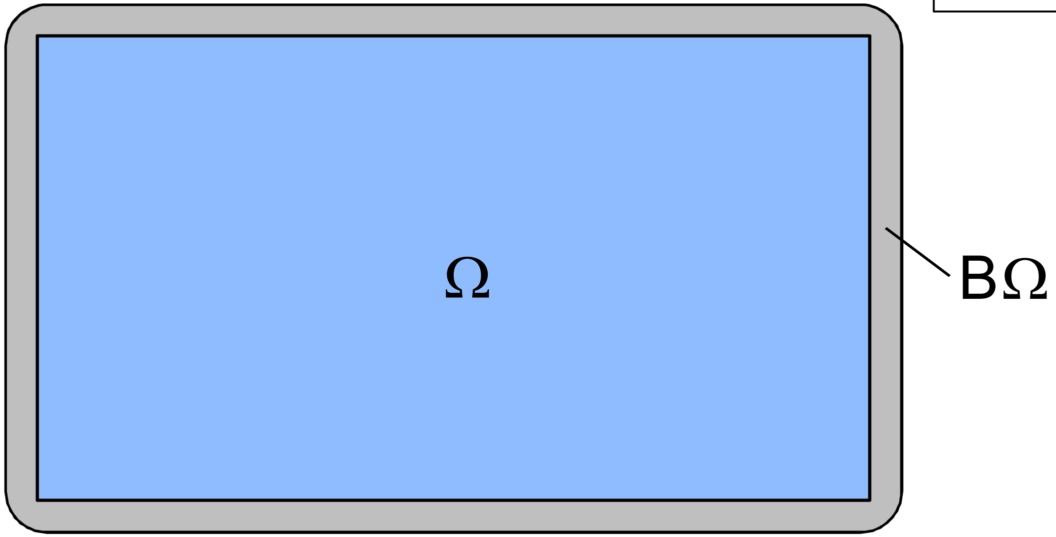
Nonlocal Boundaries

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



∂Ω interacts with all points in 👌Ω

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



Nonlocal Weak Form

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

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

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

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

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

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

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

- ❑ 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
  - □ Unnecessary in nonlocal FEM

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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

- Principle 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,

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

- This is not tight!
  - Consider lim $\delta \to 0$. Cond # estimate → ∞, 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. To Appear. 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.

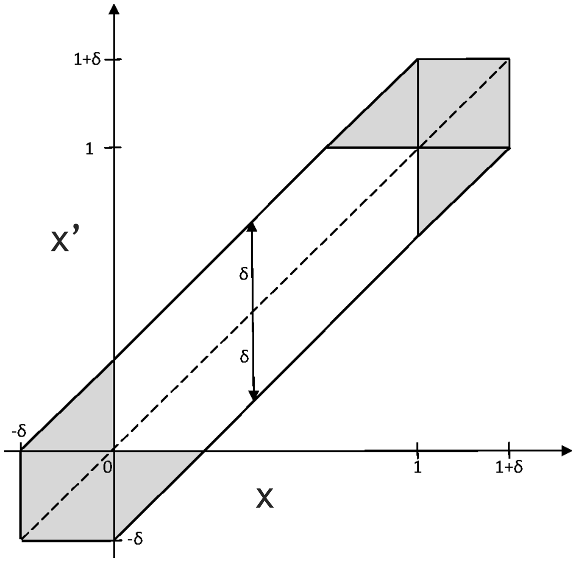
[†] Q. Du and K. Zhou. Mathematical analysis for the peridynamic nonlocal continuum theory. Mathematical Modelling and Numerical Analysis, 2010. doi:10.1051/m2an/2010040.

Conditioning Results – 1D

- ❑ Let Ω = (0,1), 👌Ω = [-δ,0]∪[1, δ].
- ❑ u=0 on 👌Ω
- ❑ Let $C(x,x') = \begin{cases} 1 & \text{if } \|x - x'\| \leq \delta \\ 0 & \text{otherwise} \end{cases}$

- ❑ Weak form becomes

$$a(u,v) = -\int_{0}^{1}\int_{x-\delta}^{x+\delta}\left[u(x') - u(x)\right]v(x)dx'dx$$



Integration
Domain in (x,x')

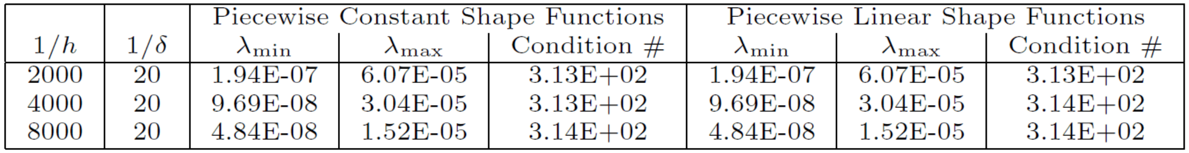
(grey = outside Ω)

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

Conditioning Results – 1D

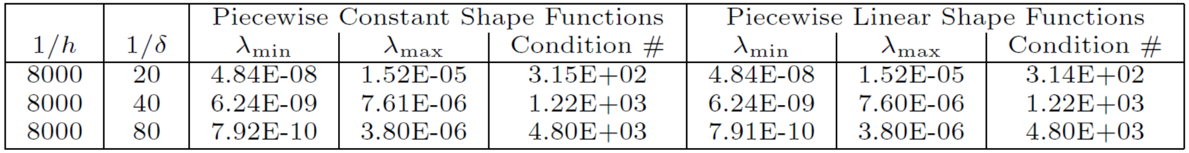
- ❑ Observations: $\kappa(K) \sim O(\delta^{-2})$, only weak h-dependence
  - ❑ At most weak h-dependence; No preconditioner!

(a) Constant δ, vary h.

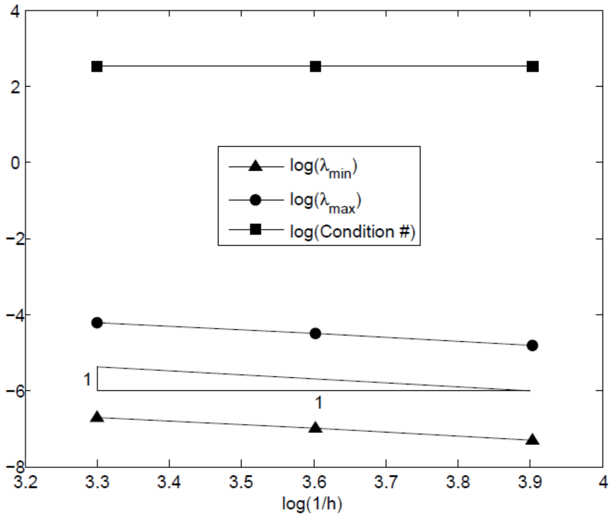


		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
2000	20	1.94E-07	6.07E-05	3.13E+02	1.94E-07	6.07E-05	3.13E+02
4000	20	9.69E-08	3.04E-05	3.13E+02	9.69E-08	3.04E-05	3.14E+02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

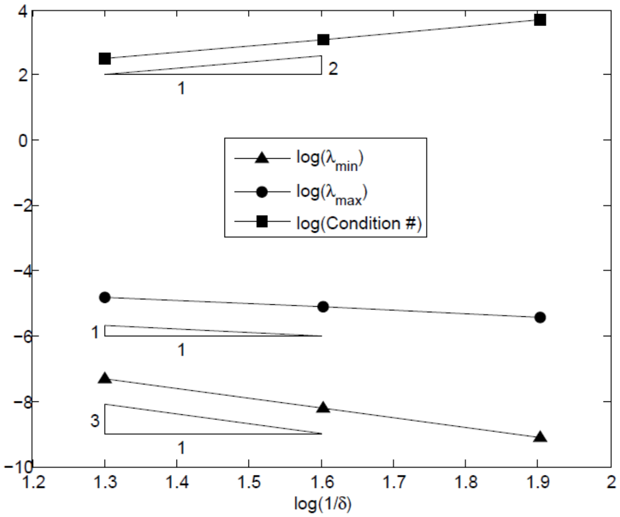
(b) Constant h, vary δ.



		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #	$\lambda_{\min}$	$\lambda_{\max}$	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



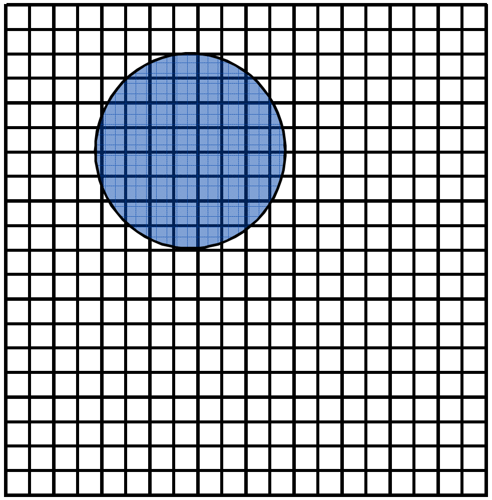
(a) Constant δ, vary h.



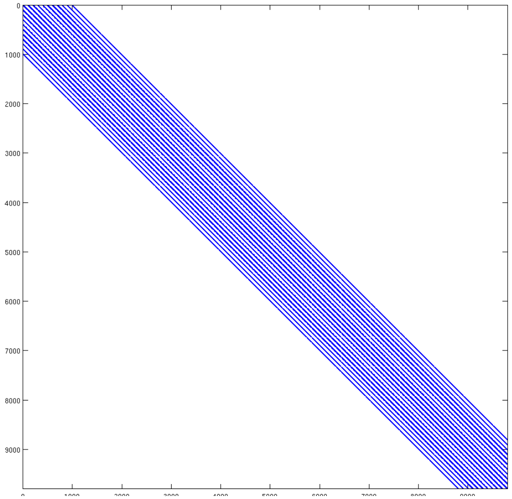
(b) Constant h, vary δ.

Conditioning Results – 2D

- ❑ Let Ω = (0,1)×(0,1), ✍Ω = [-δ,0]∪[1, δ].
- ❑ u=0 on ✍Ω
- ❑ Let $C(x,x') = \begin{cases} 1 & \text{if } \|x - x'\| \le \delta \\ 0 & \text{otherwise} \end{cases}$
- ❑ 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 fixed, vary h
  - ❑ Hold h fixed, vary δ



Integrand discontinuous over elements



Sparsity Pattern
(2D, 10,000 unknowns, 3.4M nnz)

Conditioning Results – 2D

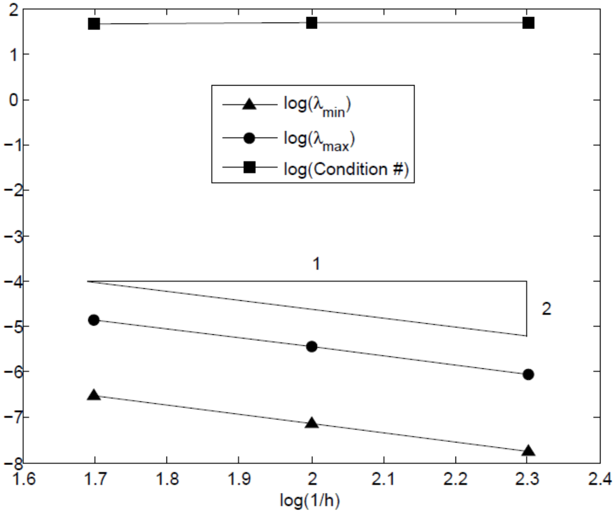
- ❑ Observations: $\kappa(K) \sim O(\delta^{-2})$, only weak h-dependence
  - ❑ At most weak h-dependence; No preconditioner!

(a) Constant δ, vary h.

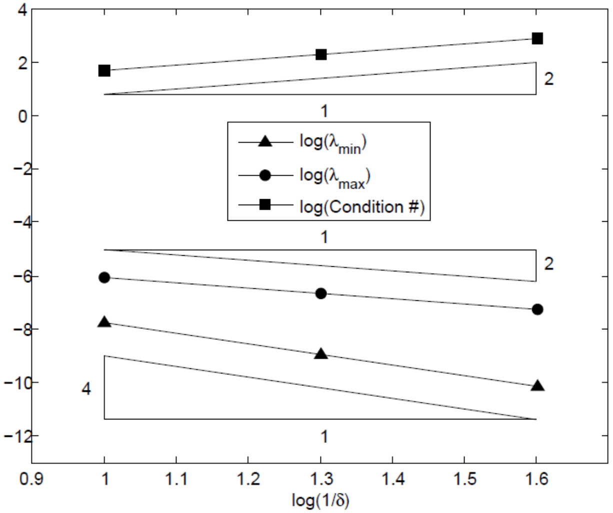
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
50	10	2.95E-07	1.40E-05	4.77E+01
100	10	7.11E-08	3.54E-06	4.97E+01
200	10	1.75E-08	8.86E-07	5.05E+01

(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.

Part IV

Nonlocal Substructuring*

[*] B. Aksoylu and M.L. Parks, *Variational Theory and Domain Decomposition for Nonlocal Problems*. Applied Mathematics and Computation. To Appear. 2011.

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!**

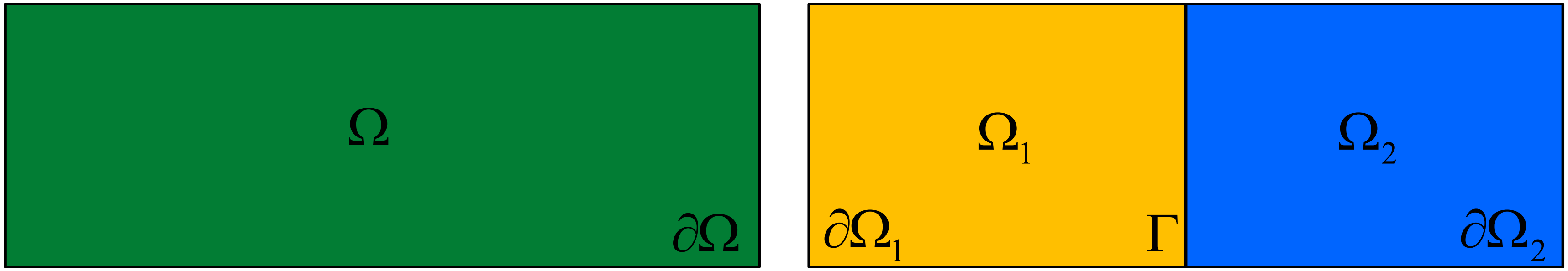
- Ideal preconditioner
  - $\kappa \approx O(1)$

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

- **Nonlocal domain decomposition theory is critical path for utilization of massively parallel leadership class supercomputers for peridynamic modeling and simulation on static & quasistatic problems.**

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

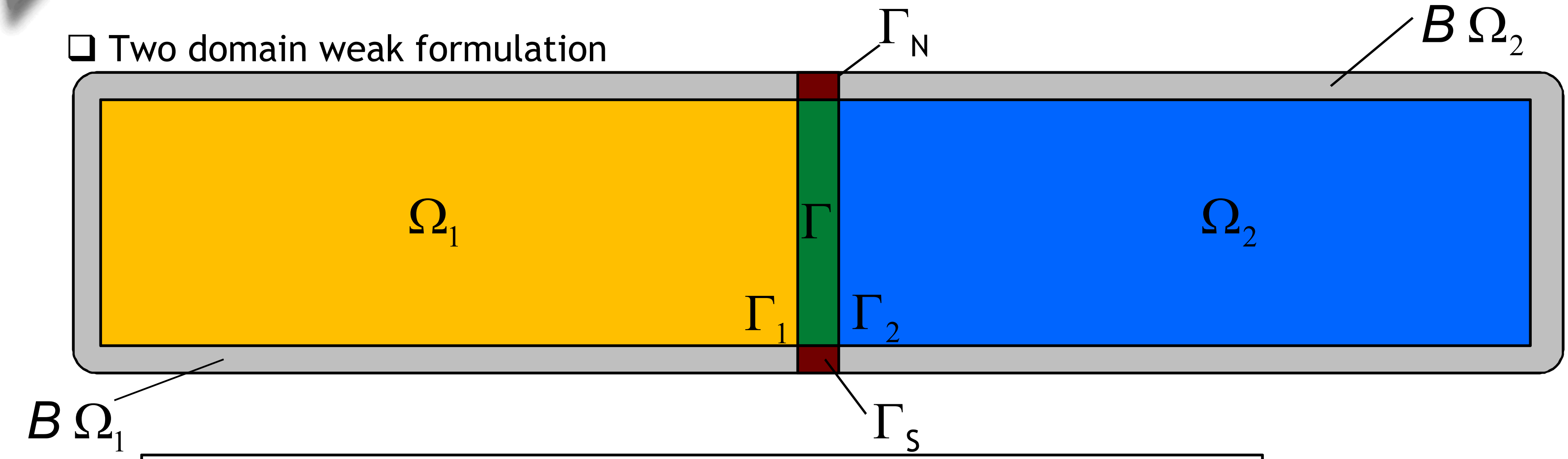
(assuming f sufficiently regular)

$$\boxed{\begin{gathered} u_1 = u_2 \quad \text{on } \Gamma \\ \frac{\partial u_1}{\partial n} = -\frac{\partial u_2}{\partial n} \quad \text{on } \Gamma \end{gathered}}$$

Transmission Conditions

Nonlocal Domain Decomposition

❑ Two domain weak formulation



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

$$\left.\begin{array}{c} u^{(1)}=u^{(2)}\quad \text{on } \overline{\Gamma} \\ \displaystyle\sum_{i=1,2} a_{\Omega^{(i)}}\left(u^{(i)},R^{(i)}\mu\right)=(u,\mu)_\Gamma+\sum_{i=1,2} a_{\Omega^{(i)}}\left(u^{(i)},R^{(i)}\mu\right)_{\Omega_i}\quad \forall\mu\in\Lambda\Gamma \end{array}\right\}\ \text{Transmission Conditions}$$

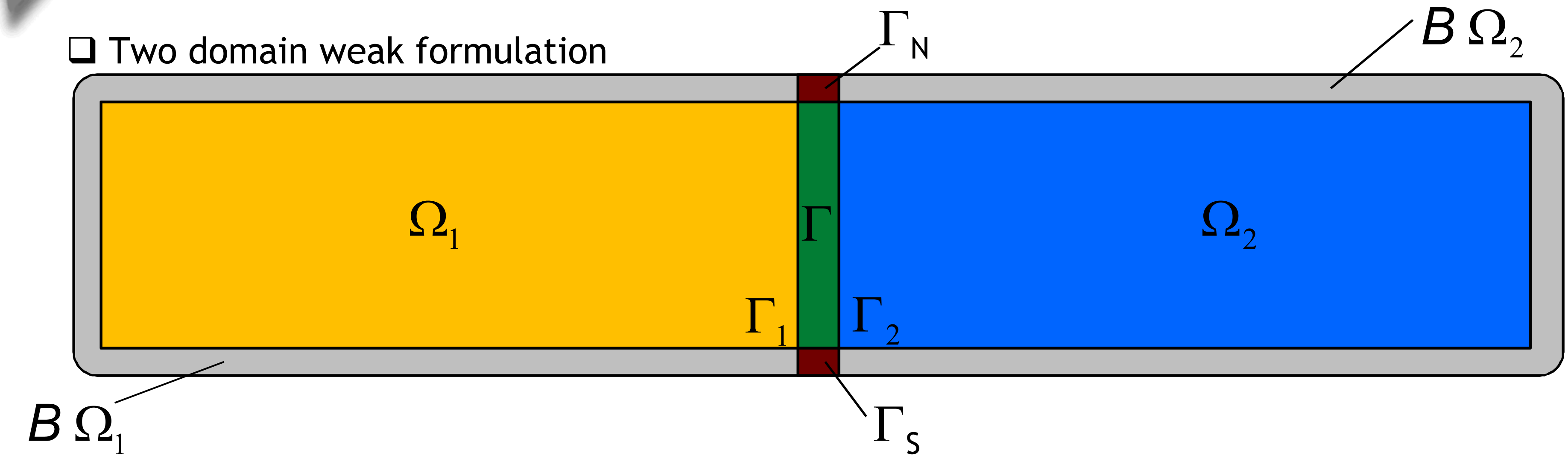
$$a_{\Omega^{(i)}}\left(u^{(i)},v_i\right)=a_{\Omega_i}\left(u^{(i)},v_i\right)+a_\Gamma(u,v)$$

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

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

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

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

- ❑ Schur complement

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

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

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

Conditioning Results – 1D

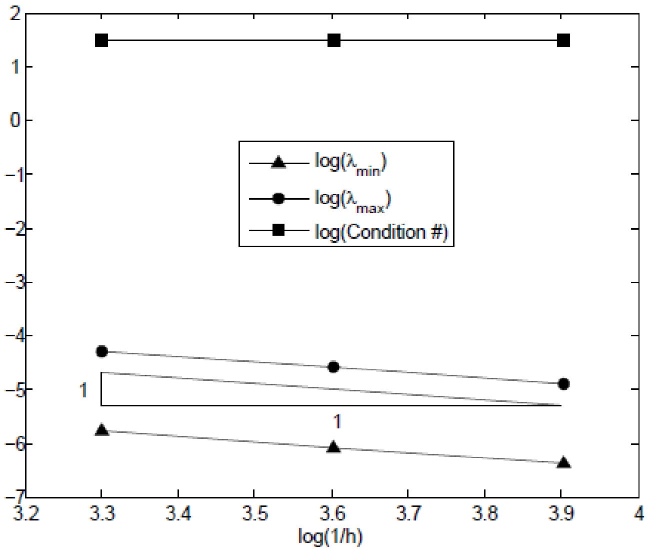
- ❑ Observations: $\kappa(S) \sim O(\delta^{-1})$, only weak h-dependence

(a) Fixed δ, vary h.

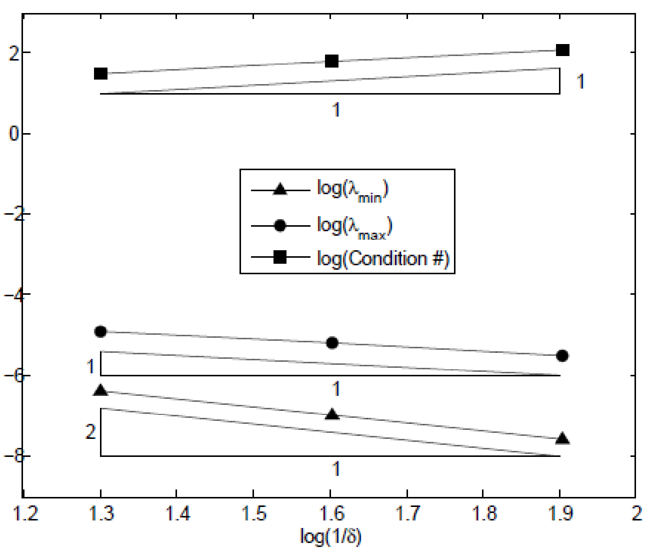
		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
2000	20	1.64E-06	5.01E-05	3.06E+01	1.63E-06	4.97E-05	3.04E+01
4000	20	8.21E-07	2.50E-05	3.05E+01	8.21E-07	2.49E-05	3.03E+01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

		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #	$\lambda_{\min}$	$\lambda_{\max}$	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.

Conditioning Results – 1D

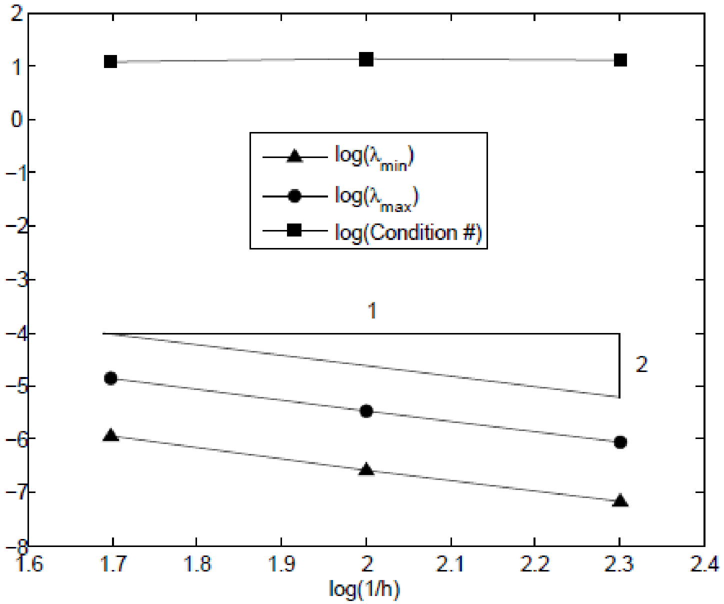
- ❑ Observations: $\kappa(S) \sim O(\delta^{-1})$, only weak h-dependence

(a) Constant δ, vary h.

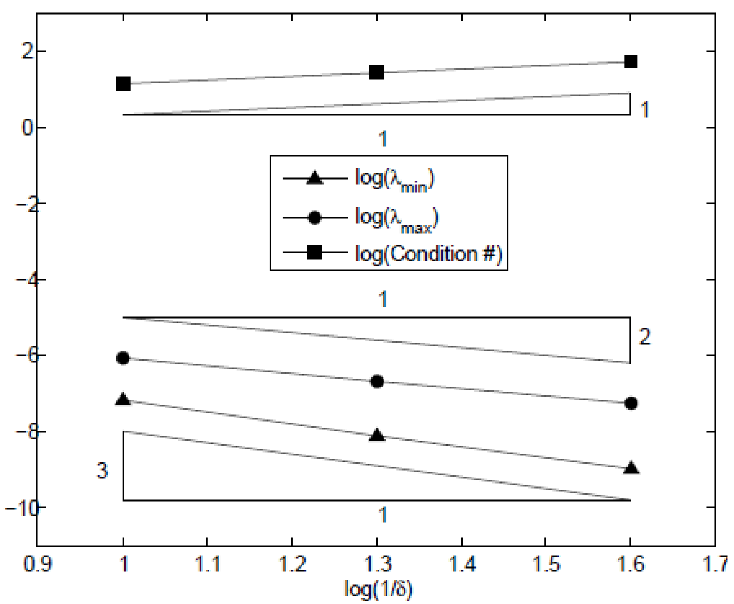
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
50	10	1.14E-06	1.38E-05	1.21E+01
100	10	2.57E-07	3.48E-06	1.36E+01
200	10	6.61E-08	8.70E-07	1.32E+01

(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

- ❑ Mercifully brief review of peridynamics
- ❑ Applications
  - ❑ Fracture, fragmentation, failure
- ❑ Codes
  - ❑ EMU, PDLAMMPS, Peridigm, more
- ❑ Discretizations & Numerical Methods
  - ❑ Particle-like discretization of strong form
- ❑ Peridynamic Finite Elements
  - ❑ Peridynamic weak forms
  - ❑ Conditioning results
- ❑ Peridynamic Domain Decomposition
  - ❑ Peridynamic Schur Complement
  - ❑ Conditioning results
- ❑ Thank you!