

Peridynamics for Material Failure

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Multiphysics Simulation Technology

Org. 1444

Sandia National Laboratories

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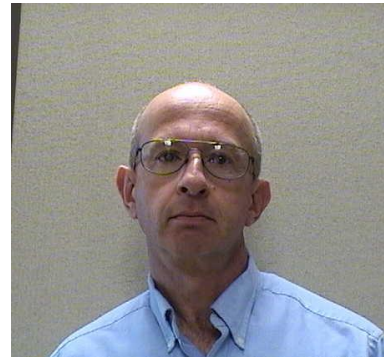
1444 Peridynamics Staff



Dave Littlewood



John Mitchell



Stewart Silling



Mike Parks



Rich Lehoucq

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

I. Peridynamics

II. Codes

III. Applications

IV. Conclusions

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

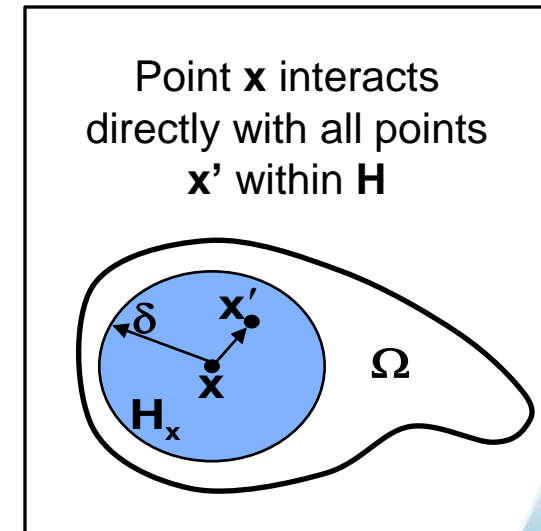
$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \nabla \cdot \boldsymbol{\sigma}(\nabla \mathbf{u}(\mathbf{x}, t)) + \mathbf{b}(\mathbf{x}, t)$$

HOW DOES PERIDYNAMICS WORK?

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

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

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



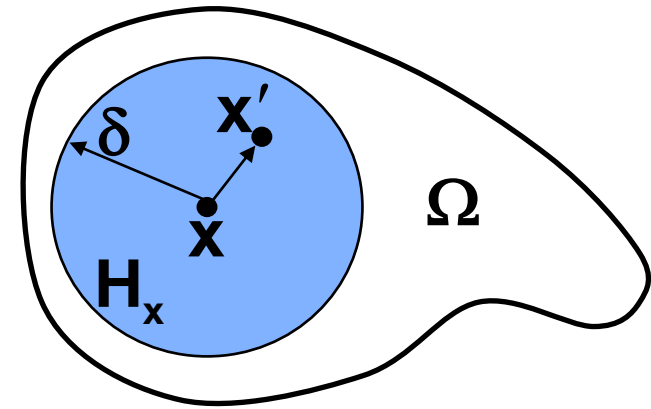
S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.

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

Peridynamics: The Basics

HORIZON AND FAMILY

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



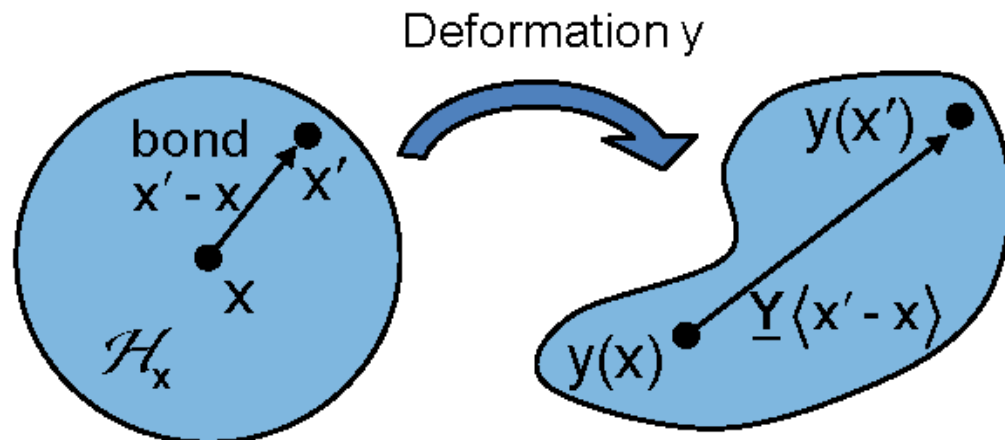
BONDS AND BOND FORCES

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

DEFORMATION STATE

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

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



Undeformed family of \mathbf{x}

Deformed family of \mathbf{x}

Peridynamics: The Basics

BONDS AND STATES

- $\mathbf{f}(\mathbf{x}', \mathbf{x})$ has contributions from material models at both \mathbf{x} and \mathbf{x}'

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

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

PERIDYNAMICS VS. CLASSICAL THEORY

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

$$\begin{aligned} \rho \ddot{\mathbf{u}}(\mathbf{x}, t) &= \lim_{\delta \rightarrow 0} \int_H \left(\mathbf{T}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \mathbf{T}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t) \\ &= \nabla \cdot \mathbf{P}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t) \end{aligned}$$

————— *Piola-Kirchhoff stress tensor*

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

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	$\underline{\mathbf{Y}} \langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho \ddot{\mathbf{u}}(\mathbf{x}) = \int_{H_x} (\underline{\mathbf{T}}[\mathbf{x}] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}'] \langle \mathbf{x} - \mathbf{x}' \rangle) dV_{x'} + \mathbf{b}(\mathbf{x})$	$\rho \ddot{\mathbf{y}}(\mathbf{x}, t) = \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular momentum balance	$\int_{H_x} \underline{\mathbf{Y}} \langle \mathbf{x}' - \mathbf{x} \rangle \times \underline{\mathbf{T}} \langle \mathbf{x}' - \mathbf{x} \rangle dV_{x'} = \mathbf{0}$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
Elasticity	$\underline{\mathbf{T}} = \mathbf{W}_{\underline{\mathbf{Y}}} \text{ (Frechet derivative)}$	$\boldsymbol{\sigma} = \mathbf{W}_{\mathbf{F}} \text{ (tensor gradient)}$
First law of thermodynamics	$\dot{\boldsymbol{\varepsilon}} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + \mathbf{h} + \mathbf{r}$	$\dot{\boldsymbol{\varepsilon}} = \boldsymbol{\sigma} \cdot \dot{\mathbf{F}} + \mathbf{h} + \mathbf{r}$

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)

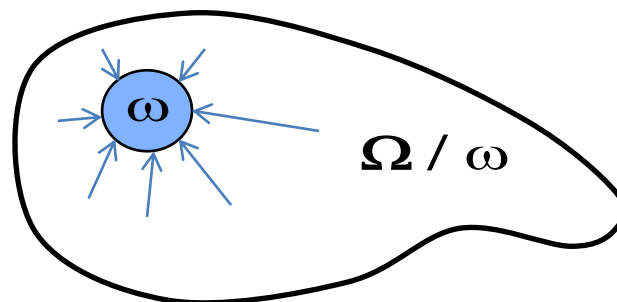
EXAMPLE: CONSERVATION OF MOMENTUM

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

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

- No self-interaction:

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



Peridynamics: The Basics

ENERGY BALANCE

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

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

where

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

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

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:

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

where

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

Peridynamic Material Modeling

LINEAR PERIDYNAMIC SOLID (LPS)*

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

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

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

- 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.

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

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

Peridynamic Damage Modeling

DAMAGE STATE

- Define a nondecreasing damage state $0 \leq \varphi\langle \mathbf{x}' - \mathbf{x} \rangle \leq 1$ for each bond $\mathbf{x}' - \mathbf{x}$ that evolves according to a given damage evolution law:

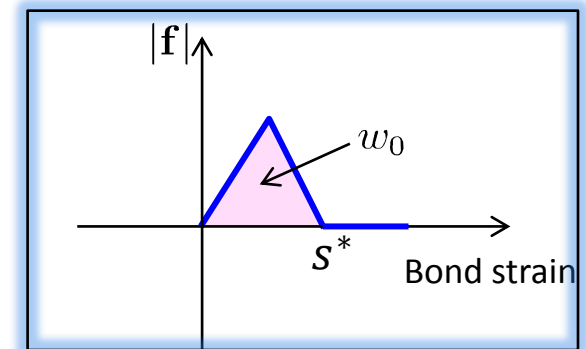
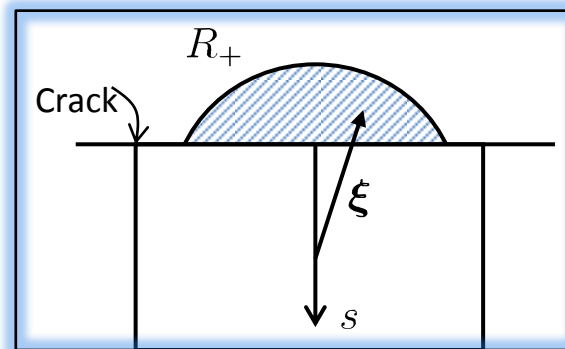
$$\varphi\langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{D}(\underline{Y}, \underline{\dot{Y}}, \dots)$$

- Simplest damage model involves bond breakage (Damage jumps discontinuously from 0 to 1)
- Damage leads to fracture and failure

ENERGY BALANCE FOR GROWING CRACK*

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

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



- Can then get the critical strain s^* for bond breakage in terms of G (value from physical experiment)
- Alternatives:
 - Could use peridynamic J-integral as bond breakage criterion
 - For composites, could use macroscale criteria such as Hashin

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

II. Codes

III. Applications

IV. Conclusions

Peridynamic Codes

Peridynamics is a continuum model, not a numerical method!

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

- Developer: Littlewood
- Peridynamic simulation capability within 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
- LAMMPS: Sandia's open-source massively parallel MD code (lammps.sandia.gov)
- More info & user guide: www.sandia.gov/~mlparks
- Time from starting implementation to running first experiment: Two weeks
 - *Peridynamics is an expedient approach for fracture modeling*

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 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

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

- ② Classical material model computes stress based on regularized deformation gradient
- ③ Convert stress to peridynamic force densities

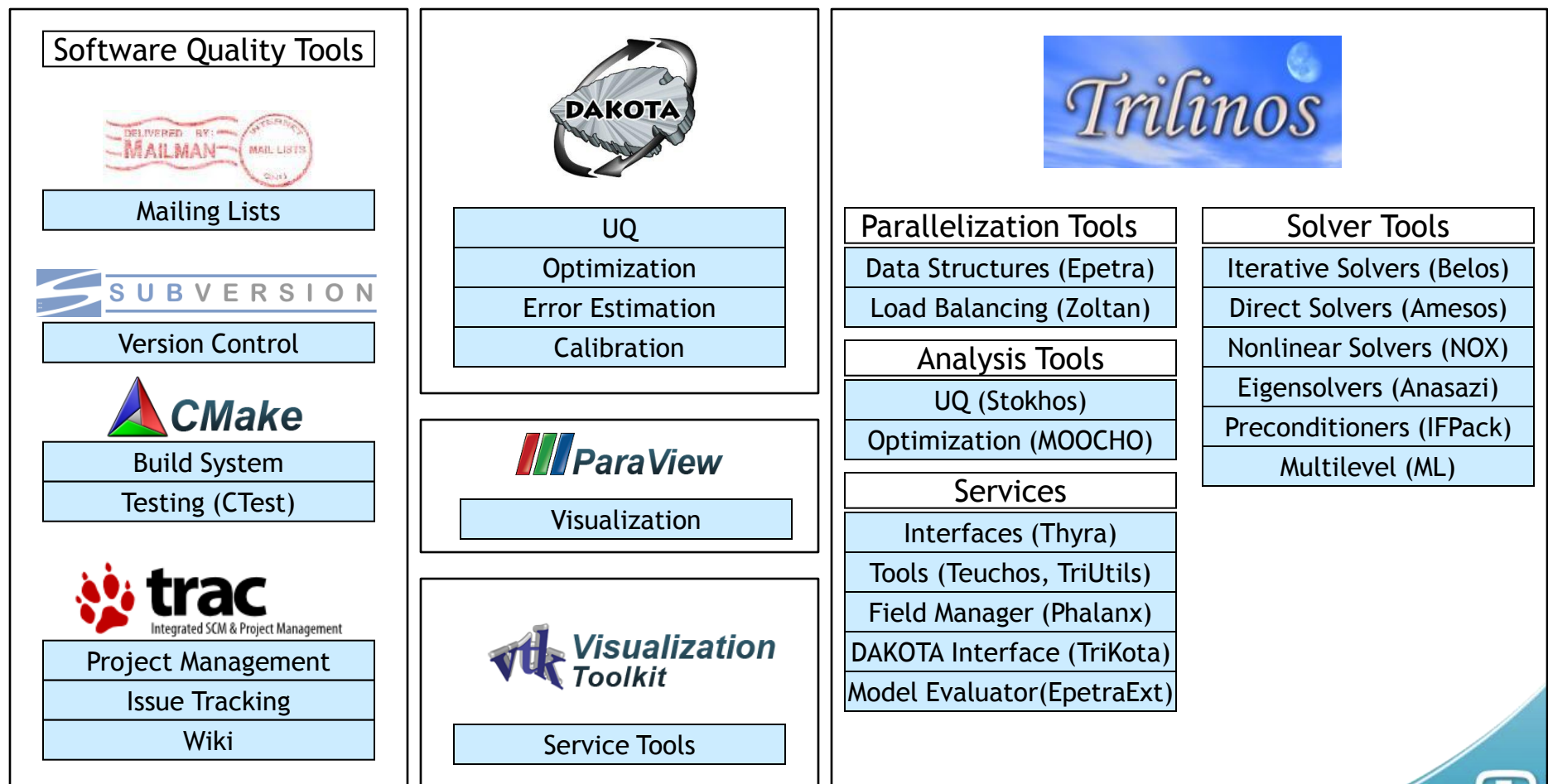
$$\underline{\mathbf{T}} \langle \mathbf{x}' - \mathbf{x} \rangle = \underline{\omega} \sigma \mathbf{K}^{-1} \langle \mathbf{x}' - \mathbf{x} \rangle$$

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

Peridigm



- Developers: Parks, Littlewood, Mitchell, Silling
- Sandia's primary open-source PD code (<https://software.sandia.gov/trac/peridigm>)
- 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)



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 (Peridynamics-in-LAMMPS)

# 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. Codes

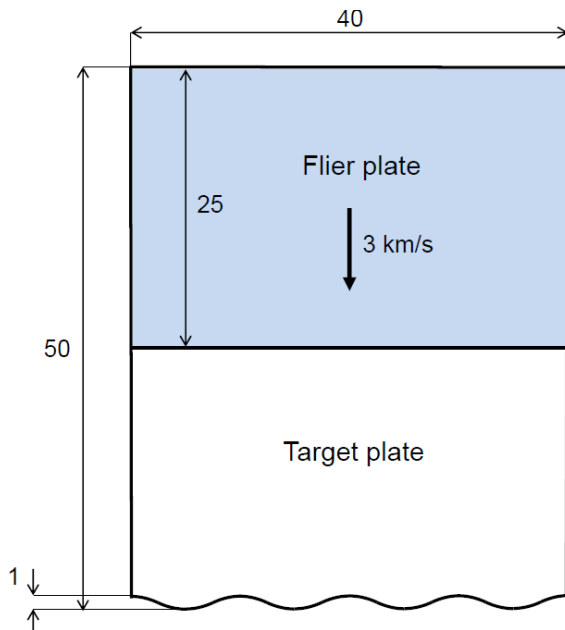
III. Applications

IV. Conclusions

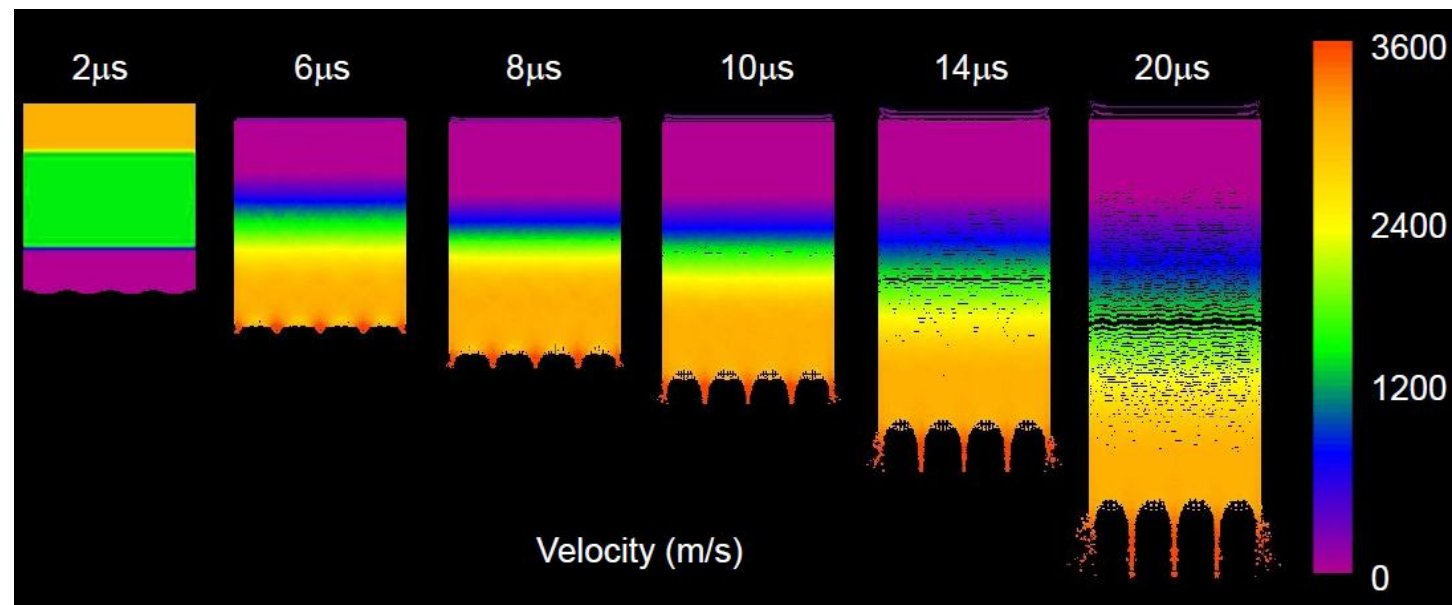
Demonstration Computation: Shockwave Ejecta

PERIDYNAMIC SIMULATION OF SHOCKWAVE EJECTA

- Preliminary work; Motivated by experiments by Ogorodnikov et al.*
- Utilize Peridynamic Eulerian model with Mie-Grüneisen EOS
- Impact aluminum flyer plate on aluminum target plate at 3 km/s, pressure 30 GPa



*Initial geometry.
Dimensions in mm.*



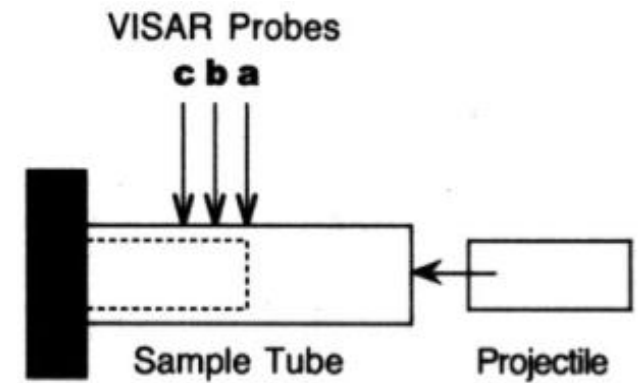
Peridynamic simulation results. Six different simulation times are shown.

- Computed shock velocity is 7.140 km/s; Expected value is 7.230 km/s.
- Computed jet tip velocity is 4.0 km/s; Experimentally measured value is 3.7 km/s.

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

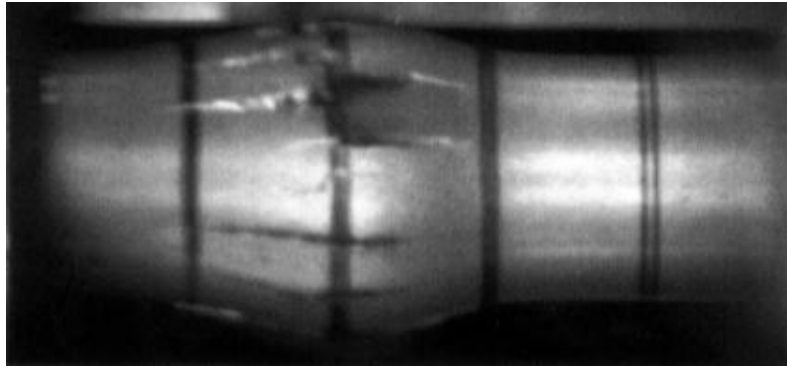
Parameter	Value
Density	7.87 g/cm ³
Young' s Modulus	194.4 GPa
Poisson' s Ratio	0.3
Yield Stress	1.72 GPa
Hardening Modulus	1.94 GPa
Critical Stretch	0.02

Lexan Projectile/Plug

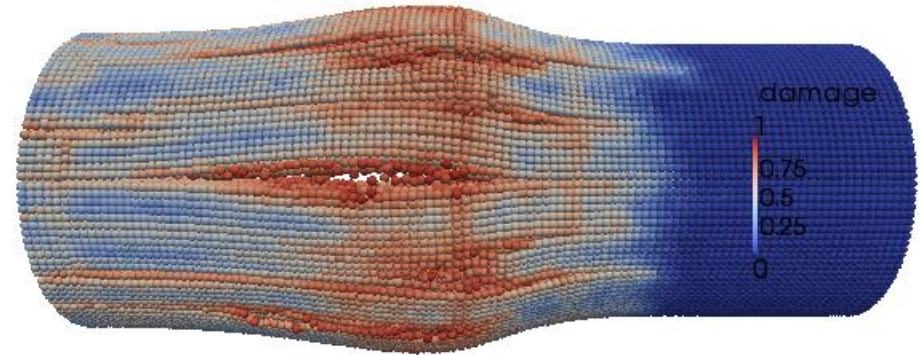
- Classical FEM
- Johnson-Cook constitutive model
- 53,214 hexahedron elements

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 <i>B</i>	68.9 MPa
Rate Constant <i>C</i>	0.0
Hardening Exponent <i>N</i>	1.0
Thermal Exponent <i>M</i>	1.85
Reference Temperature	70.0 ° F
Melting Temperature	500.0 ° F

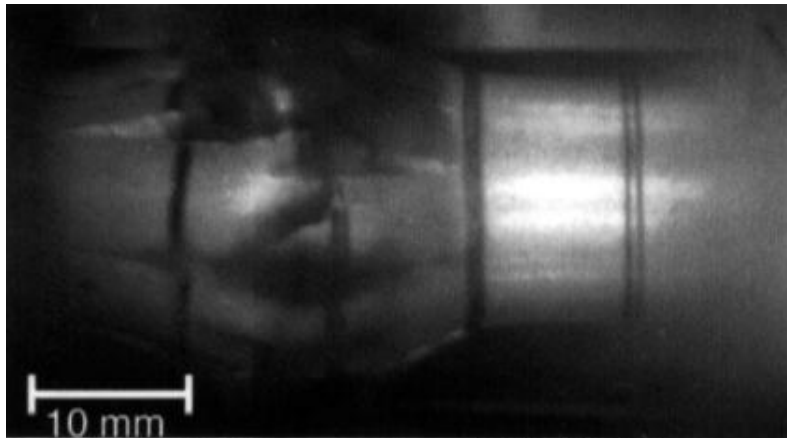
Predicted damage profiles



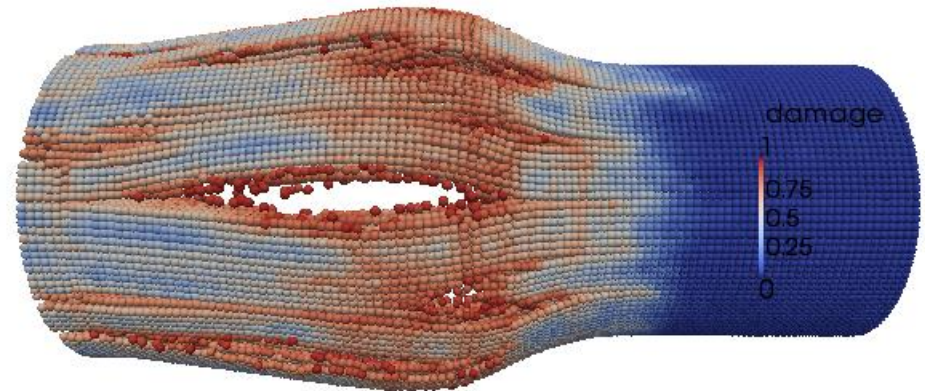
Experimental image at 15.4
microseconds [Vogler et. al]



Simulation at 15.4 microseconds



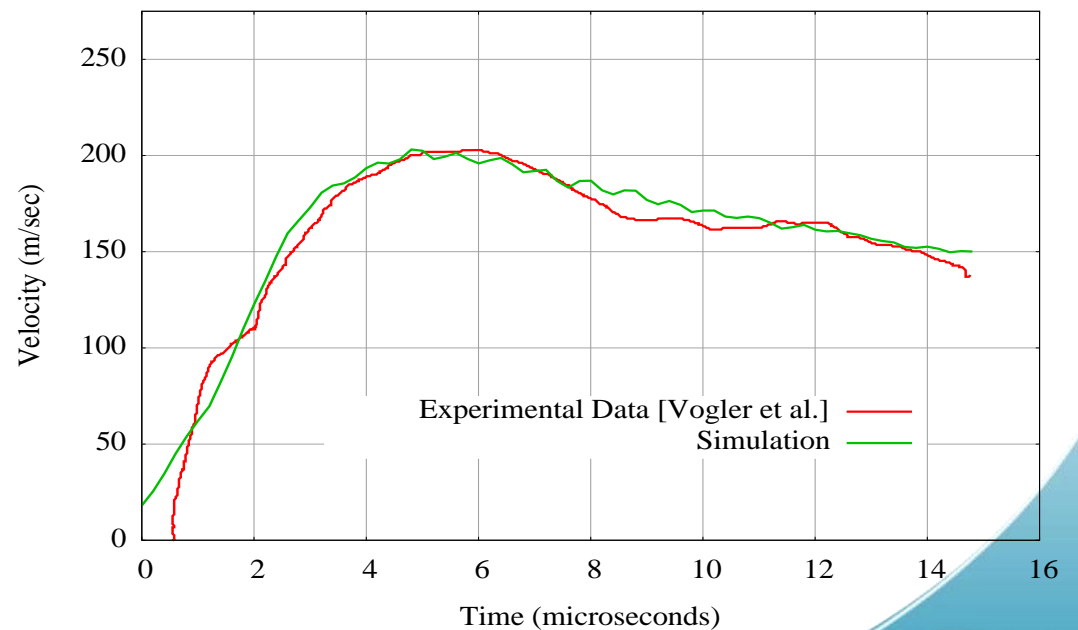
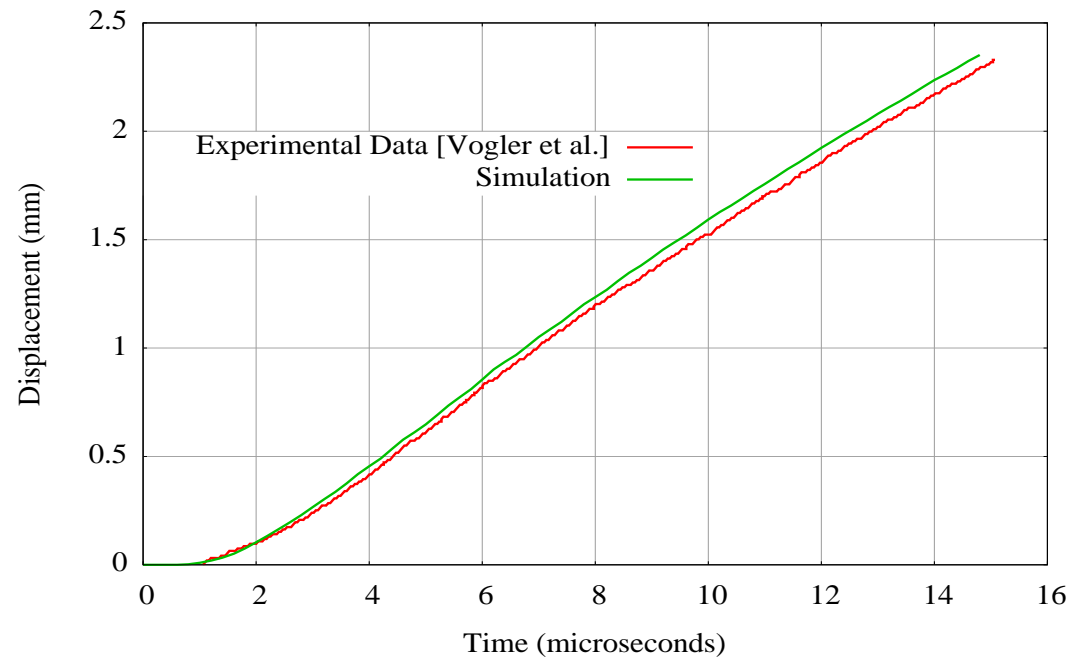
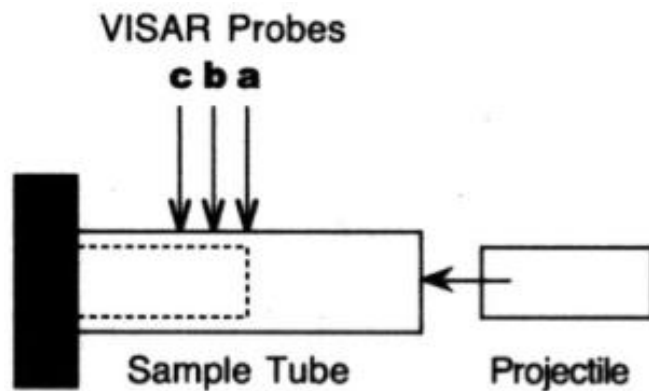
Experimental image at 23.4
microseconds [Vogler et. al]



Simulation at 23.4 microseconds

Predicted displacement and velocity on tube surface

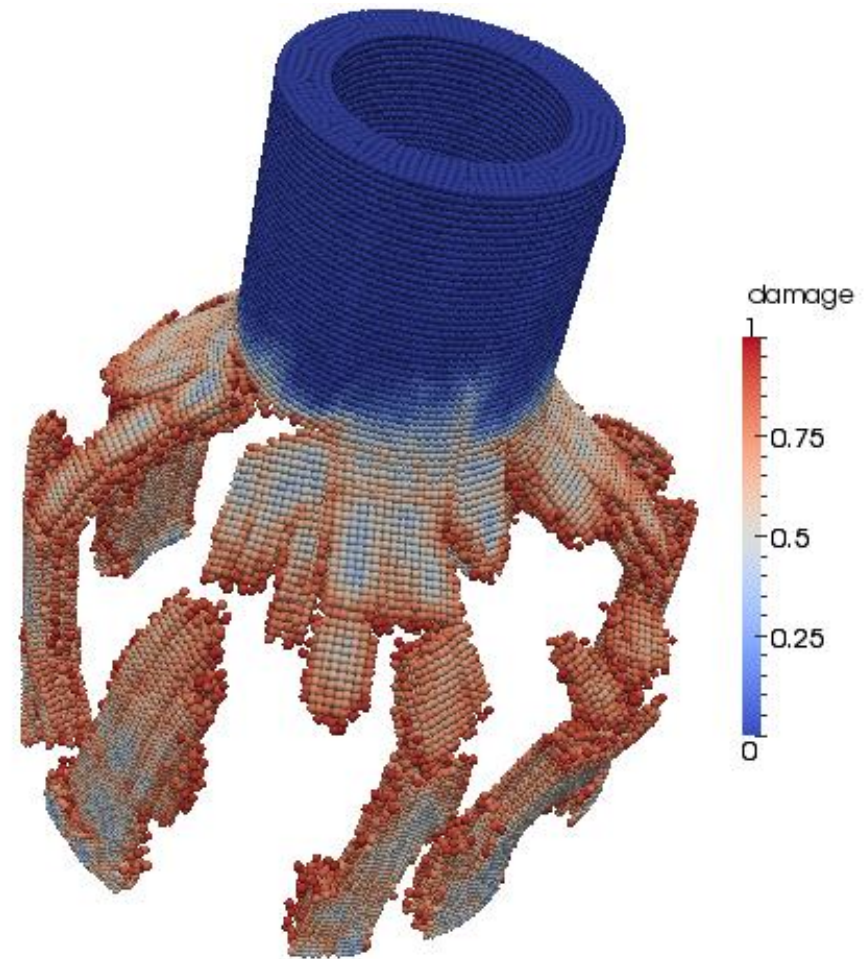
Displacement and velocity
on tube surface
at probe position A



Fragmentation pattern

Qualitative Comparison of Fragmentation Results

- 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

I. Peridynamics

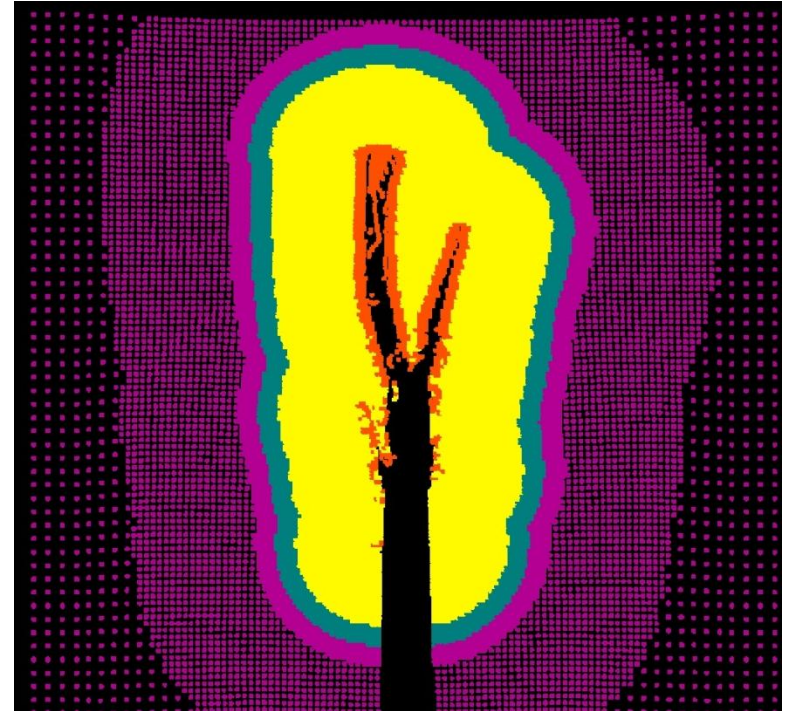
II. Numerics and Codes

III. Applications

IV. Conclusions

Summary

- Peridynamics Overview
 - The basics
 - Relationship to classical theory
 - Material modeling
 - Damage modeling
 - Analytical results
- Numerics and Codes
 - SierraMechanics
 - Peridigm
 - LAMMPS
 - EMU
- Applications
 - Shockwave ejects
 - Fragmenting cylinder



Extra Slides

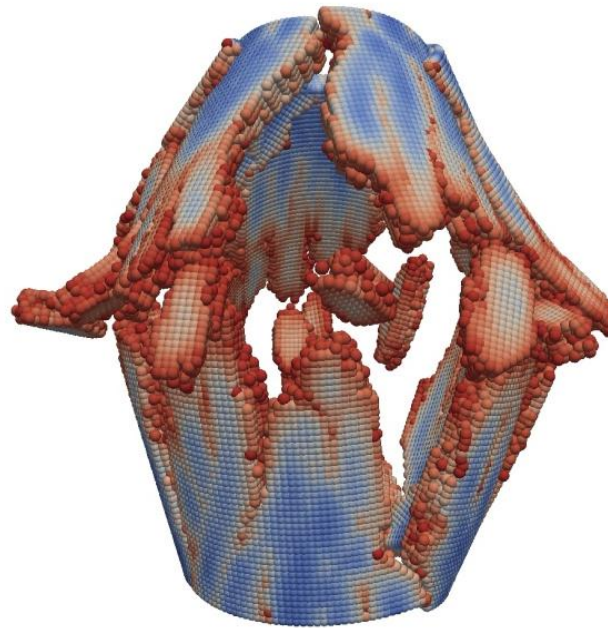
Demonstration Computation: Fragmenting Cylinder

PERIDYNAMIC SIMULATION OF FRAGMENTING CYLINDER

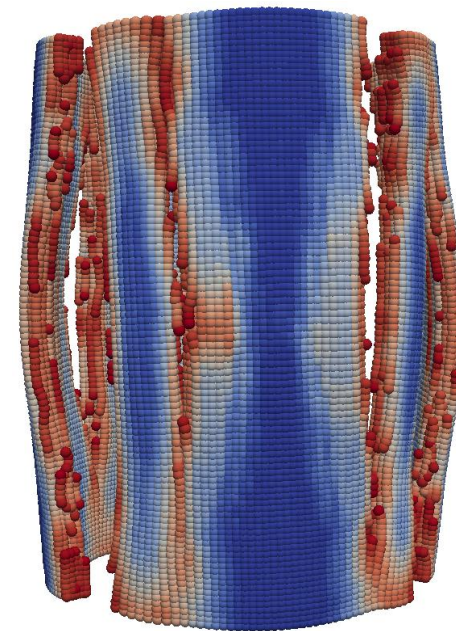
- Motivated by tube fragmentation experiments of Winter (1979), Vogler (2003)*



Before



After
(brittle model)



After
(plastic model)

*Color
indicates
damage*



Capability demonstration: Composite failure

FAILURE IN FIBER-REINFORCED COMPOSITE LAMINATE

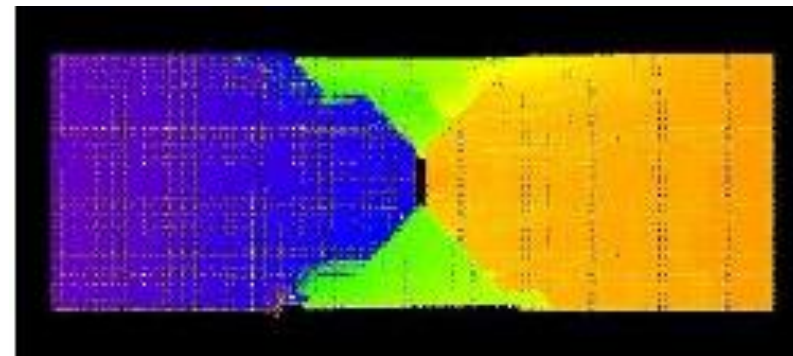
- Splitting and fracture mode changes in fiber-reinforced composites*
- Fiber orientation between plies strongly influences crack growth



Typical crack growth in notched laminate (photo courtesy Boeing)

Reproduce in peridynamic simulation by controlling bond strength orientation

45° angle of fibers within ply dictate failure direction

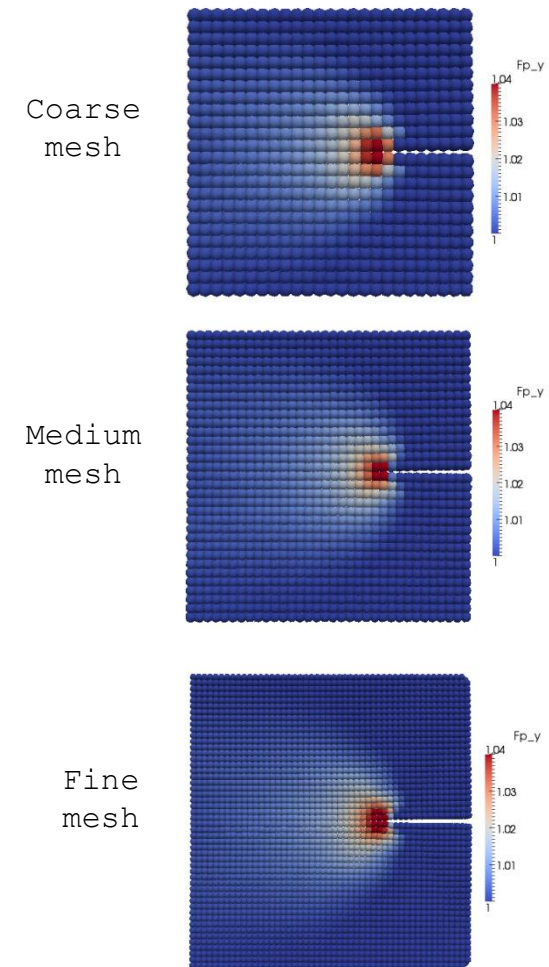
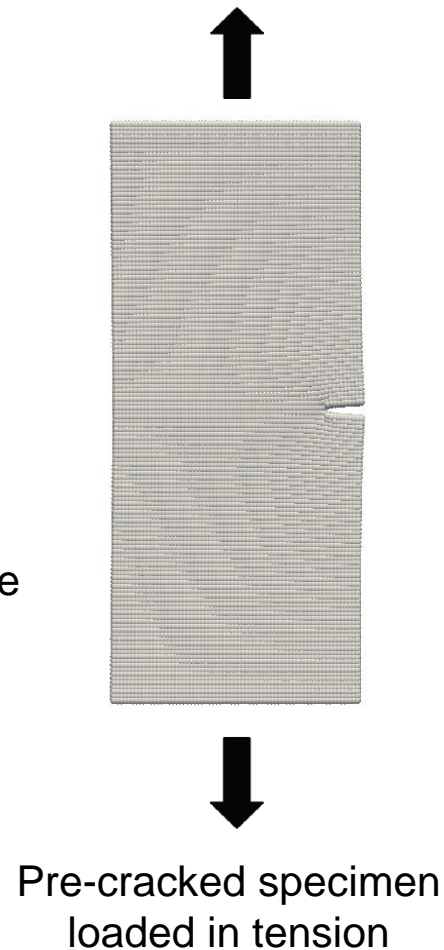


Peridynamic Model

* 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.

Capability demonstration: Mesh independent plastic zone

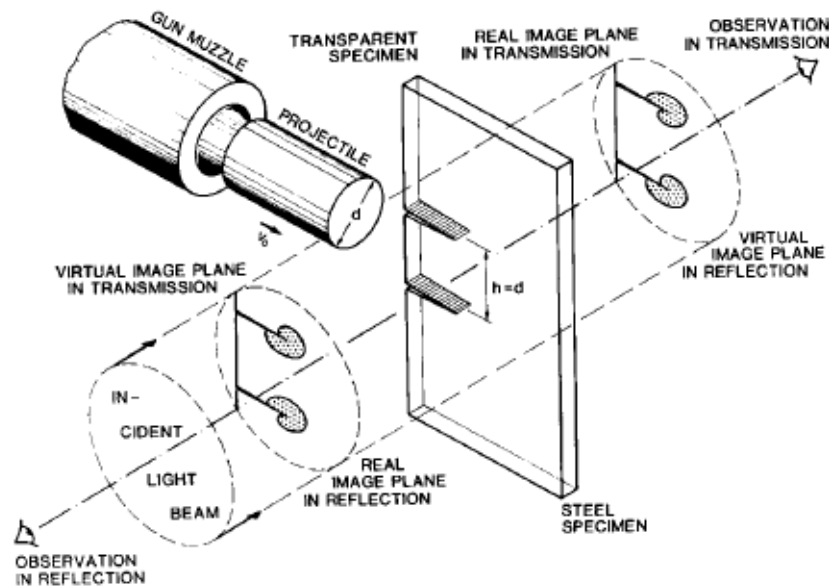
- Peridynamic horizon introduces length scale independent of mesh size
- Localization in peridynamics function of horizon (parameter of continuum model)
- Localization in classical FEM function of mesh (parameter of discrete model)
- Ongoing work: Investigation of convergence rates
- Example: Mesh independent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



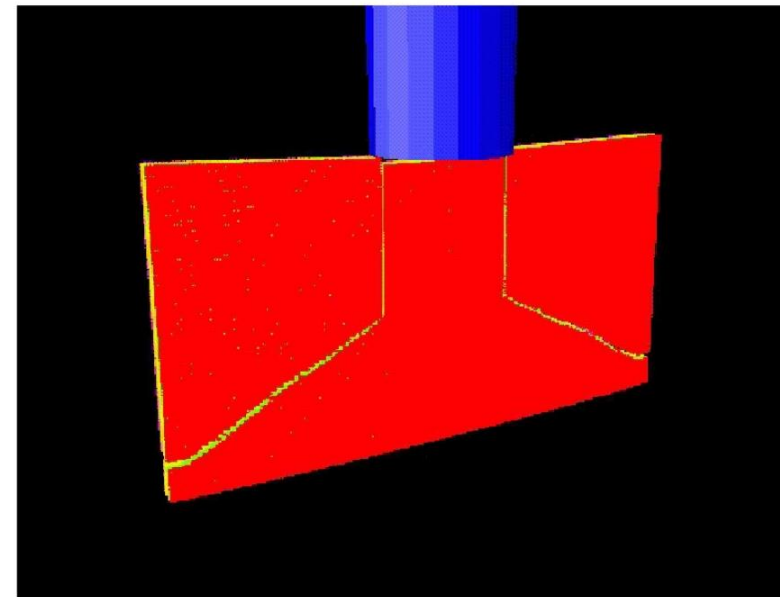
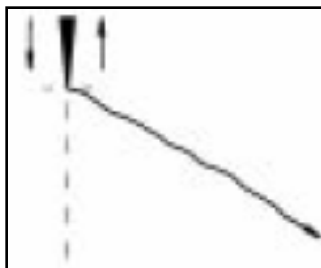
Capability demonstration: Kalthoff-Winkler experiment

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