

Computational Peridynamics

Mini-Workshop: Mathematical Analysis for Peridynamics Mathematisches Forschungsinstitut Oberwolfach

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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)

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

- □ 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
- \Box f(·, ·) is "force" function; contains constitutive model
- \Box f = 0 for particles x,x' more than δ apart (like cutoff radius in MD!)
- □ PD is "continuum form of molecular dynamics"

Impact

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

Ancestors

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

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



Peridynamic Domain





Local vs. Nonlocal Models

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

□ Local model:

- □ Contact force
- Exterior of circle imparts force to interior via surface
- Cauchy cut principle (free body diagram)

Examples:

- □ Classical elasticity, etc.
- □ Any PDE-based model

Nonlocal model:

- □ Action-at-a-distance
- $\hfill\square$ Exterior of circle imparts force to interior
 - not just at surface
- □ Examples:
 - Molecular dynamics
 - Peridynamics

Foreshadowing

Algorithms and numerical methods for nonlocal models are fundamentally different (and generally more expensive!) than local (classical) models.



Local Domains



Nonlocal Domains



Length Scales

H.

What does it mean to have a length scale?

□ Equation has no length scale; same dynamics at all scales

□ What does it mean to be multiscale?

 \Box Example #1: $\ddot{u}(x) = au''(x)$





Part I Applications and Codes



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.



Some Applications...

□ Taylor impact test of 6061-T6 aluminum*







Some Applications...

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





Peridynamic Model



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



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



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/m³

Discretization

- □ Mesh spacing: 0.005 m
- □ 100,000 particles
- □ Simulation time: 0.2 milliseconds





*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.

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

- **4**00 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)



* 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.



aboratories

Some Applications...

Content Example simulation: Dynamic brittle fracture in glass

□ Joint with Florin Bobaru, Youn-Doh Ha (Nebraska), & Stewart Silling (SNL)

□ Soda-lime glass plate (microscope slide)

Discretization (finest)

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

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



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



Some Codes...

- □ EMU (F90) **€**EMU
 - □ First Peridynamic code
 - □ Research code
 - □ EMU has many features, but export controlled...

EMU variants (F90)



Instability in slow tearing of elastic membrane* (EMU)

□ Many developers have branched EMU and started their own development line

Garaken, etc.

DLAMMPS (Peridynamics-in-LAMMPS) (C++)

- □ Core set of features, massively parallel
- Deridigm (C++) Peridigm
 - Production peridynamic code
 - □ Multiphysics
 - □ Component-based
 - □ Massively parallel
 - □ UQ/Optimization/Calibration, etc.

□ Peridynamics in SIERRA/SM (Presto)

Utilizes Sandia's LAME material library



Fragmentation of metal ring (Peridigm)



Peridynamics-in-LAMMPS (PDLAMMPS)

🗆 Goals

- □ Provide **open source** peridynamic code (distributed with LAMMPS; <u>lammps.sandia.gov</u>)
- □ 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 <u>www.sandia.gov/~mlparks</u> (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



Peridynamics-in-LAMMPS (PDLAMMPS)

LAMMPS (Sandia's open source MD package)

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

□ MPI: spatial data decomposition + ghosting



□ Added "SI" units to LAMMPS for macroscale simulations

□ MD: angstroms, femtoseconds, etc.

D PD: meters, seconds, etc.



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 Planned FY11 Development

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

Exploding Brittle Cylinder Image: Comparison of the second seco



Multiphysics Peridynamics via Agile Components

Peridigm







Part II Discretizations and Numerical Methods



Discretizing Peridynamics

Spatial Discretization

- □ Approximate integral with sum*
- Midpoint quadrature
- Piecewise constant approximation



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

$$\begin{aligned} \mathbf{v}_{i}^{n+1/2} &= \mathbf{v}_{i}^{n} + \left(\frac{\Delta t}{2m}\right) \mathbf{f}_{i}^{n} \\ \mathbf{u}_{i}^{n+1} &= \mathbf{u}_{i}^{n} + \left(\Delta t\right) \mathbf{v}_{i}^{n+1/2} \\ \mathbf{v}_{i}^{n+1} &= \mathbf{v}_{i}^{n+1/2} + \left(\frac{\Delta t}{2m}\right) \mathbf{f}_{i}^{n+1} \end{aligned}$$

 $\sum_{p} f(u(x_{p},t) - u(x_{i},t), x_{p} - x_{i}) \Delta V_{p}$

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





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...





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?

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





□ Why do we care?

- Condition number dictate convergence rates of linear solvers
- Condition numbers dictate the accuracy of computed solution
- Rule of thumb: If κ(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



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

\square New component in nonlocal modeling is peridynamic horizon δ

- $\hfill\square$ 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

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



ories

Nonlocal Weak Form

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

Prototype operator

$$\mathcal{L}\left\{u\right\}\left(x\right) = -\int_{\overline{\Omega}} C(x, x') \left[u(x') - u(x)\right] dx' \qquad \begin{array}{l} C(x, x') = C(x', x) \\ C(x, x') = 0 \text{ if } ||x - x'|| > \delta \end{array}$$

 \Box Need nonlocal weak form* \rightarrow Multiply by test function and "integrate by parts"

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

□ Compare with local Poisson operator

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



Nonlocal Quadrature

□ Review: Local Quadrature

- □ One integral required
- Compute products of gradients of shape functions and apply Gauss quadrature

(lower order quadrature scheme required)

Gradient *drops* polynomial order

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

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

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

Integration by parts is standard in local (classical) FEM.
 Discussion: Does it serve any purpose here?



Spectral Equivalence

□ For simplicity, assume

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

"Canonical" Kernel Function

□ Principle Theorem*

$$\lambda_{1}(\overline{\overline{\Omega}})\delta^{d+2} \leq \frac{a(u,u)}{\|u\|_{L_{2}(\overline{\overline{\Omega}})}} \leq \lambda_{2}(\overline{\overline{\Omega}})\delta^{d} \qquad u \in L_{2,0}(\overline{\overline{\Omega}})$$

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

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

□ This is not tight!

□ Consider lim $\delta \rightarrow 0$. Cond # estimate $\rightarrow \infty$, true $\kappa(K) \rightarrow h^{-2}$.

Condition number not mesh independent (bound is mesh independent).

□ In practice, observe **very** weak mesh dependence.

\Box Bound descriptive when h < δ .

□ Alternative approach: Zhou & Du[†]

 $\hfill\square$ Dominant length scale in nonlocal model set by $\delta.$

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.



Nonlocal Weak Form – 1D





Nonlocal Finite Elements and Conditioning – 1D

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

		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
1/h	$1/\delta$	λ_{\min}	$\lambda_{ m max}$	Condition $\#$	λ_{\min}	$\lambda_{ m max}$	Condition $\#$
2000	20	1.94E-07	$6.07 \text{E}{-}05$	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

(a) Constant δ , vary h.

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







Nonlocal Weak Form – 2D

Let $\Omega = (0,1) \times (0,1)$, $\mathcal{B}\Omega = [-\delta,0] \cup [1, \delta]$. u=0 on $\mathcal{B}\Omega$

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

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
 - \Box Hold δ constant, vary h
 - $\hfill\square$ Hold h constant, vary δ



Discussion: Is there a better way to do accurate nonlocal quadrature?



Nonlocal Finite Elements and Conditioning – 2D

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

1/h	$1/\delta$	$\lambda_{ m min}$	$\lambda_{ m max}$	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	$1.75 \text{E}{-}08$	8.86E-07	5.05E + 01

(a) Constant δ , vary h.

(b) Constant h, vary δ .

1/h	$1/\delta$	$\lambda_{ m min}$	$\lambda_{ m max}$	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.

2 1 $log(\lambda_{min})$ - log(λ_{max}) log(Condition #) 1 -10-1 -12 0.9 1.1 1.2 1.3 1.4 1.5 1.6 1 $log(1/\delta)$

(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!

□ Questions for me...?

