

# Peridynamics for Material Failure

NECDC 2012  
Lawrence Livermore National Laboratory  
October 22-26, 2012

Multiphysics Simulation Technology  
Org. 1444  
Sandia National Laboratories



Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



# 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

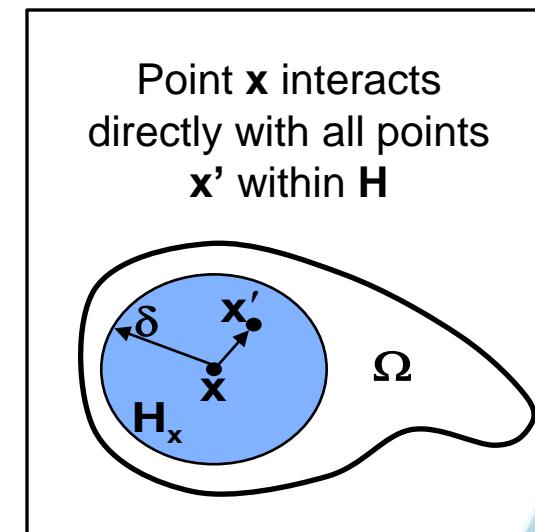
$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \nabla \cdot \boldsymbol{\sigma}(\nabla \mathbf{u}(\mathbf{x}, t)) + \mathbf{b}(\mathbf{x}, t)$$

## HOW DOES PERIDYNAMICS WORK?

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

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

- 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.

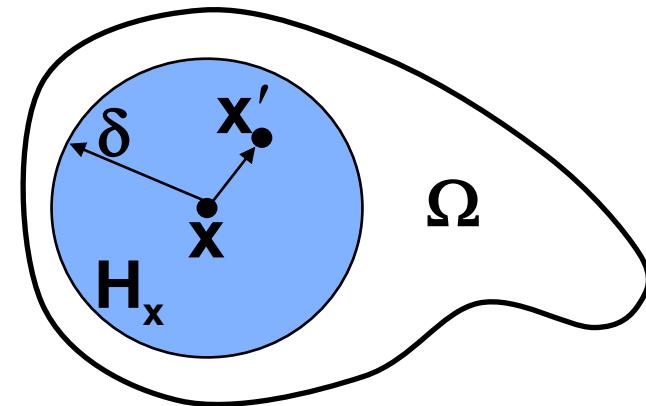
4 Silling, S.A. and Lehoucq, R. B. Peridynamic Theory of Solid Mechanics.

*Advances in Applied Mechanics* 44:73-168, 2010.

# Peridynamics: The Basics

## HORIZON AND FAMILY

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



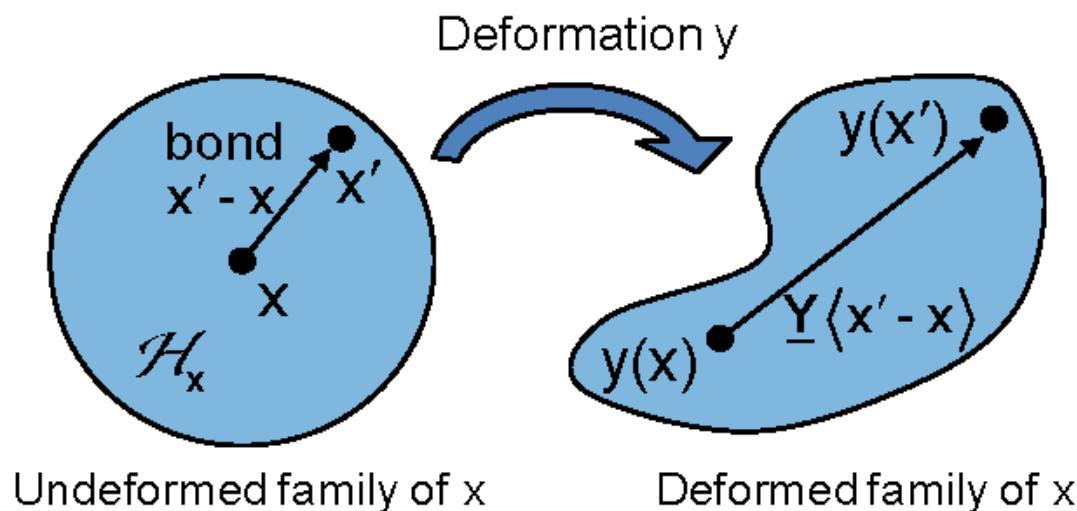
## BONDS AND BOND FORCES

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

## DEFORMATION STATE

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

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



# Peridynamics: The Basics

## BONDS AND STATES

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

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

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

## PERIDYNAMICS VS. CLASSICAL THEORY

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

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

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

# 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)

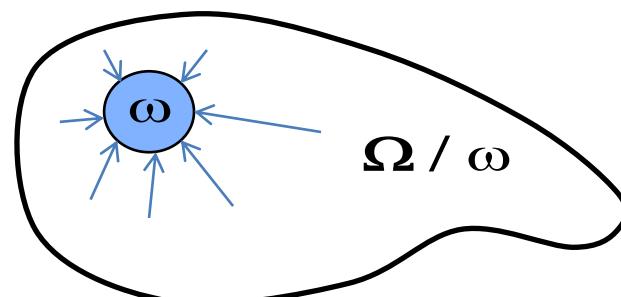
## EXAMPLE: CONSERVATION OF MOMENTUM

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

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

- No self-interaction:

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



# Peridynamics: The Basics

## ENERGY BALANCE

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

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

where

- $\varepsilon$  = 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):

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

where

- $\theta$  = absolute temperature
- $\eta$  = entropy density

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

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

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,  $\mu$  is shear modulus

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

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

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

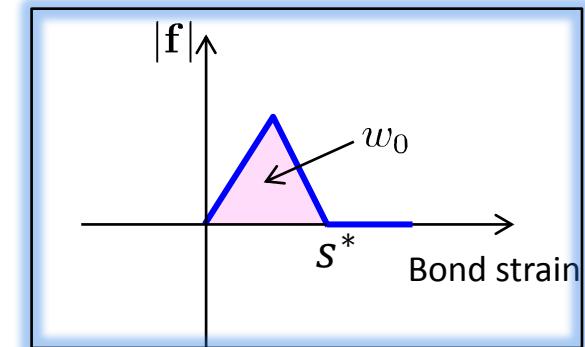
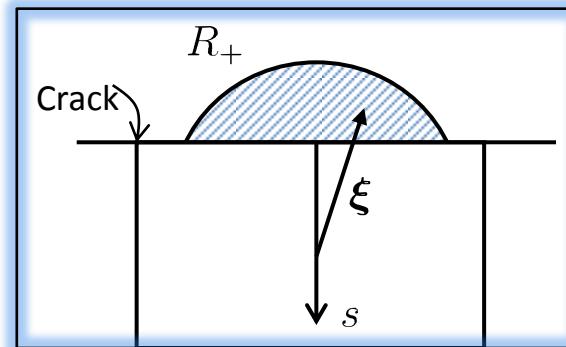
$$\varphi_{\langle x' - x \rangle} = D(\underline{Y}, \dot{\underline{Y}}, \dots)$$

- 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  $\xi$  is  $w_0(\xi)$ , 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  $s^*$  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

11 \*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.

# Analytical Results

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

<sup>a</sup> 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.

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

<sup>c</sup> 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

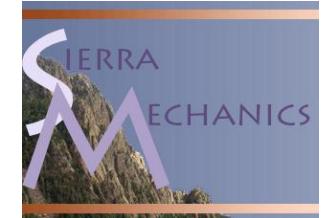
# IV. Conclusions

# 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](http://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](http://lammps.sandia.gov))
- More info & user guide: [www.sandia.gov/~mlparks](http://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](http://www.sandia.gov/emu/emu.htm))
- Research 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

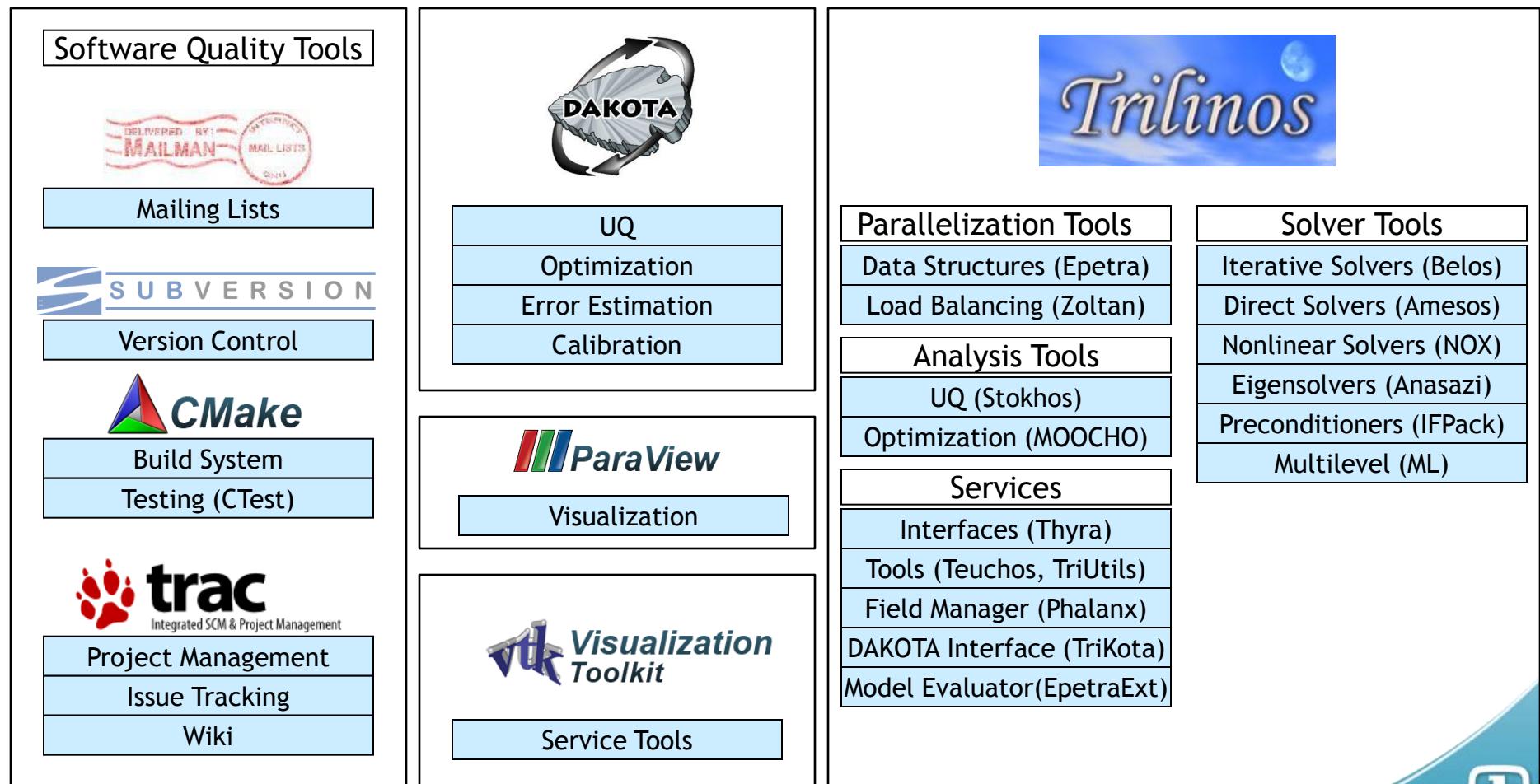
$$\bar{\mathbf{F}} = \left( \sum_{i=0}^N \underline{\omega}_i \underline{\mathbf{Y}}_i \otimes \underline{\mathbf{X}}_i \Delta V_{\mathbf{x}_i} \right) \mathbf{K}^{-1} \quad \mathbf{K} = \sum_{i=0}^N \underline{\omega}_i \underline{\mathbf{X}}_i \otimes \underline{\mathbf{X}}_i \Delta V_{\mathbf{x}_i}$$

- 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)

- 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](http://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](http://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
- Largest peridynamic simulations in history



*Dawn at LLNL*

## 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

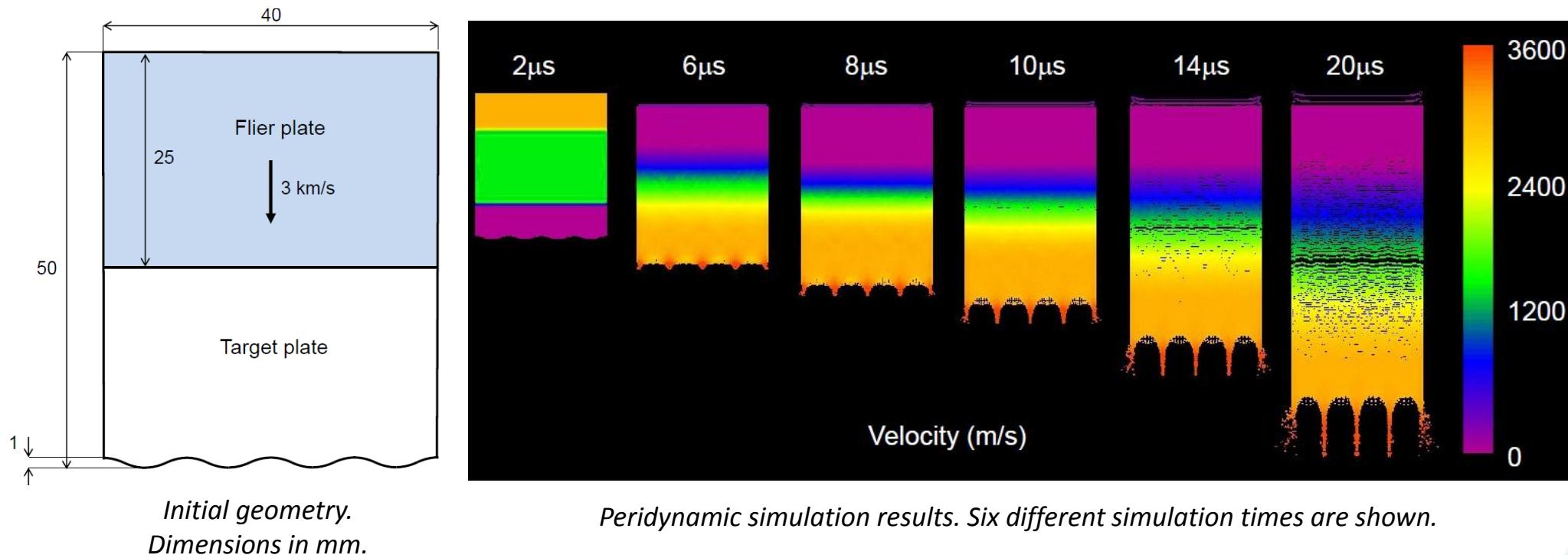
# III. Applications

# 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

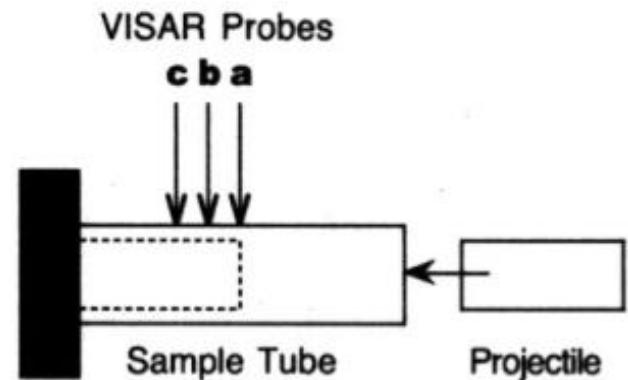


- Computed shock velocity is 7.140 km/s; Expected value is 7.230 km/s.
- Computed jet tip velocity is 4.0 km/s; Experimentally measured value is 3.7 km/s.

# 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

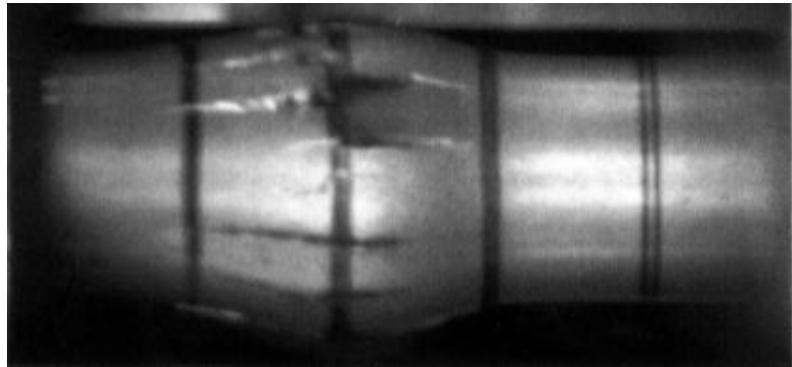
Parameter	Value
Density	7.87 g/cm <sup>3</sup>
Young's Modulus	194.4 GPa
Poisson's Ratio	0.3
Yield Stress	1.72 GPa
Hardening Modulus	1.94 GPa
Critical Stretch	0.02

## Lexan Projectile/Plug

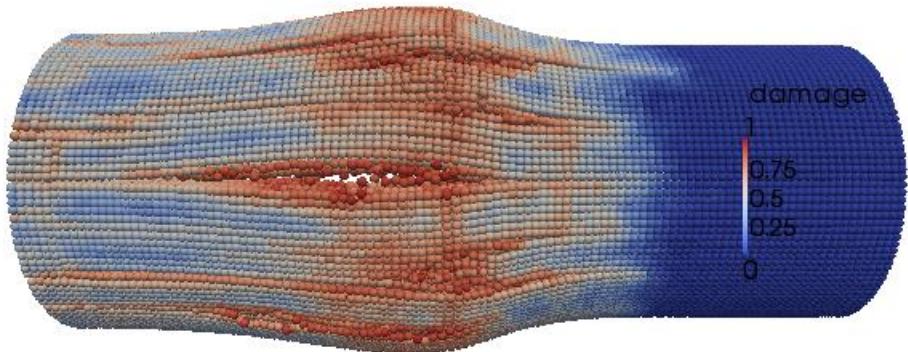
- Classical FEM
- Johnson-Cook constitutive model
- 53,214 hexahedron elements

Parameter	Value
Density	1.19 g/cm <sup>3</sup>
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

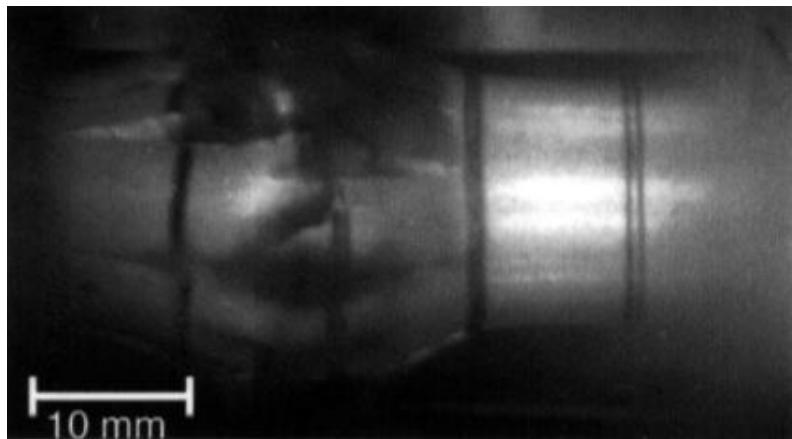
# Predicted damage profiles



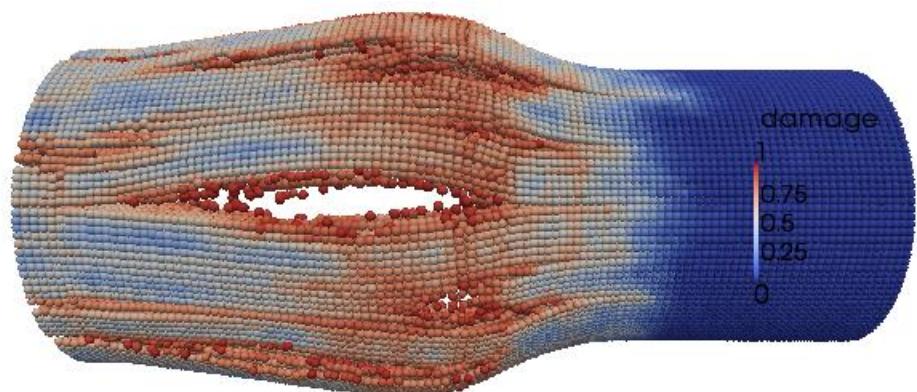
Experimental image at 15.4  
microseconds [Vogler et. al]



Simulation at 15.4 microseconds



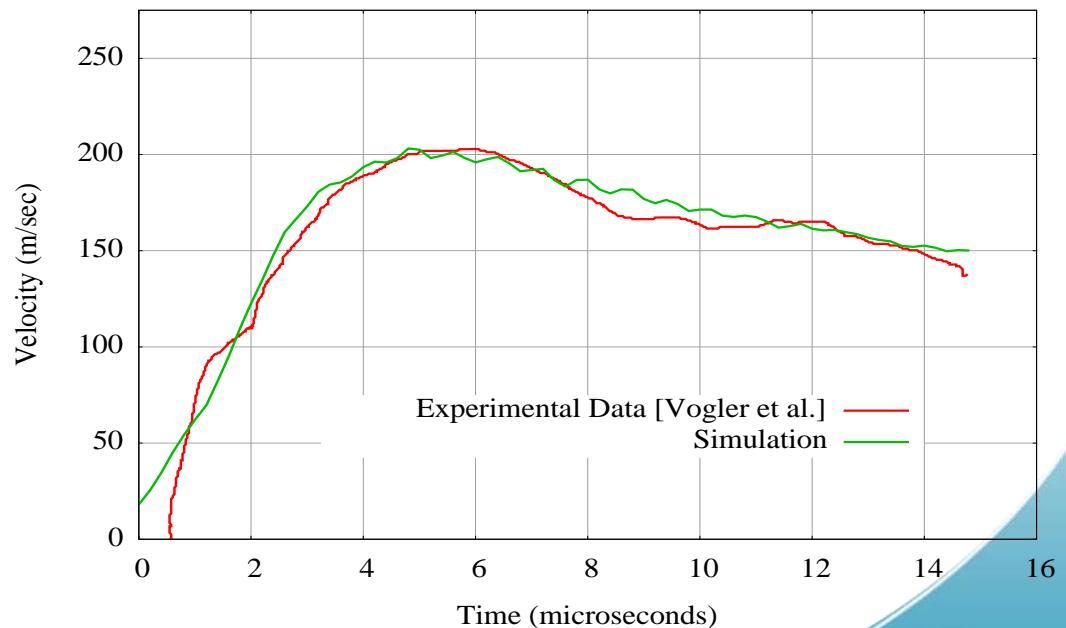
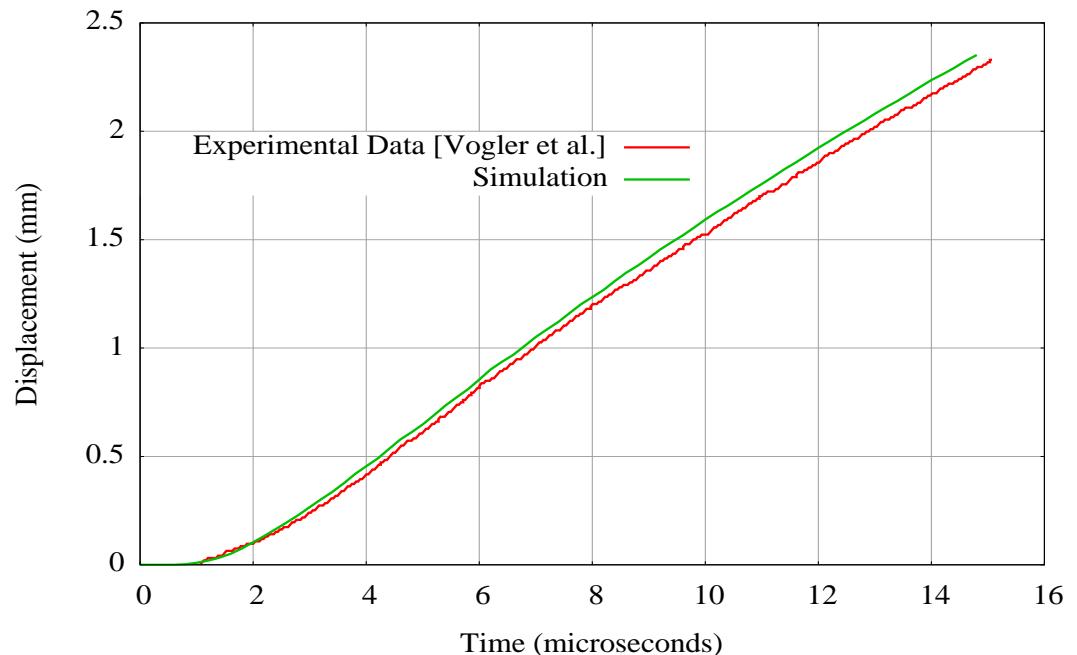
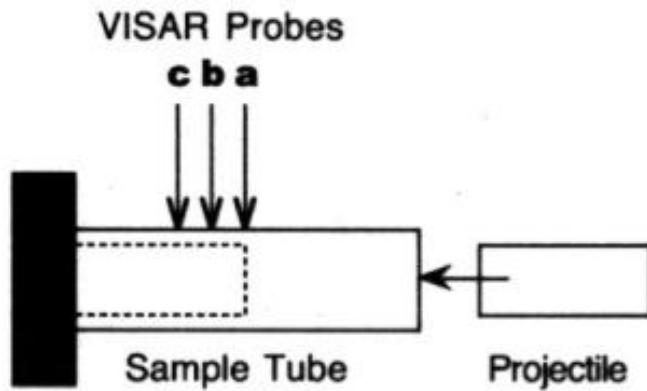
Experimental image at 23.4  
microseconds [Vogler et. al]



Simulation at 23.4 microseconds

# Predicted displacement and velocity on tube surface

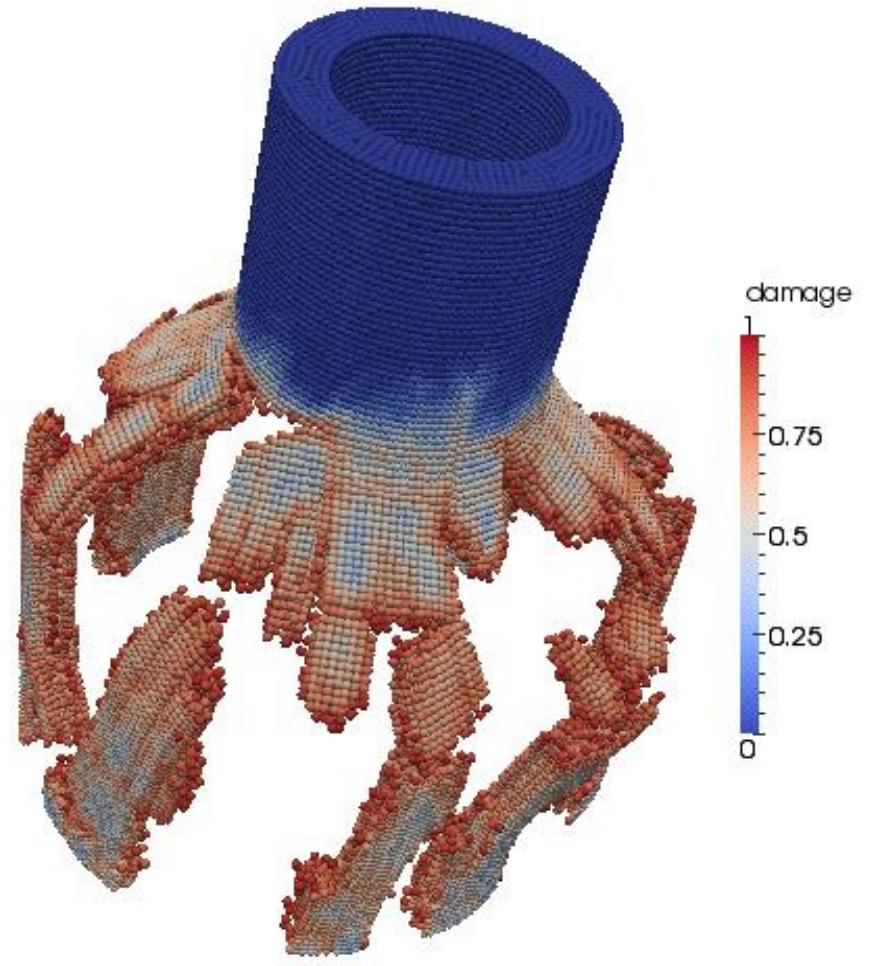
Displacement and velocity  
on tube surface  
at probe position A



# 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

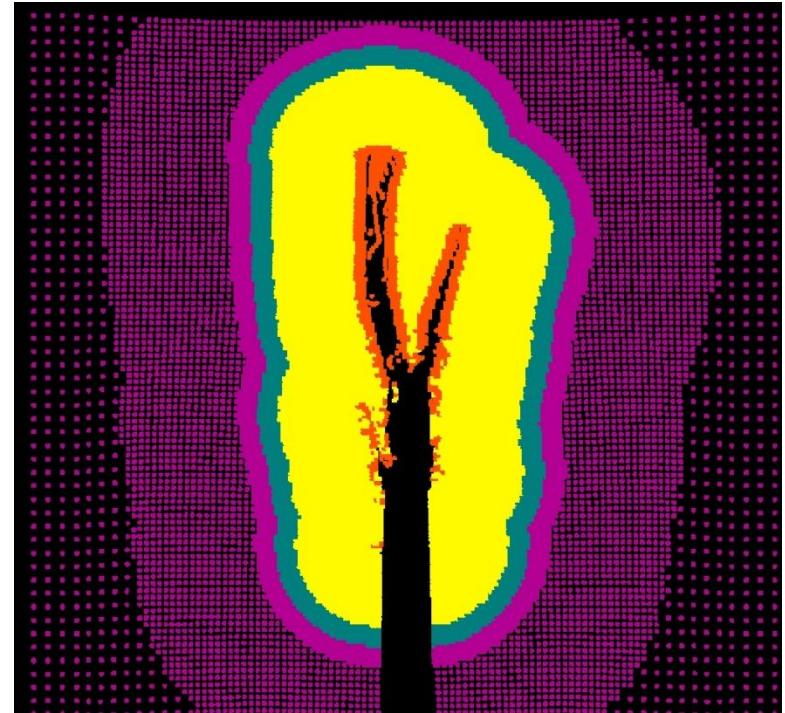
# II. Numerics and Codes

# 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

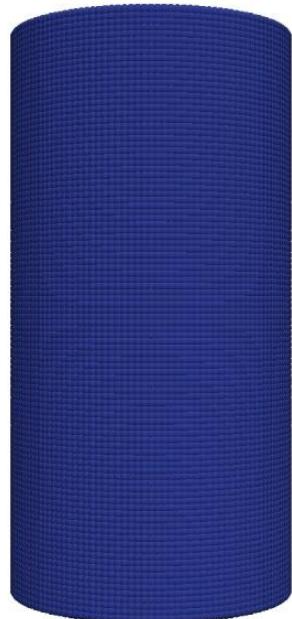


# Extra Slides

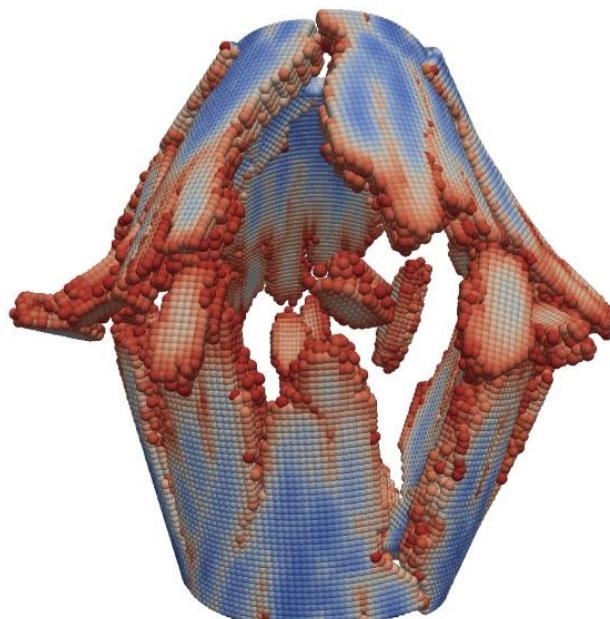
# Demonstration Computation: Fragmenting Cylinder

## 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

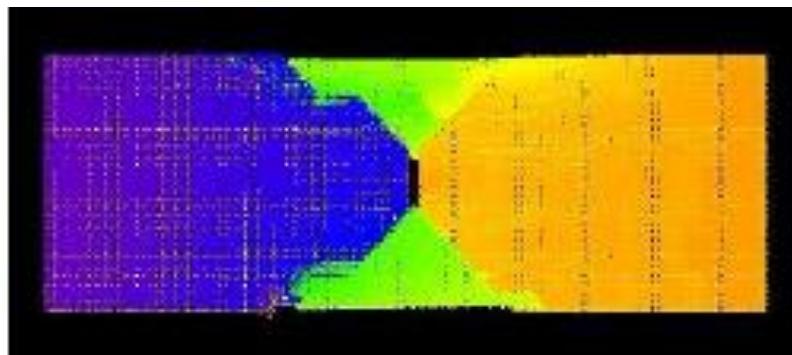
- Splitting and fracture mode changes in fiber-reinforced composites\*
- Fiber orientation between plies strongly influences crack growth



*45° angle of fibers within ply  
dictate failure direction*

Typical crack growth in notched laminate (photo courtesy Boeing)

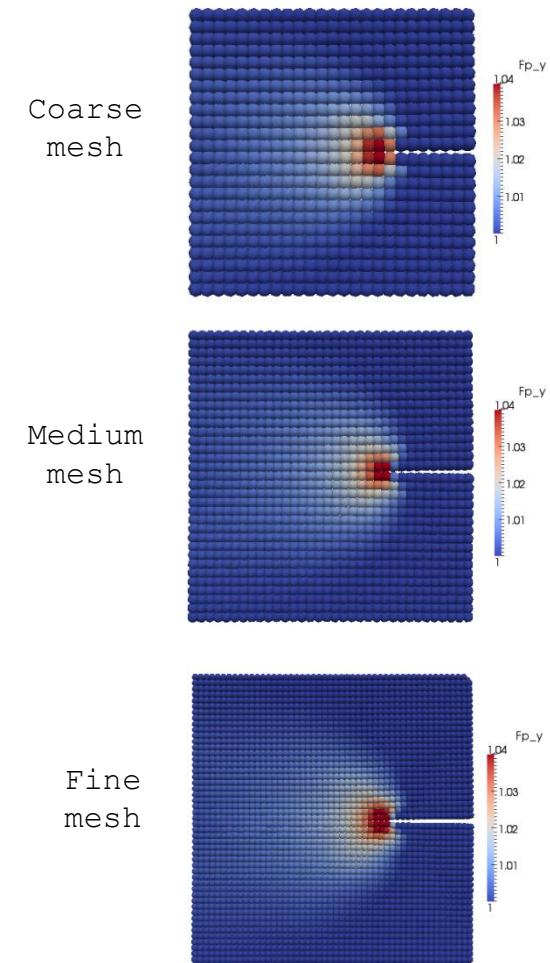
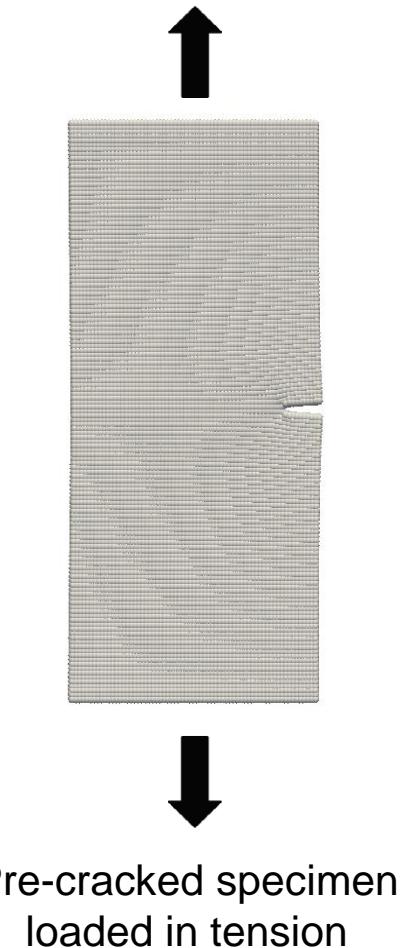
*Reproduce in peridynamic  
simulation by controlling bond  
strength orientation*



Peridynamic Model

# 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

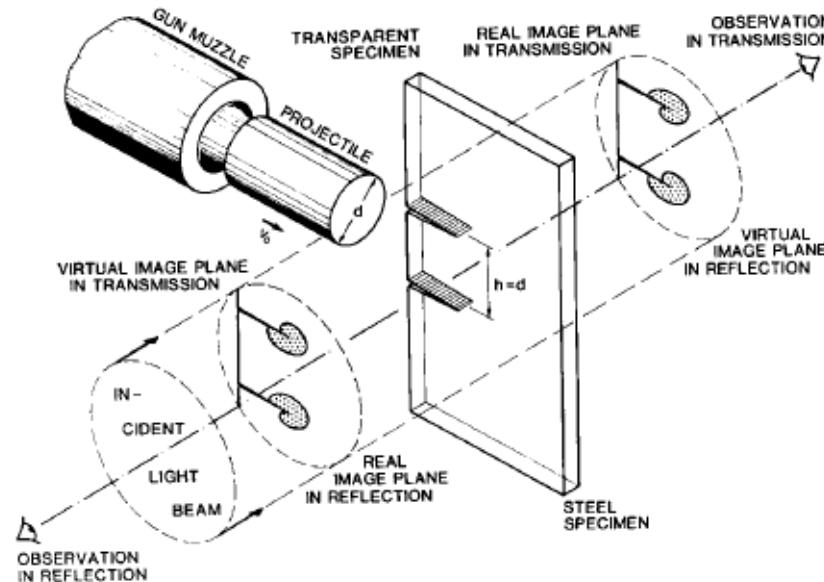


Component of plastic deformation gradient in loading direction

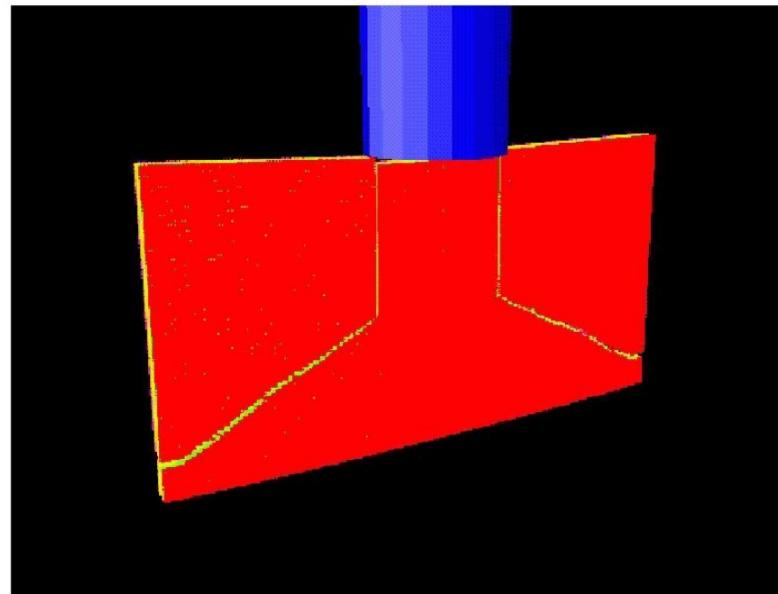
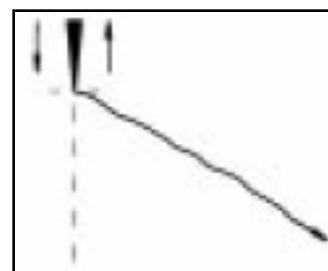
# Capability demonstration: Kalthoff-Winkler experiment

## 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  $70^\circ$  angle
- *Peridynamic model reproduces  $70^\circ$  crack angle\**



Experimental  
Results



Peridynamic Model