SAND2012-2877P

Peridynamics for Material Failure

Multiphysics Simulation Technology

Org. 1444

Sandia National Laboratories

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1444 Peridynamics Staff

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- Other Sandia collaborators (including Jim Kamm)
- Dozens of external collaborators (academia, labs, industry)

I. Peridynamics

II. Numerics and Codes

III. Applications

IV. Current & Future Work

Peridynamics

WHAT IS PERIDYNAMICS?

Peridynamics is a continuum mechanical model that unifies the mechanics of continuous and discontinuous media within a single, consistent set of equations

WHY NOT USE CLASSICAL OF SOLID MECHANICS?

- Can't differentiate at a crack; Cracks treated as pathological solution.
- Must apply special techniques at discrete level to support desired fracture solutions

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

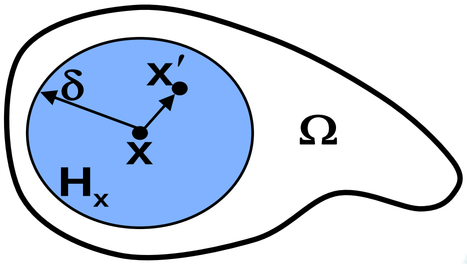
HOW DOES PERIDYNAMICS WORK?

- Peridynamics is a *nonlocal* extension of continuum mechanics
- Replace PDEs with integral equations
- Peridynamic equation of motion (*integral*, *nonlocal*)

$$\rho \ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathbf{H_x}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

- No obstacle to integrating nonsmooth functions
- Remains valid in presence of discontinuities, including cracks
- Impact: larger solution space (fracture), length scales (multiscale material model)

Point **x** interacts directly with all points **x'** within **H**



S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.

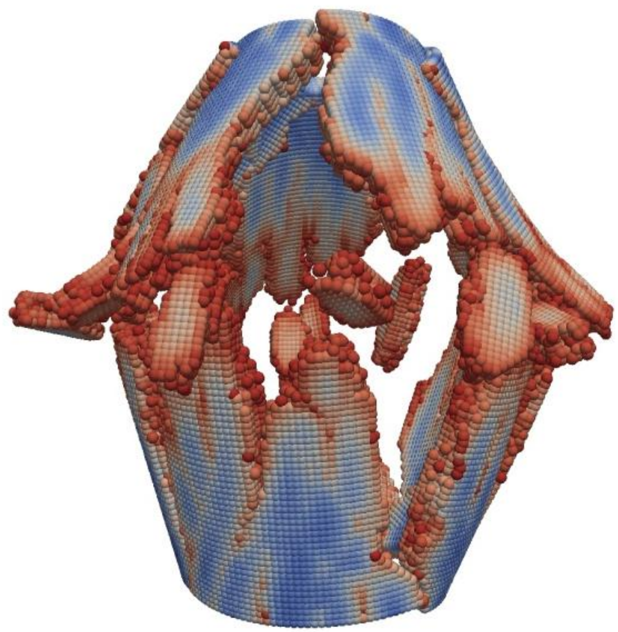
Silling, S.A. and Lehoucq, R. B. Peridynamic Theory of Solid Mechanics. *Advances in Applied Mechanics* 44:73-168, 2010.

Demonstration Computation: Fragmenting Cylinder

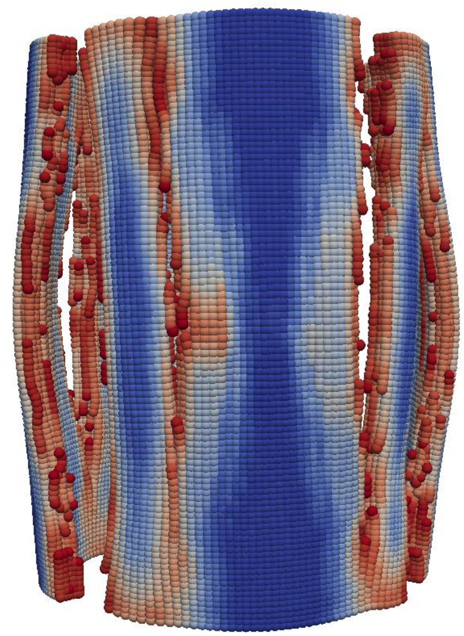
PERIDYNAMIC SIMULATION OF FRAGMENTING CYLINDER

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

Before



After
(brittle model)

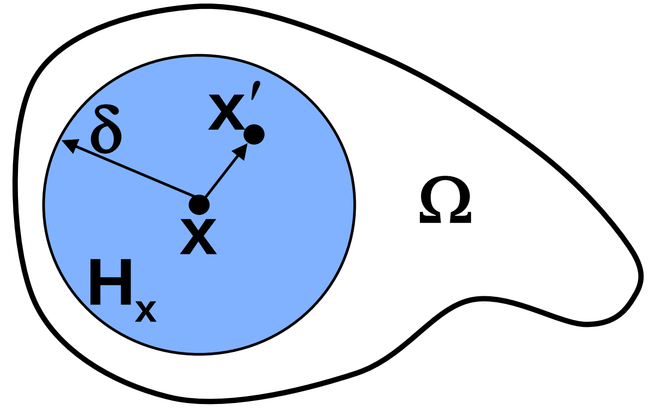


After
(plastic model)

Color indicates damage

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

Peridynamics: The Basics



HORIZON AND FAMILY

- Point **x** interacts directly with all points with distance δ (***horizon***)
- Material within distance δ of **x** is denoted $\mathbf{H_x}$ (***family of x***)

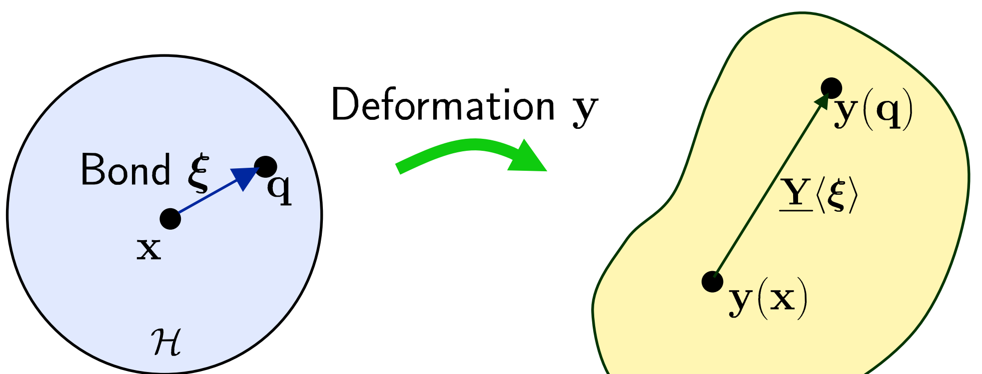
BONDS AND BOND FORCES

- Vector between **x** and any point in its family is called a ***bond:* ξ = x' - x**
- Each bond has ***pairwise force density vector*** applied at both points: **f(x', x, t)**
- This vector is determined jointly by collective deformation of $\mathbf{H_x}$ and collective deformation of $\mathbf{H_{x'}}$
- Bond forces are antisymmetric: **f(x', x, t) = - f(x, x', t)**

DEFORMATION STATE

- Deformation state operator $\underline{\mathbf{Y}}$ maps each bond ξ into its deformed image

$$\underline{\mathbf{Y}}\langle \xi \rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$$



Undeformed family of $\mathbf{x}$ Deformed family of $\mathbf{x}$

Peridynamics: The Basics

BONDS AND STATES

- **f(x', x)** has contributions from material models at both **x** and **x'**

$$\mathbf{f}(\mathbf{x}',\mathbf{x}) = \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x}-\mathbf{x}'\rangle$$

- $\underline{\mathbf{T}}[\mathbf{x}]$ is the ***force state*** – it maps bonds onto bond force densities
- $\underline{\mathbf{T}}[\mathbf{x}]$ is determined by the constitutive model $\underline{\mathbf{T}} = \hat{\mathbf{T}}(\underline{\mathbf{Y}})$, where $\hat{\mathbf{T}}$ maps deformation state to force state

PERIDYNAMICS VS. CLASSICAL THEORY

- If displacement smooth, convergence to classical equation in limit as $\delta \to 0$

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t) = \lim_{\delta\to 0}\int_{H}\left(\underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x}-\mathbf{x}'\rangle\right)dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

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

Piola-Kirchhoff stress tensor

- Peridynamics can be viewed as nonlocal extension of classical theory
  - Classical theory is a special case of peridynamics

S.A. Silling, R.B. Lehoucq, Convergence of Peridynamics to Classical Elasticity Theory. *J. Elasticity,* 93:1, pp. 13-37, 2008.

Peridynamics: The Basics

PERIDYNAMICS VS. STANDARD EQUATIONS

- Peridynamic operators and relationships between them are nonlocal analogues of standard theory

Relation	*Peridynamic theory*	*Standard theory*
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q}) - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \int_{\mathcal{H}} \Big(\mathbf{t}(\mathbf{q},\mathbf{x}) - \mathbf{t}(\mathbf{x},\mathbf{q})\Big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\mathbf{t}(\mathbf{q},\mathbf{x}) = \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular momentum balance	$\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle\, dV_{\mathbf{q}} = \mathbf{0}$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{\mathbf{Y}}}$ (Fréchet derivative)	$\boldsymbol{\sigma} = W_{\mathbf{F}}$ (tensor gradient)

Peridynamics: The Basics

MECHANICAL PROPERTIES OF PERIDYNAMICS

- Conserves energy (in absence of fracture, plastic deformation, etc.)
- Conserves linear & angular momentum (always)
- Basis in statistical mechanics*
- Obeys the laws of thermodynamics (restrictions on constitutive models)

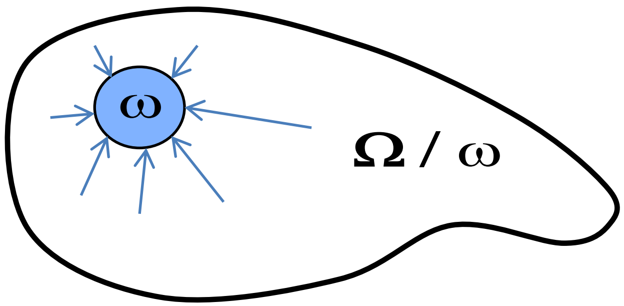
EXAMPLE: CONSERVATION OF MOMENTUM

- Rate of change of momentum of material within ω equals force of body outside ω acting upon ω plus external body force upon ω:

$$\frac{d}{dt}\int_{\omega} \rho \dot{u}(x,t)dV_x = \int_{\omega}\int_{\Omega/\omega}\left(T[x,t]\langle x'-x\rangle - T[x',t]\langle x-x'\rangle\right)dV_{x'}dV_x + \int_{\omega} b(x,t)dV_x$$

- No self-interaction:

$$\int_{\omega}\int_{\omega}\left(T[x,t]\langle x'-x\rangle - T[x',t]\langle x-x'\rangle\right)dV_{x'}dV_x = 0$$



*R.B. Lehoucq and M. Sears. *Statistical mechanical foundation of the peridynamic nonlocal continuum theory: Energy and momentum conservation laws. Phys. Rev. E 84, 031112 (2011).*

Peridynamics: The Basics

ENERGY BALANCE

- $\underline{\mathbf{T}}$ is work conjugate to $\underline{\mathbf{Y}}$:
- This leads to energy balance (first law of thermodynamics)

$$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + \mathbf{q} + \mathbf{r}$$

Peridynamic equivalent of stress power $\sigma \cdot \dot{\mathbf{F}}$

where

- ε = internal energy density
- $\mathbf{q}$ = rate of heat transport
- $\mathbf{r}$ = energy source rate

THERMODYNAMIC ADMISSIBILITY FOR CONSTITUTIVE MODELS

- Second law of thermodynamics (Clausius-Duhem inequality):

$$\theta\dot{\eta} \geq \mathbf{q} + \mathbf{r}$$

where

- θ = absolute temperature
- η = entropy density

- Combining with first law gives thermodynamic admissibility condition for constitutive models:

$$\underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} - \dot{\theta}\eta - \dot{\psi} \geq \mathbf{0}$$

where

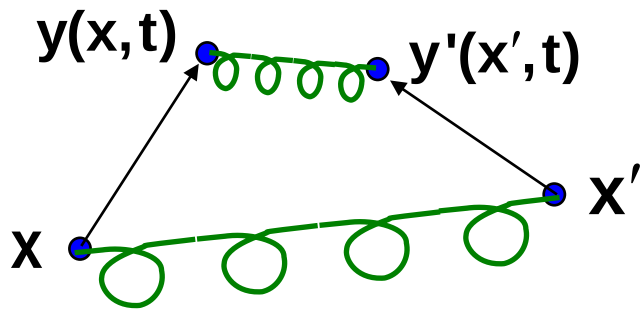
- $\psi = \varepsilon - \theta\eta$ is free energy density

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

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

$$T[x,t]\langle x' - x\rangle = \frac{1}{2} f(y'-y, x'-x)$$

*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.

Peridynamic Material Modeling

*PROPORTIONAL MICROELASTIC BRITTLE (PMB) MATERIAL MODEL**

$\mathbf{x} \equiv$ **initial position**

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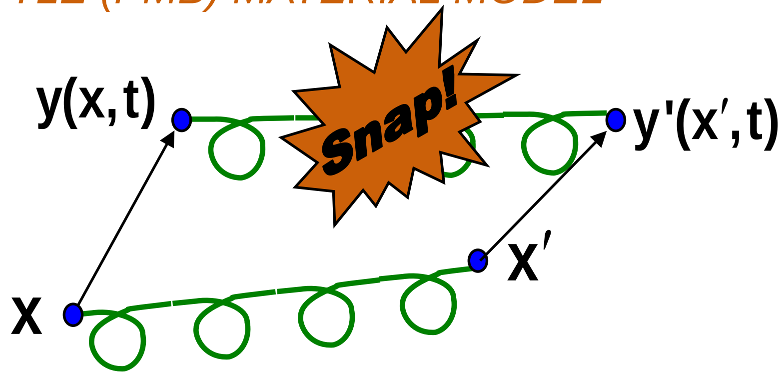
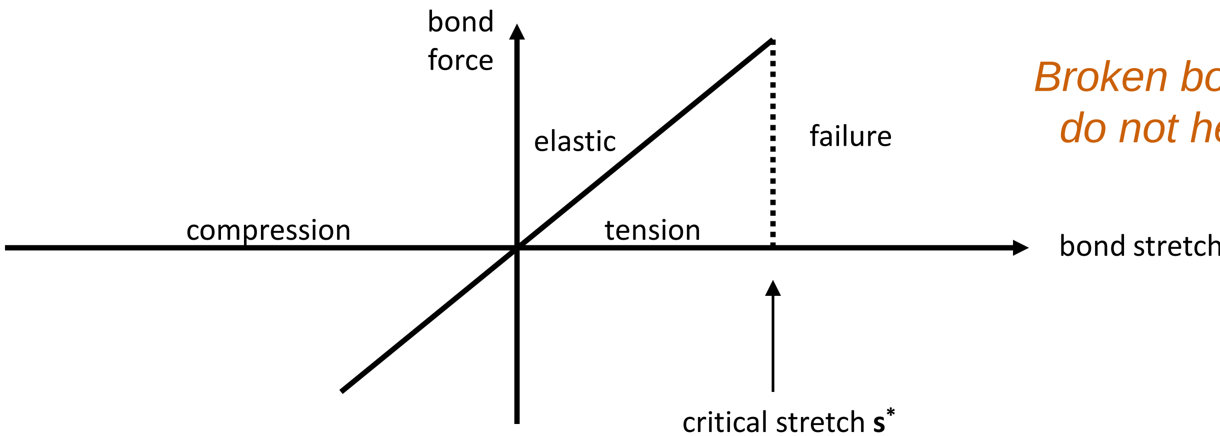


$$s = \frac{\|\mathbf{y}' - \mathbf{y}\| - \|\mathbf{x}' - \mathbf{x}\|}{\|\mathbf{x}' - \mathbf{x}\|}$$

Bond fails when stretch too large

Broken bonds do not heal



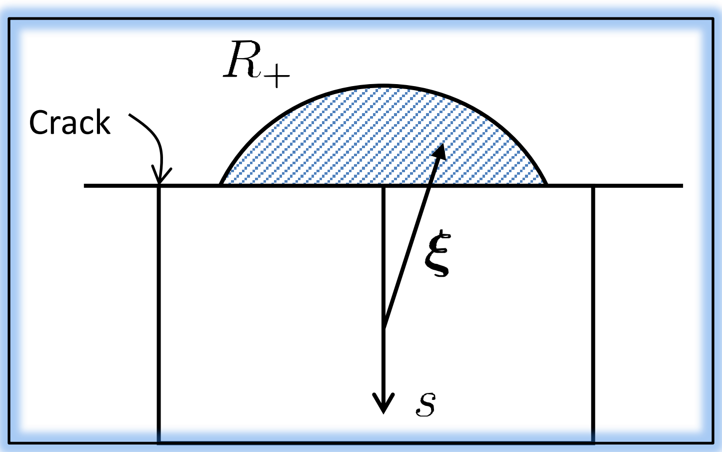
*S.A. Silling and E. Askari, A meshfree method based on the peridynamic model of solid mechanics, Computers and Structures, 83, pp. 1526-1535, 2005.

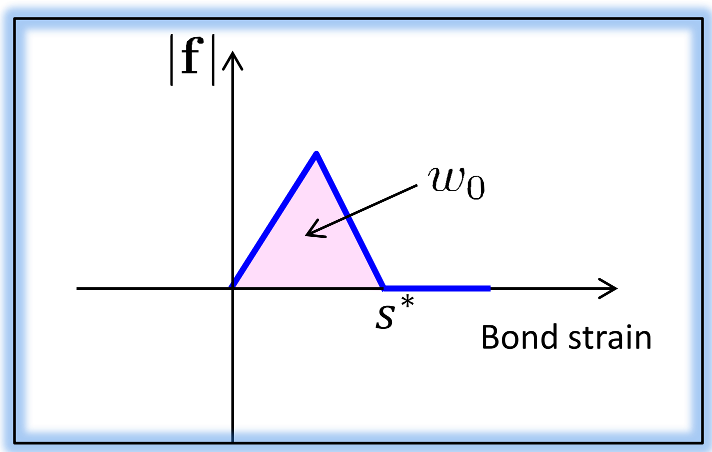
Peridynamic Material Modeling

ENERGY BALANCE FOR GROWING CRACK

- If work to break bond ξ is $\mathbf{w_0(\xi)}$, then energy release rate found by summing this work per unit crack area

$$G = \int_0^\delta \int_{R_+} w_0(\xi) dV_\xi ds$$





- Can then get the critical strain $\mathbf{s^*}$ for bond breakage in terms of G.
- Alternatives:
  - Could use peridynamic J-integral as bond breakage criterion
  - For composites, could use macroscale criteria such as Hashin

Peridynamic Material Modeling

*LINEAR PERIDYNAMIC SOLID (LPS)**

- Nonlocal analogue to linear isotropic elastic solid
- k is bulk modulus, μ is shear modulus

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

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

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

- **Can wrap classical material models (e.g., LAME material library) in a peridynamic “skin” (more on this later!)**

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

Peridynamic Material Modeling

*ELASTIC-PLASTIC MODEL**

- Nonlocal analogue to perfect plasticity model
- Relevant to ductile materials and ductile failure

RATE EQUATIONS AND CONSTRAINTS

- Additive decomposition of extension state: $\underline{\mathbf{e}}^{d} = \underline{\mathbf{e}}^{de} + \underline{\mathbf{e}}^{dp}$
- Elastic force state relations:

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

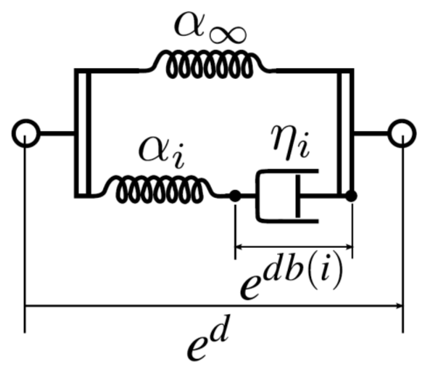
- Elastic force state domain defined by yield surface/function that depends upon deviatoric force state:
  - $\mathbf{f}(\underline{\mathbf{t}}^{d}) = \psi(\underline{\mathbf{t}}^{d}) - \psi_0 \leq 0$, where $\psi(\underline{\mathbf{t}}^{d}) = \frac{1}{2} \|\underline{\mathbf{t}}^{d}\|^2$
- Flow rule describing rate of plastic deformation: $\dot{\mathbf{e}}^{dp} = \lambda \nabla^{d} \Psi$
- Loading/un-loading conditions (Kuhn-Tucker constraints):
  - $\lambda > 0, \quad \mathbf{f}(\underline{\mathbf{t}}^{d}) \leq 0, \quad \lambda\, \mathbf{f}(\underline{\mathbf{t}}^{d}) = 0$
- Consistency condition: $\lambda \dot{\mathbf{f}}(\mathbf{t}^{d}) = 0$

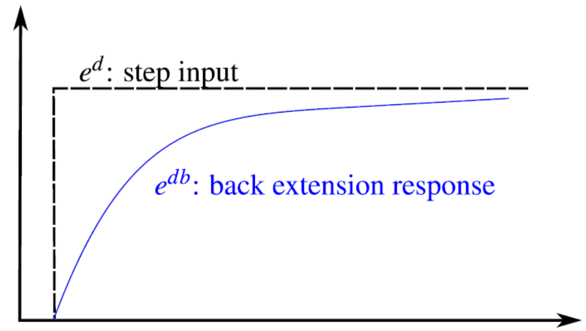
*J. Mitchell, A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics, SAND2011-3166, 2011.

Peridynamic Material Modeling

*VISCOELASTIC MODEL**

- Nonlocal analog to standard linear solid
- Applicable where rate effects may be important
- Adds viscous terms to deviatoric portion of extension state; bulk response remains elastic
- Logical intermediate step between fluid and solid
  - viscous fluid: little or no elastic resistance to shear (fluids flow) but resists compressive volumetric deformations
  - elastic solid: elastic resistance to both shear and volumetric deformations



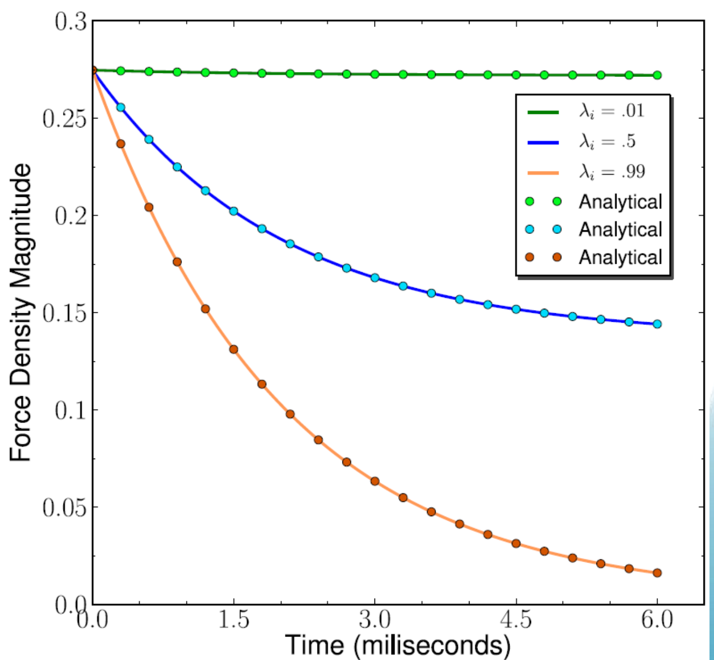


GOVERNING EQUATIONS

- Scalar deviatoric force: $\mathbf{t}^d = \eta_i \dot{\mathbf{e}}^{db}$

$$= \alpha_i (\mathbf{e}^d - \mathbf{e}^{db})$$

- Evolution equation: $\dot{\mathbf{e}}^{db} = \frac{1}{\tau^b}(\mathbf{e}^d - \mathbf{e}^{db})$



*J. Mitchell, A Non-local, Ordinary-State-Based Viscoelasticity Model for Peridynamics, SAND2011-8064, 2011.

Analytical Results

- Weak form of linear peridynamic solid (LPS) model is well-posed.[a]
- Weak form of nonlocal diffusion equation is well-posed.[b]
- Weak form of nonlocal wave equation is well-posed.[b]
- Finite element error bounds established for bond-based models on 2D plate.[c]

[a] Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou, Application of a nonlocal vector calculus to the analysis of linear peridynamic materials. Technical report SAND 2011-3870J.

[b] Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou, Analysis and approximation of nonlocal diffusion problems with volume constraints. SIREV (to appear).

[c] K. Zhou and Q. Du. Mathematical and numerical analysis of linear peridynamic models with nonlocal boundary conditions. SIAM Journal on Numerical Analysis, 48(5):1759 - 1780.

I. Peridynamics

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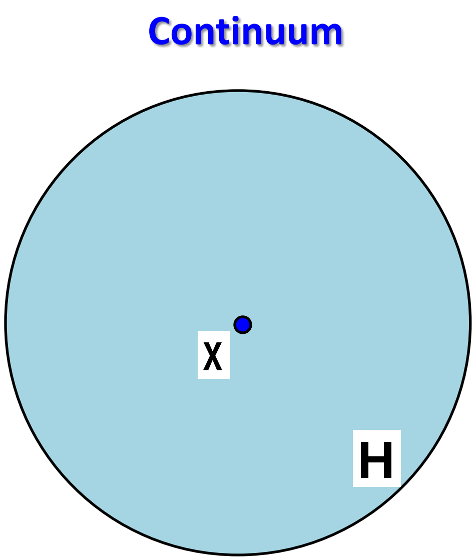
Discretizing Peridynamics

*SPATIAL DISCRETIZATION**

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



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

*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

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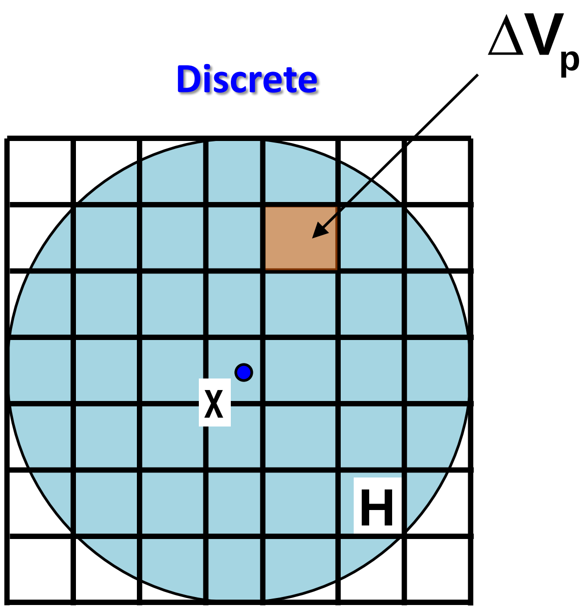


$$\sum_p f(u(x_p,t)-u(x_i,t),x_p-x_i)\Delta V_p$$

*TEMPORAL DISCRETIZATION**

- Explicit central difference in time

$$\ddot{u}(x,t) \approx \ddot{u}_i^n = \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2}$$

- Velocity-Verlet

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

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

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

- Must satisfy nonlocal CFL condition
- Larger timesteps allowed than in local models

- **Peridynamics is a continuum theory; Discretize it how you want**
  - Finite element; finite volume, etc.

*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.

Peridynamic Codes

PERIDYNAMICS IN SIERRA/SOLIDMECHANICS (Export controlled, C++)

- Developer: Littlewood
- Sandia engineering analysis code

PERIDIGM (Open source, C++)

- Developers: Parks, Littlewood, Mitchell, Silling
- Sandia's primary open-source PD code
- Built upon Sandia's Trilinos Project (trilinos.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

EMU (Export Controlled, F90)

- Developer: Silling (www.sandia.gov/emu/emu.htm)
- Research code

Peridynamics is a capability that can be added to (almost) any analysis code!

Peridynamics in Sierra/SolidMechanics

Peridynamics is available in Sierra/SolidMechanics for the modeling of material failure

- Available for explicit dynamics
- Current work: quasi-statics and implicit dynamics
- Material models
  - Linear peridynamic solid material model
  - Interface to full set of Sierra/SM classical material models (LAME library)
- User defined peridynamic horizon and influence function
- Bond failure laws
  - Critical stretch bond failure rule
  - Bond failure based on element variables (e.g. material model data)
- Contact algorithm
- Full set of pre- and post-processing tools
  - Meshing, visualization, initialization of peridynamic bonds

Key feature: Interface to LAME material library

Full set of classical material models is available via peridynamics in Sierra/SolidMechanics

MATERIAL MODELS: LIBRARY OF ADVANCED MATERIALS FOR ENGINEERING (LAME)

- Traditional models: Elastic, Thermo-elastic, Elastic-plastic, others…
- Advanced models: Johnson-Cook, BCJ, K&C Concrete, others…
- Suitable for geo modeling: Soil and Crushable Foam, Orthotropic Crush, others…

APPROACH: NON-ORDINARY STATE-BASED PERIDYNAMICS

① Compute regularized deformation gradient

$$\bar{\mathbf{F}} = \left(\sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{Y}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i} \right) \mathbf{K}^{-1} \qquad \mathbf{K} = \sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{X}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i}$$

② Classical material model computes stress based on regularized deformation gradient

③ Convert stress to peridynamic force densities

$$\underline{\mathbf{T}} \langle \mathbf{x}' - \mathbf{x} \rangle = \underline{\omega} \, \sigma \mathbf{K}^{-1} \langle \mathbf{x}' - \mathbf{x} \rangle$$

④ Apply peridynamic hourglass forces as required to stabilize simulation (optional)

S. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari. Peridynamic states and constitutive modeling. *Journal of Elasticity*, 88(2):151-184, 2007.

Peridigm

- Developers: Parks, Littlewood, Mitchell, Silling
- Sandia's primary open-source PD code
- Component based -- Built upon Sandia's Trilinos Project (trilinos.sandia.gov)
- Notable features: Massively parallel, Exodus mesh input/output multiple material blocks, explicit, implicit time integration, state-based linear elastic, elastic-plastic, viscoelastic models
- DAKOTA interface for UQ/optimization/calibration, etc. (dakota.sandia.gov)

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)
- Model Evaluator(EpetraExt)

Solver Tools

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

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
- 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: ????
- *Peridynamics is an expedient approach for fracture modeling*

Parallel Performance

- **Dawn (LLNL): IBM BG/P System**
  - 500 teraflops; 147,456 cores
- **Part of Sequoia procurement**
  - 20 petaflops; 1.6 million cores
- **Large-scale simulation**
  - Mesh spacing: 35 microns
  - Approx. 82 million mesh points
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores

***Dawn* at LLNL**

- **Largest peridynamic simulations in history**

Weak Scaling Results (PDLAMMPS)

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

I. Peridynamics

II. Numerics and Codes

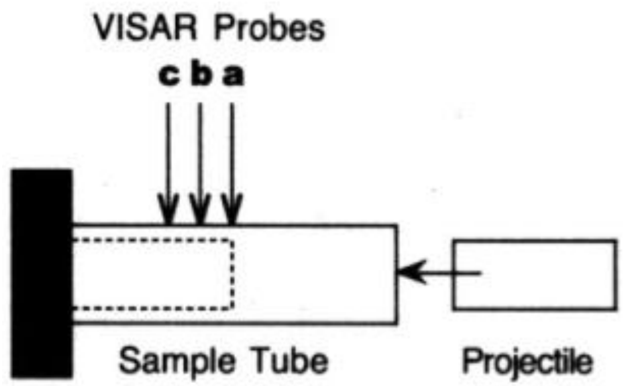
III. Applications

IV. Current & Future Work

Application: Expanding tube experiment

Experimental Setup

- Tube expansion via collision of Lexan projectile and plug within AerMet tube
- Accurate recording of velocity and displacement on tube surface



Experimental setup [Vogler et. Al]

Modeling Approach

- AerMet tube modeled with peridynamics, elastic-plastic material model with linear hardening
- Lexan plugs modeled with classical FEM, equation-of-state Johnson-Cook material model
- Interaction via contact algorithm

Model discretization

Vogler, T.J., Thornhill, T.F., Reinhart, W.D., Chhabidas, L.C., Grady, D.E., Wilson, L.T., Hurricane, O.A., and Sunwoo, A. Fragmentation of materials in expanding tube experiments. *International Journal of Impact Engineering*, 29:735-746, 2003.

D. Littlewood. 2010. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition, British Columbia, Canada.

Application: Expanding tube experiment

AerMet Tube

- Peridynamics
- Elastic-plastic constitutive model
- 73,676 sphere elements
- Horizon set to five times element radius

Parameter	Value
Density	7.87 g/cm^3
Young’s Modulus	194.4 GPa
Poisson’s Ratio	0.3
Yield Stress	1.72 GPa
Hardening Modulus	1.94 GPa
Critical Stretch	0.02

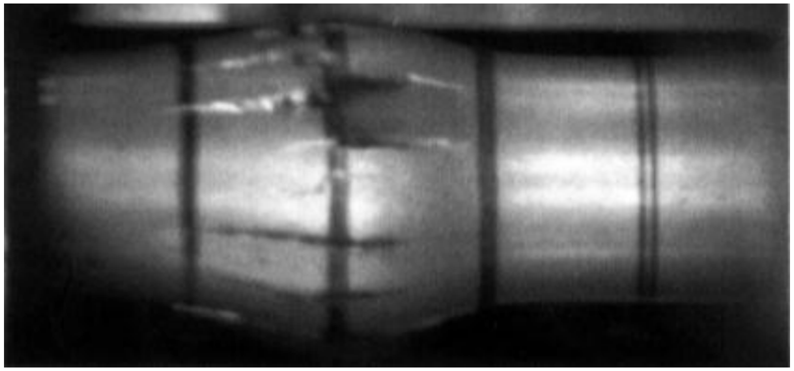
Lexan Projectile/Plug

- Classical FEM
- Johnson-Cook constitutive model
- 53,214 hexahedron elements

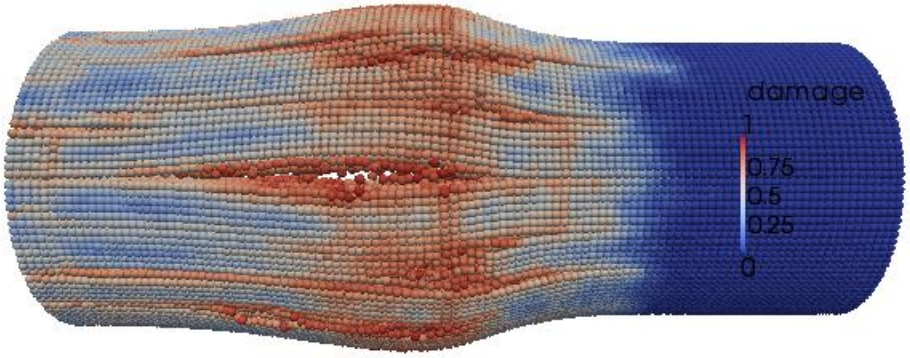
Parameter	Value
Density	1.19 g/cm^3
Young’s Modulus	2.54 GPa
Poisson’s Ratio	0.344
Yield Stress	75.8 MPa
Hardening Constant *B*	68.9 MPa
Rate Constant C	0.0
Hardening Exponent *N*	1.0
Thermal Exponent *M*	1.85
Reference Temperature	70.0 ° F
Melting Temperature	500.0 ° F

Simulation performed with Sierra/SolidMechanics

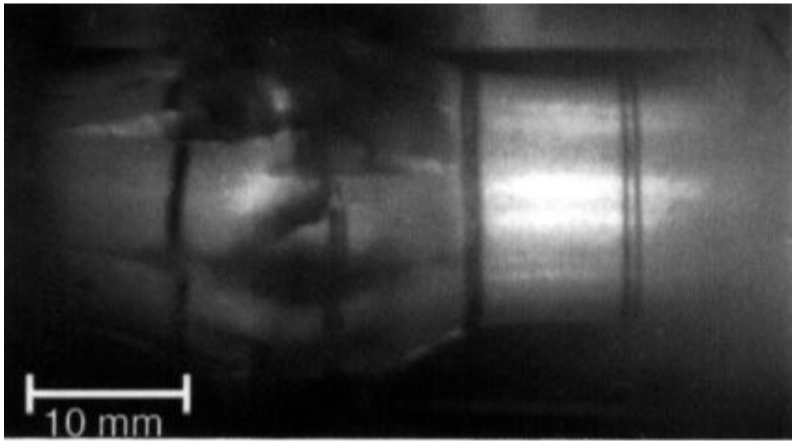
Predicted damage profiles



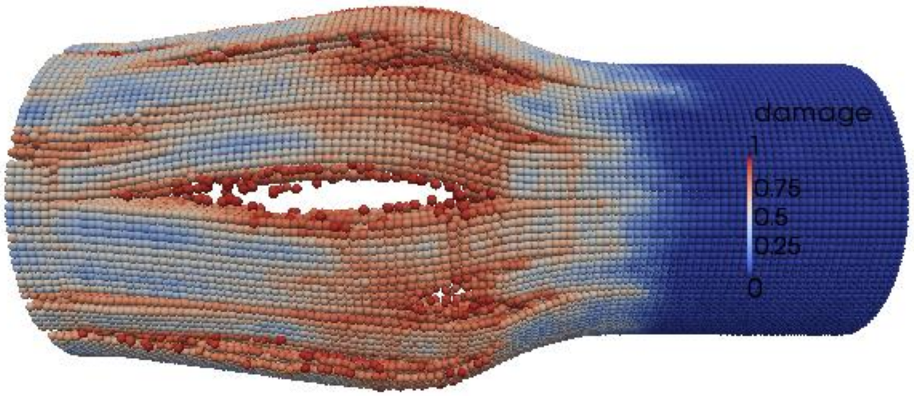
Experimental image at 15.4 microseconds [Vogler et. al]



Simulation at 15.4 microseconds



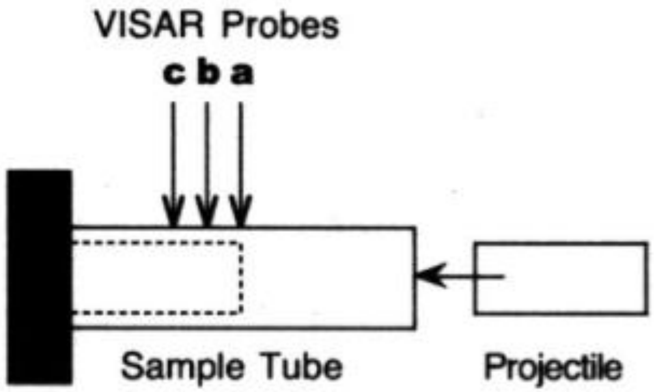
Experimental image at 23.4 microseconds [Vogler et. al]

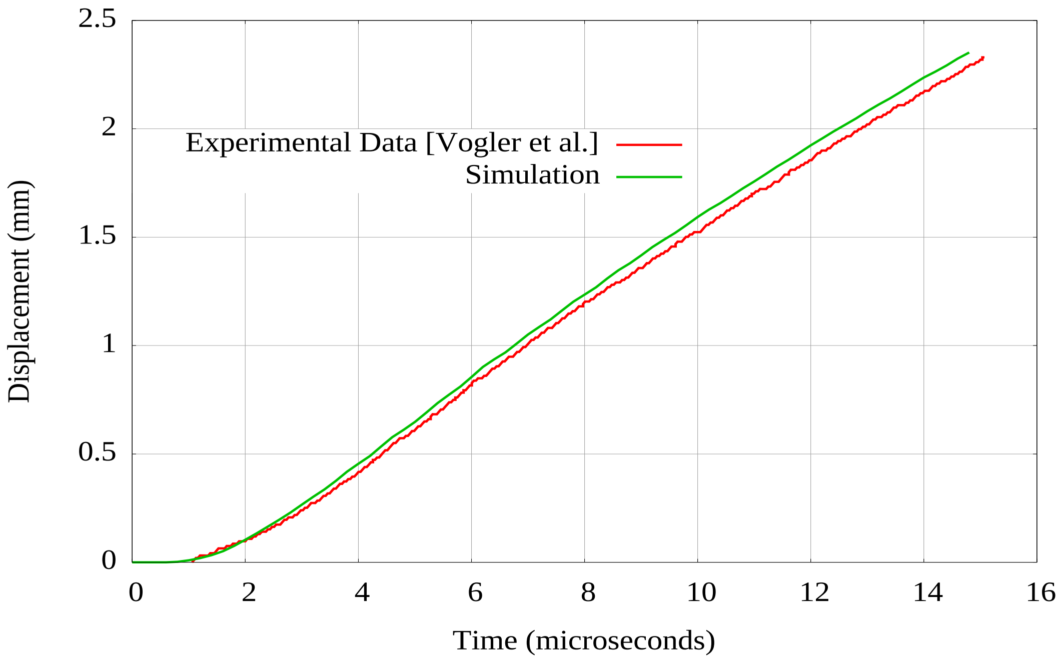


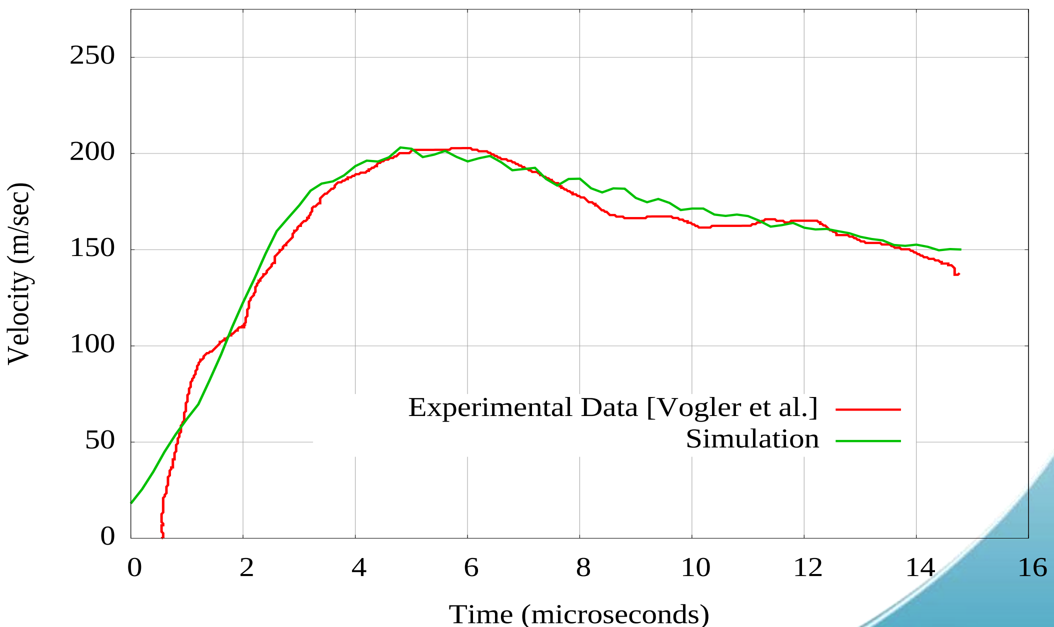
Simulation at 23.4 microseconds

Predicted displacement and velocity on tube surface

Displacement and velocity
on tube surface
at probe position A





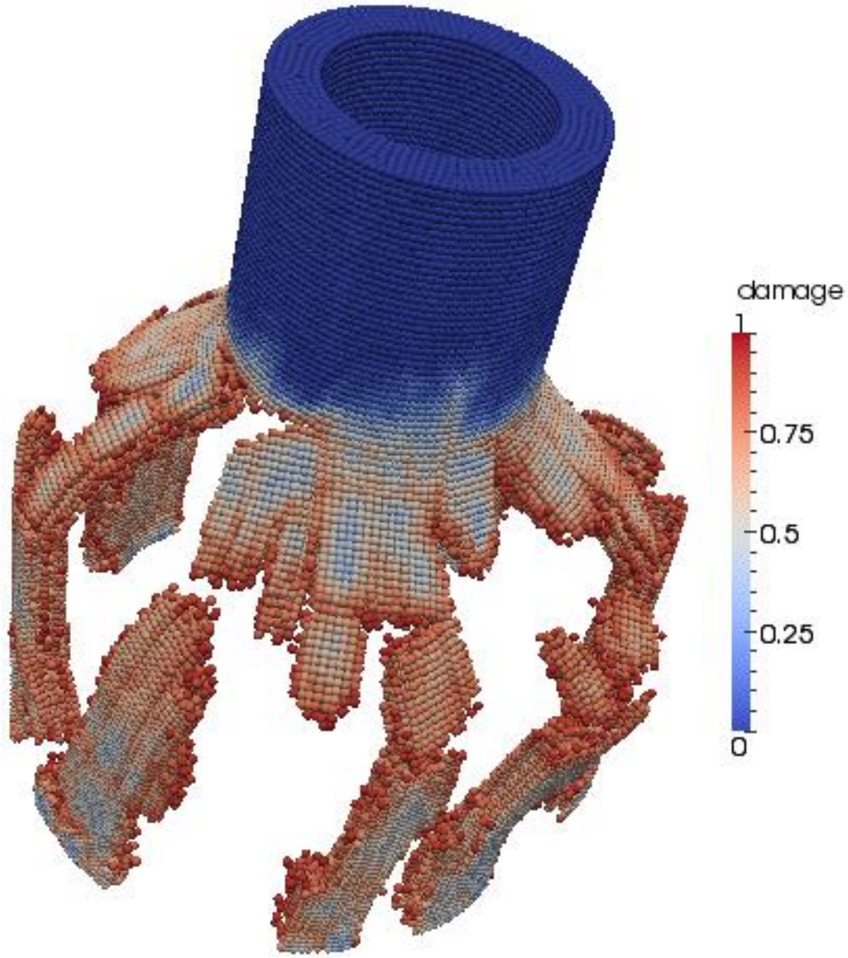


Simulation performed with Sierra/SolidMechanics

Fragmentation pattern

<u>Qualitative Comparison of Fragmentation Results</u>

- Vogler et. al reported significant uncertainty in results at late time
- Approximately half the tube remained intact
- Vogler et. al recovered 14 fragments with mass greater than one gram



Simulation at 84.8 microseconds

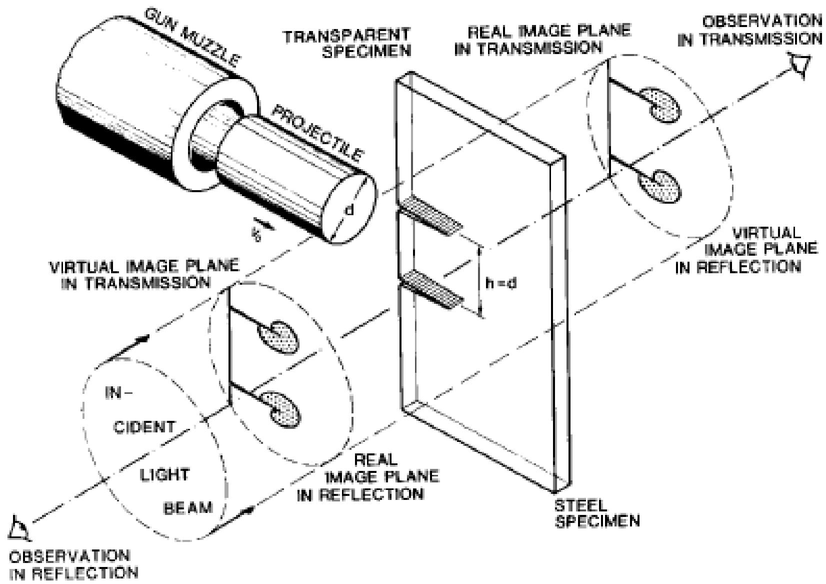
Sandia National Laboratories

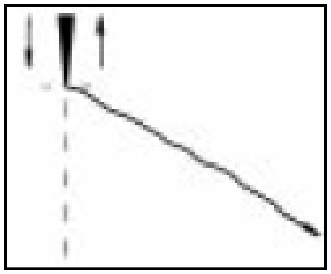
Simulation performed with EMU

Capability demonstration: Kalthoff-Winkler experiment

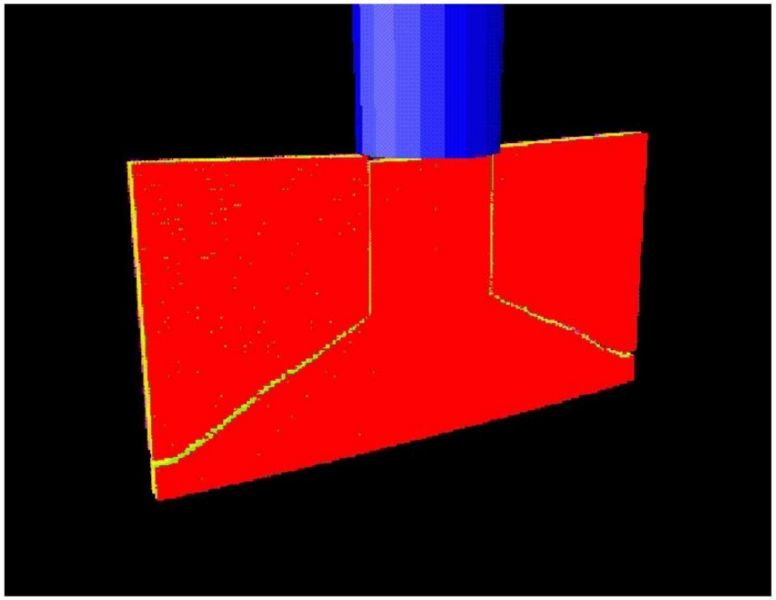
PERIDYNAMIC MODELING OF THE KALTHOFF-WINKLER EXPERIMENT

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





Experimental Results



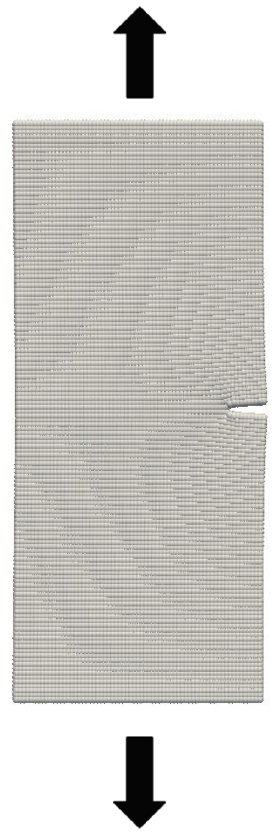
Peridynamic Model

* 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.

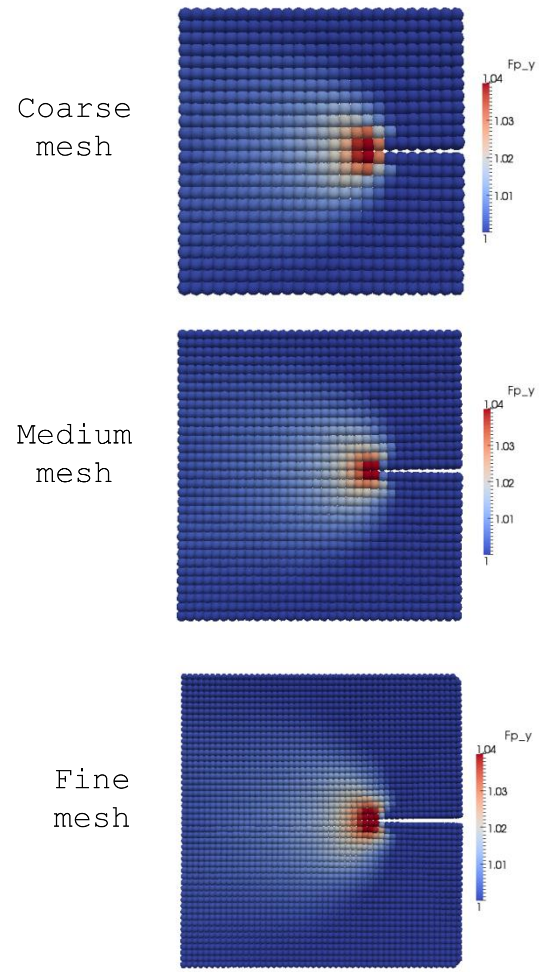
Simulation performed with Sierra/SolidMechanics

Capability demonstration: Mesh independent plastic zone

- Peridynamic horizon introduces length scale independent of mesh size
- Localization in peridynamics function of horizon (parameter of continuum model)
- Localization in classical FEM function of mesh (parameter of discrete model)
- Ongoing work: Investigation of convergence rates
- Example: Mesh independent plastic zone in the vicinity of crack
- Similar phenomena occur in necking and shear banding



Pre-cracked specimen loaded in tension



Component of plastic deformation gradient in loading direction

Simulation performed with EMU

Capability demonstration: Composite failure

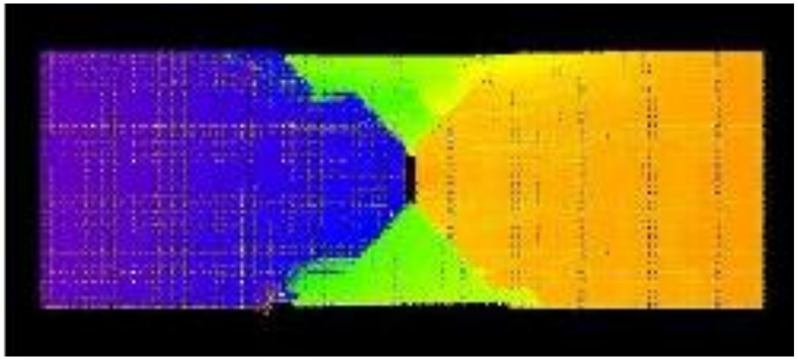
FAILURE IN FIBER-REINFORCED COMPOSITE LAMINATE

- 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)

45° angle of fibers within ply dictate failure direction

Reproduce in peridynamic simulation by controlling bond strength orientation



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.

I. Peridynamics

II. Numerics and Codes

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IV. Current & Future Work

Current & Future Work

- Multiscale dynamic fracture modeling

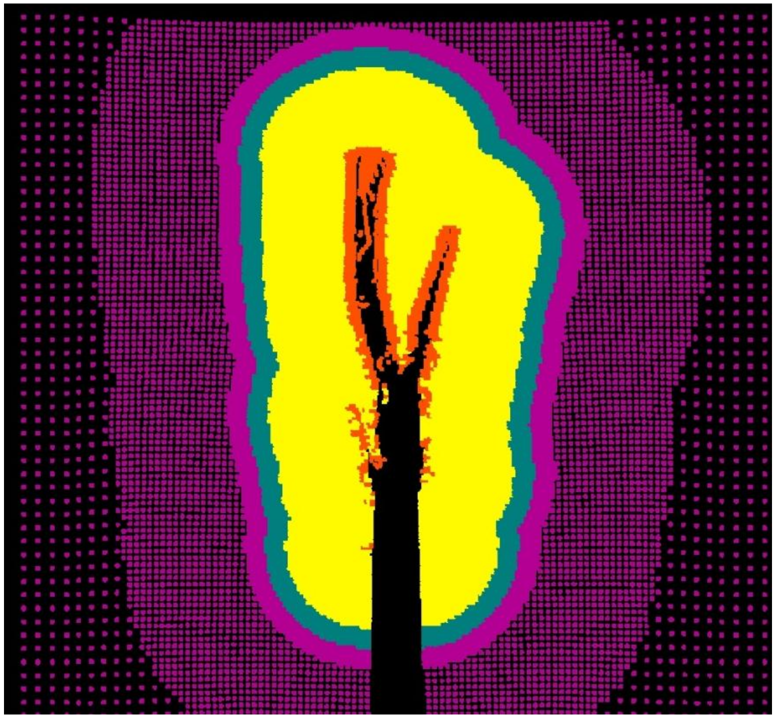
- Advanced solvers; nonlocal domain decomposition;
- Condition number bounds for peridynamic models; nonlocal preconditioners

- Develop peridynamic viscoplastic model

- Local/nonlocal coupling,
  (to enable FEM/PD coupling)

- Continued error/convergence/verification studies

- Continued mathematical and numerical analyses



Summary

- Peridynamics Overview
- Numerics and Codes
- Applications
- Current & Future Work

- Some Current Customers…
  - Army Research Labs (ARL): Munitions fragmentation, penetration
  - Boeing: Failure in composite laminates
  - ExxonMobil: Driven fracture in shale
  - Orica: Bench-blasting (mining)
  - X-Prize: Predictive failure modeling