SAND2011-2602P

Recent Advancements in Peridynamics with Applications to Failure Modeling

Sandia Failure Modeling Workshop

December 2010

David Littlewood

Multiphysics Simulation Technologies (Org. 1444)

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Outline

- Mercifully brief review of peridynamics
- Recent advancements in peridynamic theory
- Implementation efforts
- Peridynamics in action
- Strengths and weaknesses
- Current and future work (timeline)

What is Peridynamics?

- Peridynamics is a *nonlocal* extension of continuum mechanics
- Balance of linear momentum is based on an *integral equation*
- Capable of modeling bodies in which discontinuities occur spontaneously
- Well suited for *fracture modeling*

S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48(1):175-209, 2000.

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

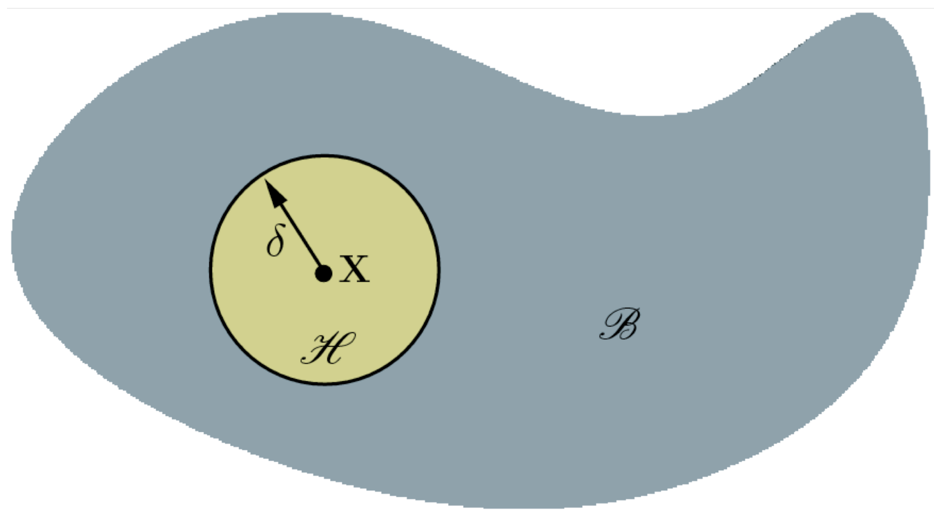
S.A. Silling and R.B. Lehoucq. Peridynamic theory of solid mechanics. SAND Report 2010-1233J, Sandia National Laboratories, Albuquerque, NM, 2010.

Peridynamics is a Nonlocal Formulation of Continuum Mechanics

Balance of linear momentum formulated as an integral equation

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}' - \mathbf{x} \right\rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\left\langle \mathbf{x} - \mathbf{x}' \right\rangle \right\} \, \mathrm{d}V_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

$\mathbf{X}$	Point in body $\mathscr{B}$
δ	Horizon of $\mathbf{X}$
$\mathscr{H}$	Family of $\mathbf{X}$

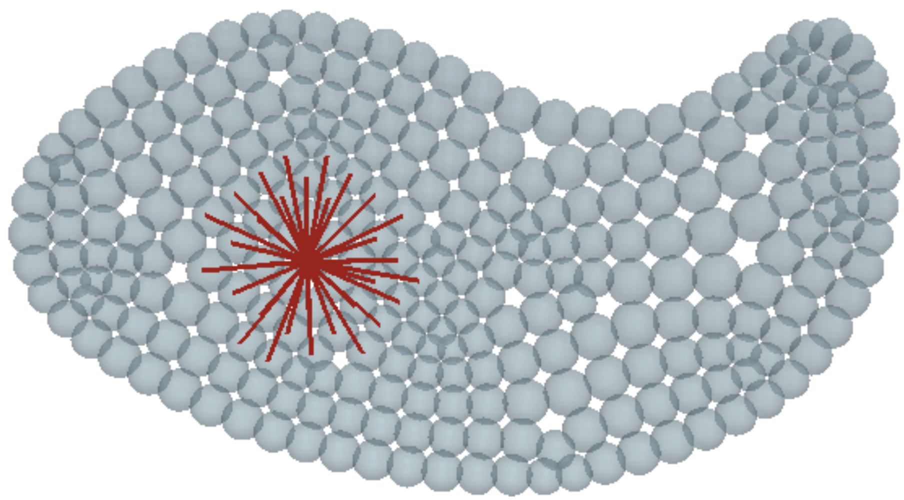


Discretization of a Peridynamic Body

Body may be represented with a finite number of sphere elements

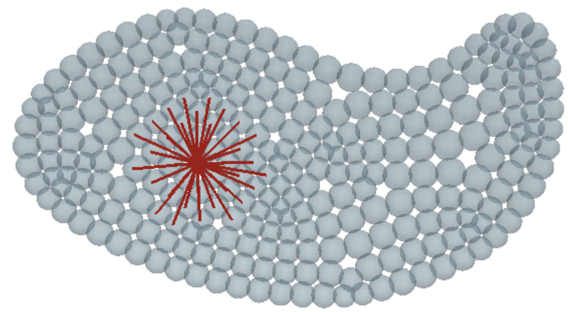
$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}'_i - \mathbf{x} \right\rangle - \underline{\mathbf{T}}'[\mathbf{x}'_i,t]\left\langle \mathbf{x} - \mathbf{x}'_i \right\rangle \right\} \Delta V_{\mathbf{x}'_i} + \mathbf{b}(\mathbf{x},t)$$

- Each element interacts with all elements within its neighborhood
- A *bond* connects any two elements that interact directly
- Pairwise forces determined by a force state, $\underline{\mathbf{T}}[\mathbf{x},t]$, acting on a bond, $\langle \mathbf{x}'_i - \mathbf{x} \rangle$
- Material failure occurs through the accumulation of broken bonds



Constitutive Laws in Peridynamics

$$\underbrace{\underline{\mathbf{T}}[\mathbf{x}, t]}_{\text{Force State}} \quad \underbrace{\langle \mathbf{x}_i' - \mathbf{x} \rangle}_{\text{Bond}}$$



- Force states are determined by constitutive laws
- Force states are functions of the deformations of all points within a neighborhood
- Force states act on bonds, resulting in a pairwise force between elements
- Pairwise forces combine to determine the net force on a given element

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Mathematical Theory

- Well-posedeness of the linear peridynamic bond-based equation of motion (and its equilibrium equation)
  - Sufficient conditions on the existence and uniqueness of the solution given a load and initial conditions
  - Discontinuous displacement depends upon the load and constitutive relation
- Developed a nonlocal vector calculus for a general formulation of bond-based and state-based peridynamics
  - Rewrite peridynamic equations in terms of nonlocal div, grad, curl
  - Well-posedeness of the volume constrained peridynamic equation of motion and energy in progress
- Verification now possible (e.g. rates of convergence)

[Lehoucq]

Theoretical Mechanics

- Coleman-Noll restrictions on peridynamic elastic materials so that the second law of thermodynamics is not violated
- Peridynamic principle of virtual work leads to a variational formulation
- Peridynamic first law of thermodynamics available (heat conduction)
- Statistical mechanical basis for the balance of momentum and energy
- Nonlocal advection and diffusion leading to a conservative formulation of balance laws is possible

[Lehoucq]

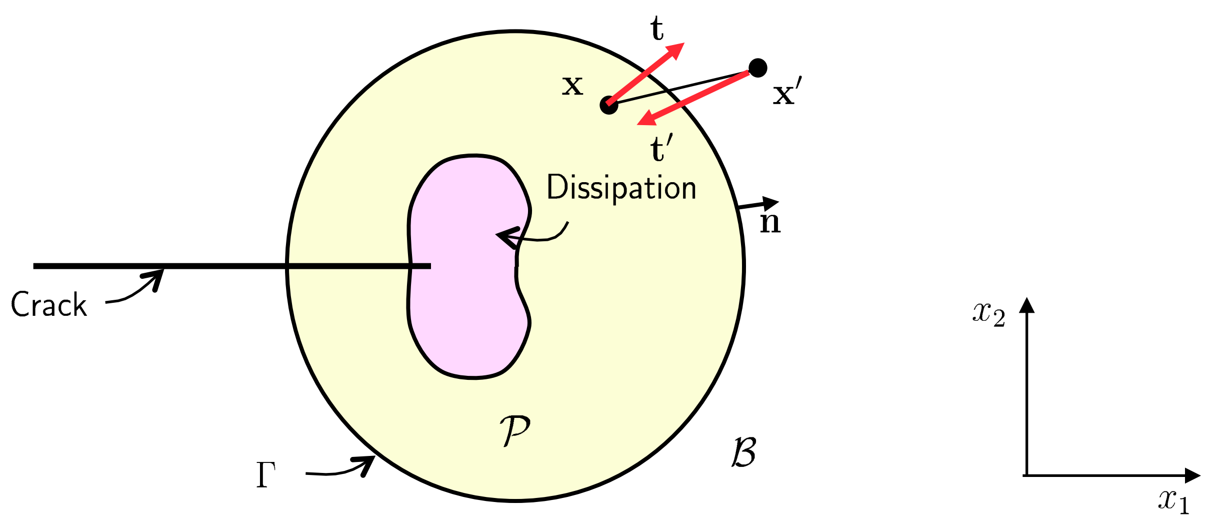
J-Integral for State-Based Peridynamics: Power Term Involves Nonlocal Forces

Nonlocal power term: $\mathbf{t}$, $\mathbf{t}'$ are bond forces

Peridynamic : $$J = \int_\Gamma W n_2 \, ds + h \int_\mathcal{P} \int_{\mathcal{B}\setminus\mathcal{P}} \left(\frac{\partial \mathbf{u}}{\partial x_1} \cdot \mathbf{t}' - \frac{\partial \mathbf{u}'}{\partial x_1} \cdot \mathbf{t} \right) dA' \, dA$$

Compare standard : $$J = \int_\Gamma W n_2 \, ds + \int_\Gamma \boldsymbol{\tau} \cdot \frac{\partial \mathbf{u}}{\partial x_1} \, ds$$

Local power term: $\boldsymbol{\tau}$ is traction



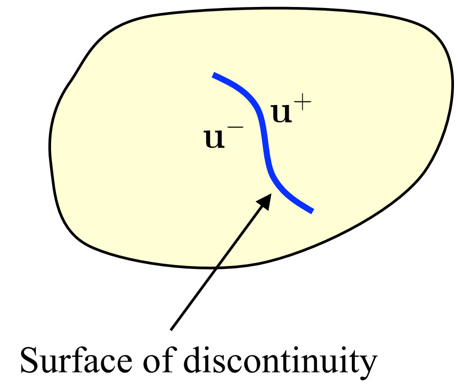
[Silling]

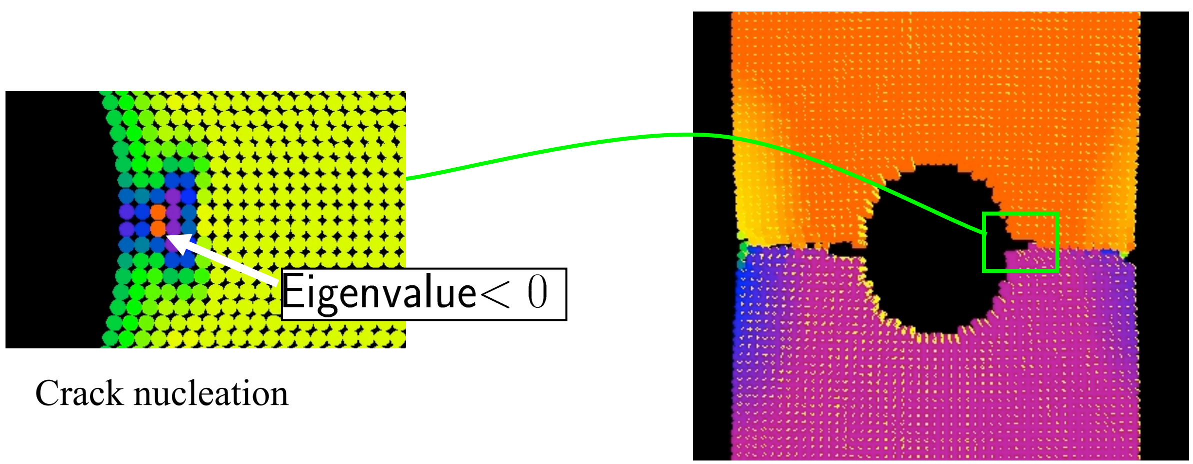
Crack Nucleation Condition

- In peridynamics, cracks nucleate and grow spontaneously.
- What mathematical condition exists when this occurs?
- Newly developed material stability condition answers this question.
- Define a tensor field $\mathbf{P}$ by

$$\mathbf{P}(\mathbf{x}) = \int_{\mathcal{B}} \mathbf{C}(\mathbf{x}, \mathbf{x}')\, dV_{\mathbf{x}'}$$

  where $\mathbf{C}$ is the micromodulus function.
- A discontinuity in displacement can appear if $\mathbf{P}$ has a negative eigenvalue at some $\mathbf{x}$.





Crack nucleation

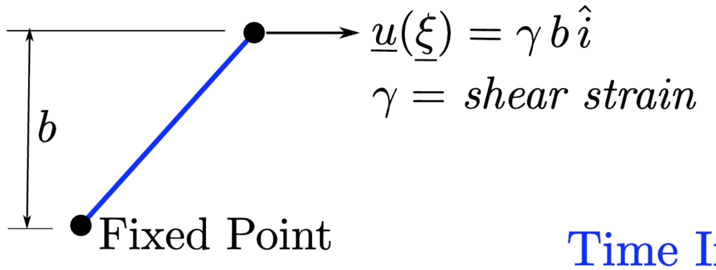
[Silling]

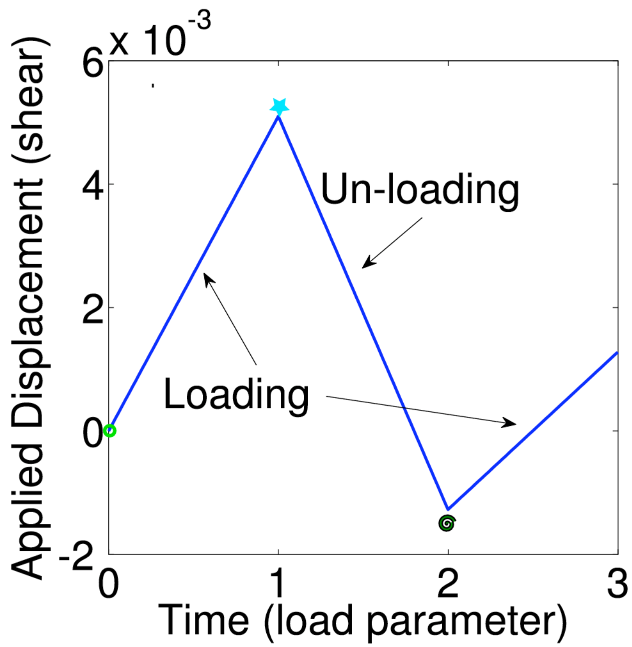
Elastic-Plastic Constitutive Law

- Elastic-plastic material model specific to peridynamics
  - Dilatation based on deformation of all points in neighborhood
  - Individual bonds deform plastically if yield condition is met
- Characteristics of constitutive law:
  - Perfect plasticity, no hardening (possible future work)
  - Flow rule describing rate of plastic deformation
  - Loading / un-loading conditions (Kuhn-Tucker constraints)
  - Shown to satisfy 2^{nd} law of thermodynamics
- SAND report forthcoming

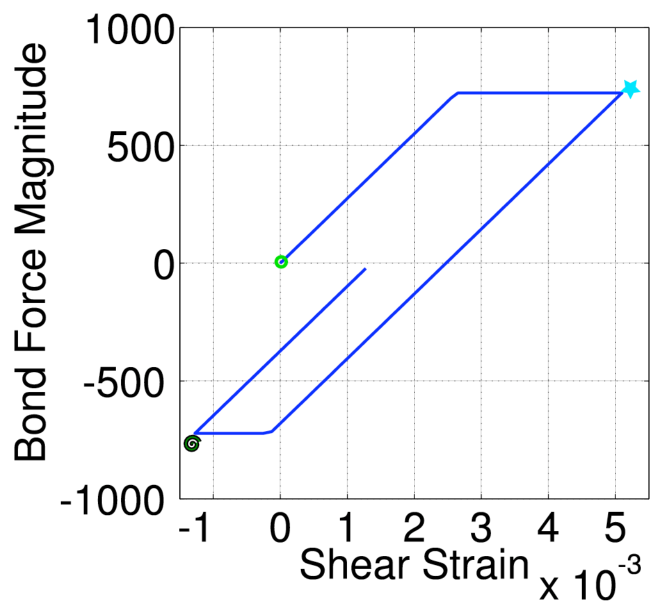
[Mitchell]

Elastic-Plastic Constitutive Law: Behavior of Single Bond





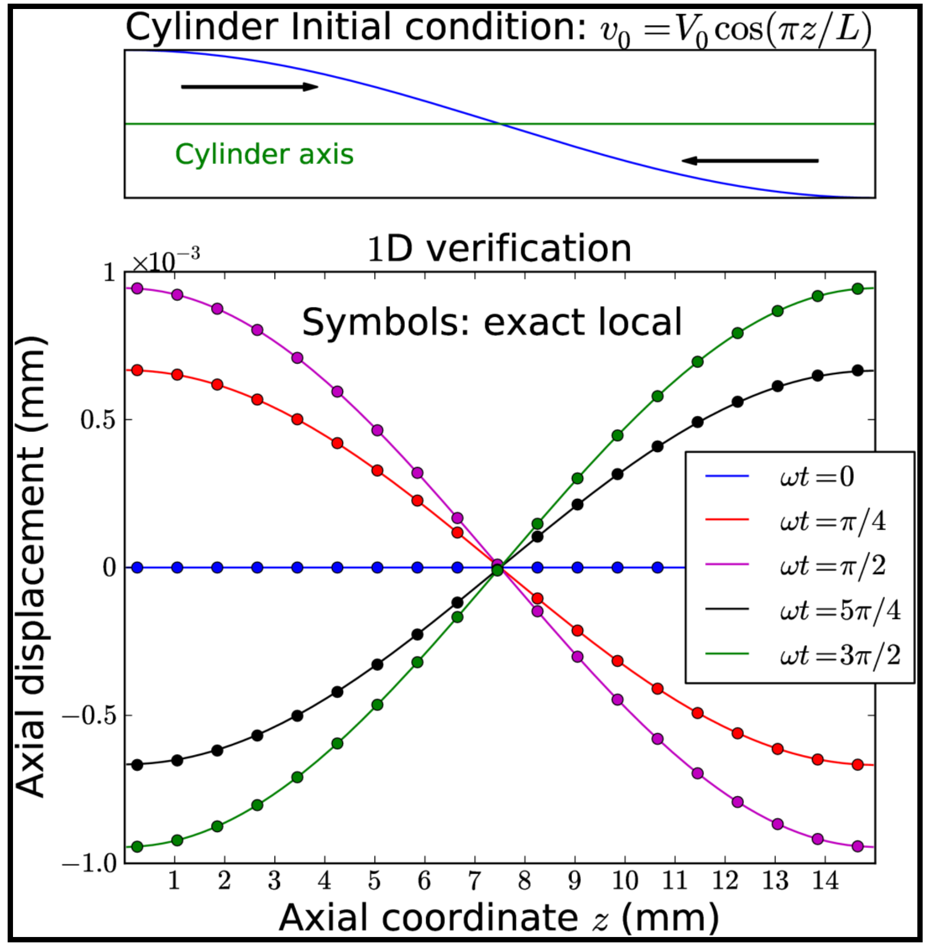
Time Integration of Single Bond



[Mitchell]

Implicit Time Integration for Peridynamics

- Application to implicit dynamics and quasistatics
- Prototype implementation complete
- Analytical Jacobian
- Demonstration of implicit dynamics: Linear vibrations



[Mitchell]

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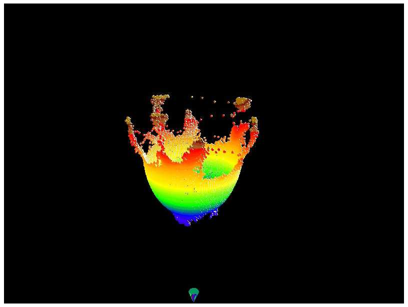
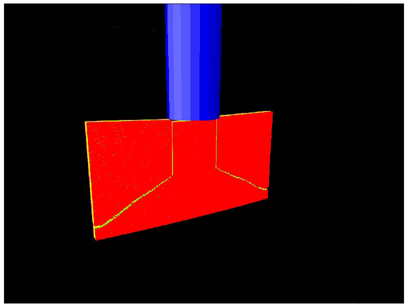
Emu
(Silling, et. al)

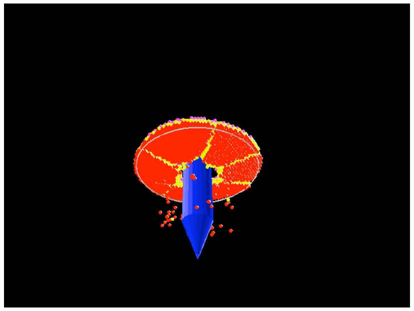
- First code based on the peridynamic theory
- Bond-based and state-based peridynamics
- Invaluable research tool for development of peridynamics
- Applied to wide variety of engineering applications



Balloon popped by sharp fragment



Kalthoff-Winkler experiment



Projectile impacting brittle target

[Silling]

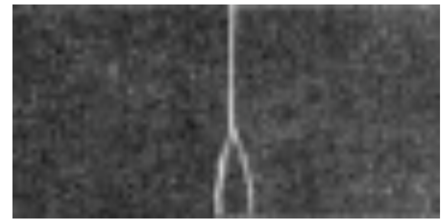
Peridynamics in LAMMPS
(Parks, et al.)

- Peridynamics and molecular dynamics have similar computational structure

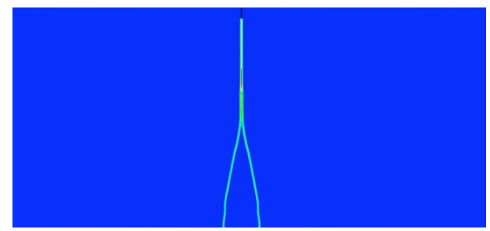
→ Put peridynamics into a MD code

- Leverage portability, fast parallel implementation of LAMMPS
- Open source distribution

Example application:
Notched glass plate under tension



Physical Experiment
[Bowden, et al]



Peridynamics

Weak scaling results

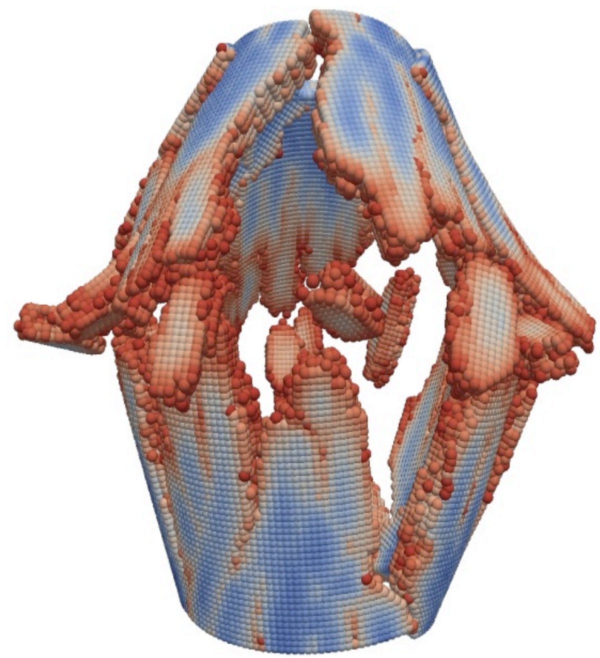
Dawn (LLNL) BG/P system

# 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

[Parks]

Peridigm
(Parks, Littlewood, Mitchell, Silling)

- Next-generation peridynamics code
  - Production quality analysis tool
  - Research platform
- Built on Trilinos components
  - Rich set of software components
  - Suitable for distribution to external collaborators
- Project goals:
  - Multi-physics peridynamics analyses
  - Massively scalable
  - Born-in optimization / UQ



Fragmenting **Brittle Cylinder**
(color indicates damage)

Peridynamics via Agile Components

Peridigm

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)

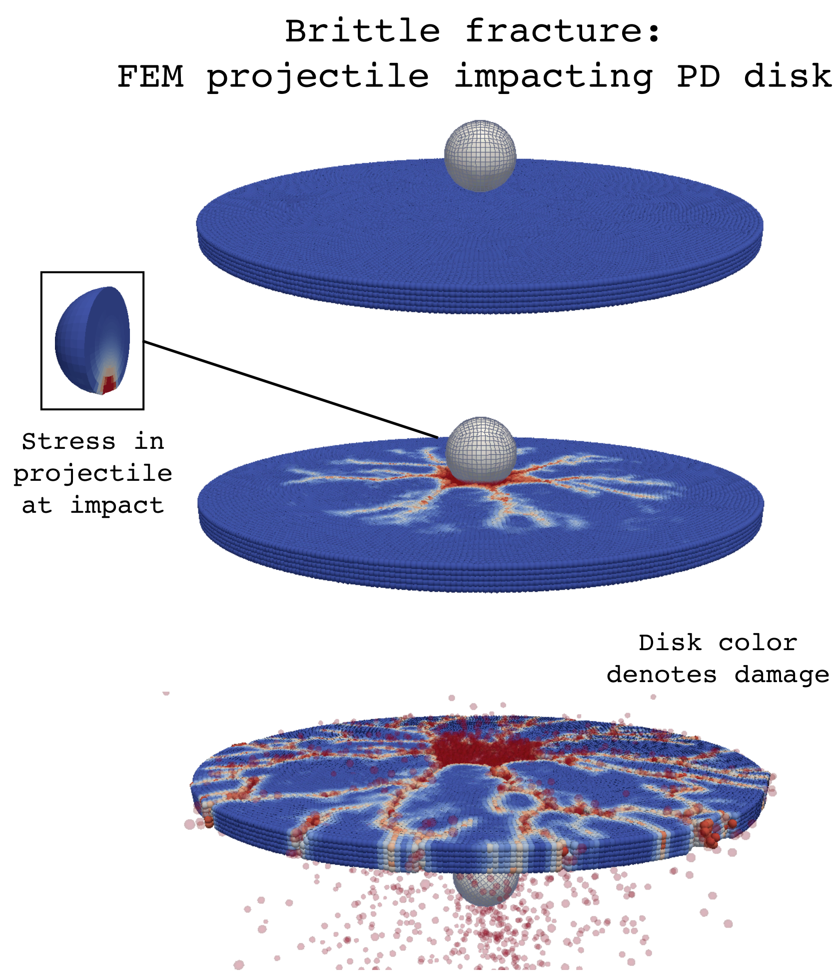
Solver Tools

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

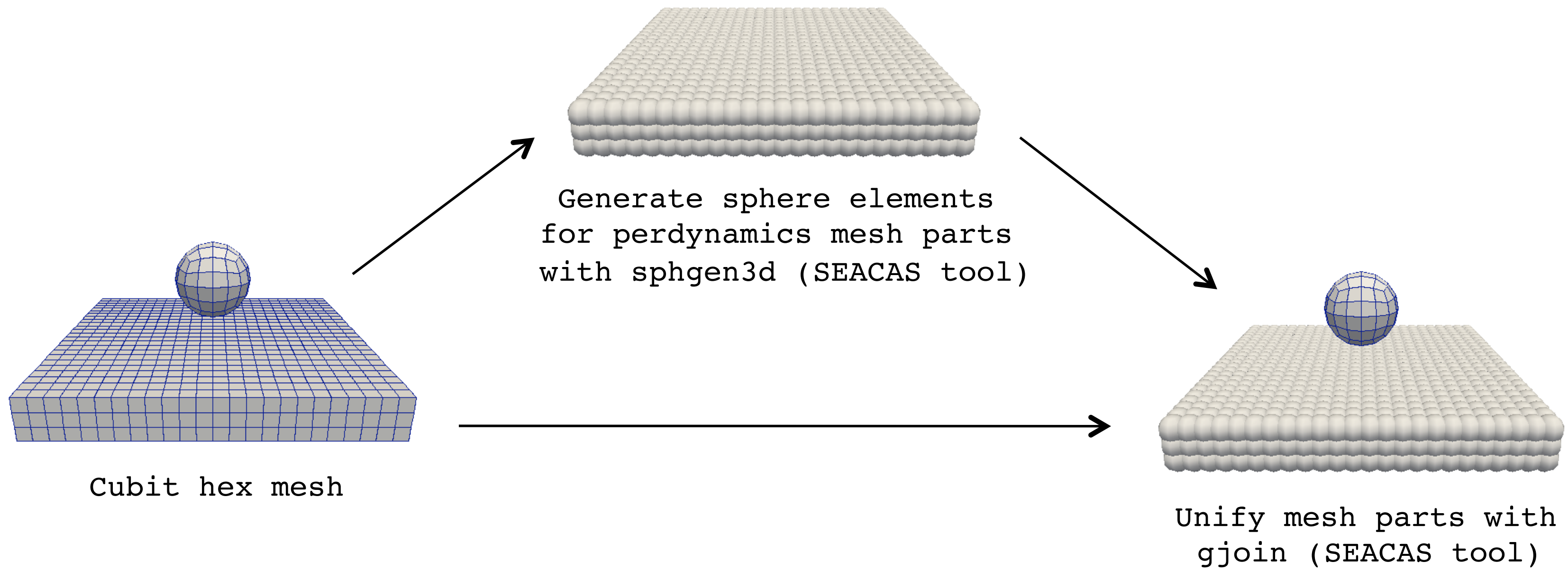
[Parks]

Peridynamics in Sierra/SM (Presto)

- Peridynamics included in 4.18 release of Sierra/SM
- Interface to Sandia's LAME material library
- Interaction of perdynamics and classical FEM via contact
- Collaborative effort between orgs. 1444 and 1542



Workflow: Model Creation and Input Deck




```
BEGIN PERIDYNAMICS SECTION
  MATERIAL MODEL FORMULATION = CLASSICAL|PERIDYNAMICS
  HORIZON = <real>peridynamics_horizon [SCALE BY ELEMENT RADIUS]
  BOND DAMAGE MODEL = NONE|CRITICAL_STRETCH [<real>critical_stretch]
  HOURGLASS STIFFNESS = <real>stiffness
  BOND CUTTING BLOCK = <string list>block_names
  BOND VISUALIZATION = ON|OFF
END PERIDYNAMICS SECTION
```

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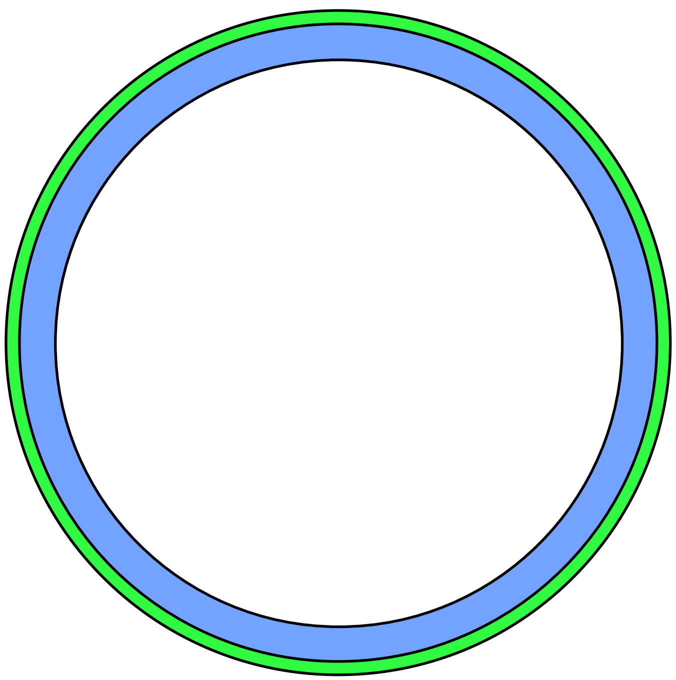
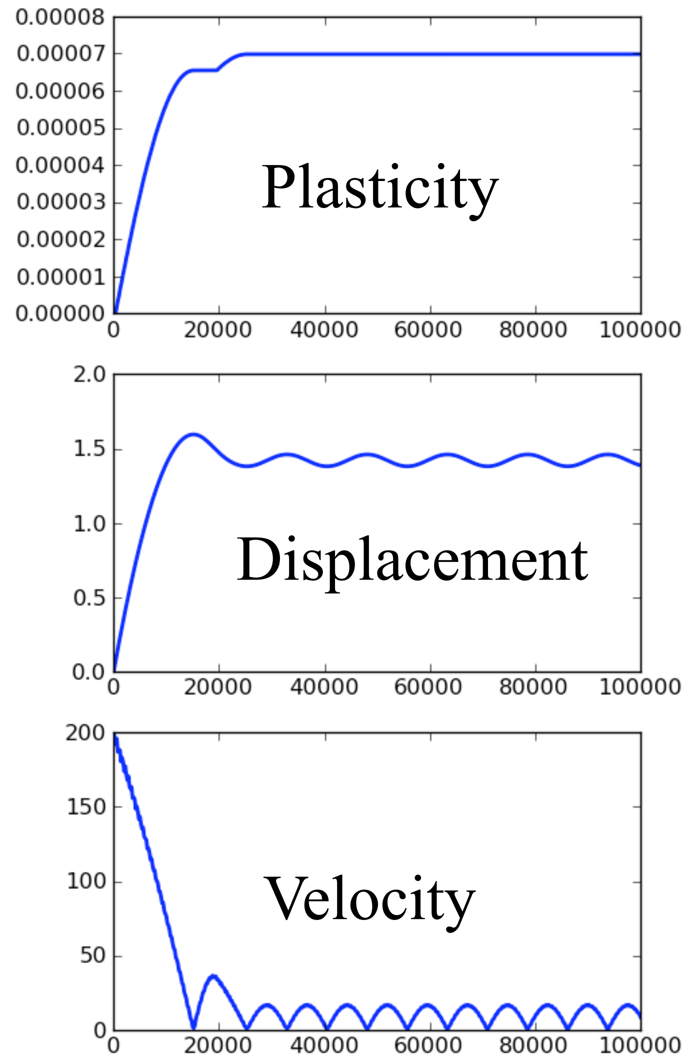
Elastic-Plastic Constitutive Law: Expanding Ring Simulation

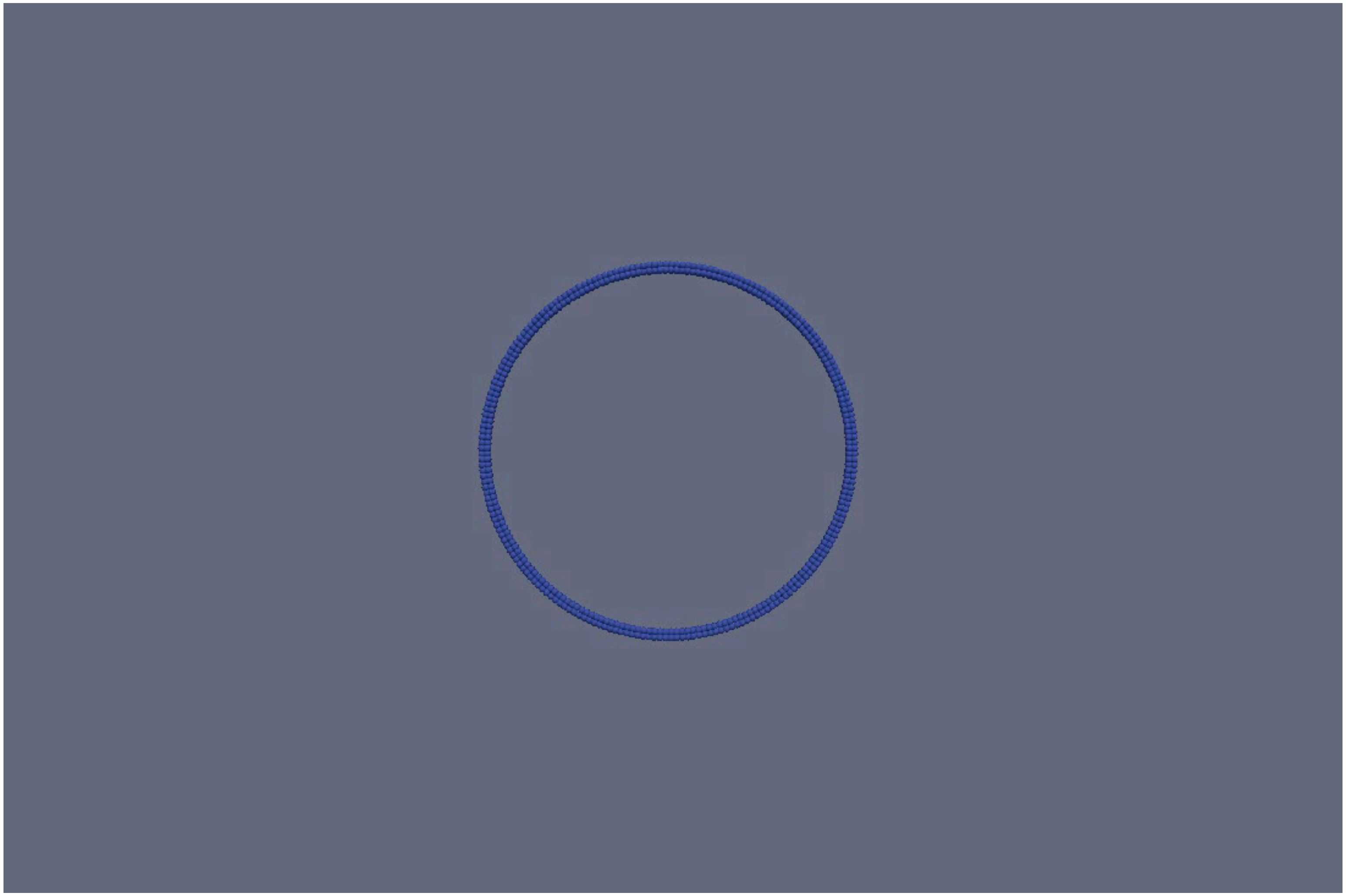
Initial condition: Radial velocity

Explicit time integration: Peridigm



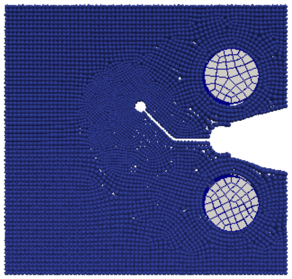


Elastic-Plastic Constitutive Law: Expanding Ring Simulation with Damage

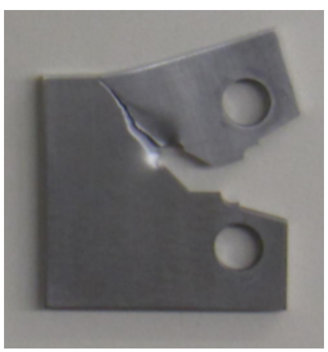


Ductile Failure X-Prize Challenge 1

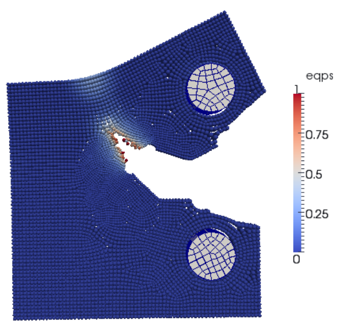
- Input mesh created with Cubit & SEACAS tools
- Precut channel created with bond cutting block
- LAME multilinear elastic-plastic material
- Interaction with pins via contact
- Visualization using ParaView



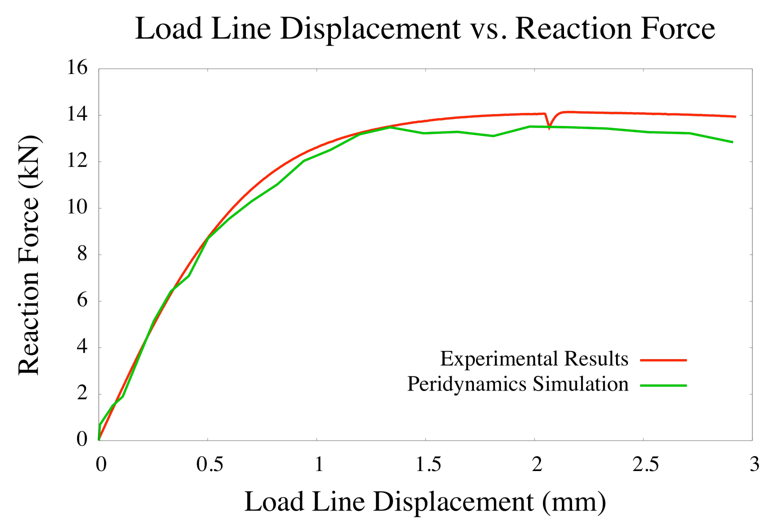
Undeformed Model



Experimental Results
[Theresa Córdova]

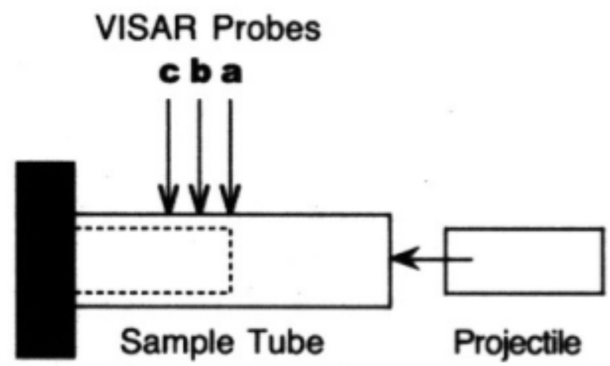


Sierra/SM Simulation



Expanding Tube Experiment of Vogler et. al

- Experimental setup:
  - Tube expansion via collision of Lexan projectile and plug within AerMet tube
  - Accurate recording of velocity and displacement on tube surface
- Modeling approach:
  - AerMet tube modeled with peridynamics, elastic-plasitic material model with linear hardening
  - Lexan plugs modeled with traditional FEM, EOS-enabled Johnson-Cook material model



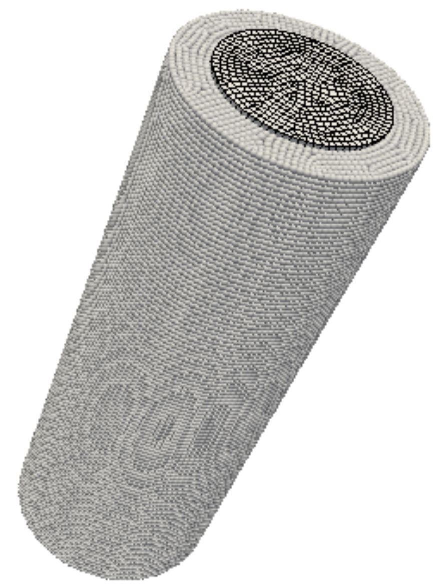
[Vogler et. al]

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.

Model Discretization

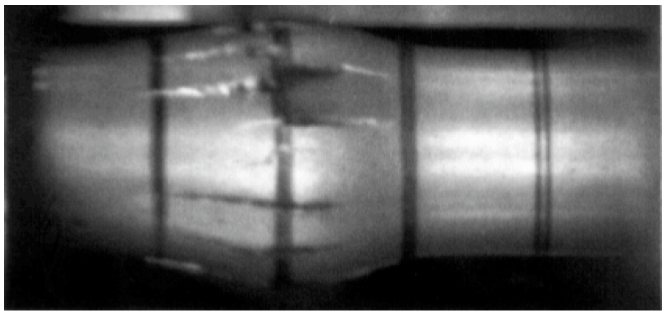
- AerMet tube
  - Peridynamics
  - Elastic-plastic material model
  - 73,676 sphere elements
  - Horizon set to five times element radius

- Lexan projectile / plug
  - Classical FEM
  - Johnson-Cook material model
  - 53,214 hexahedron elements

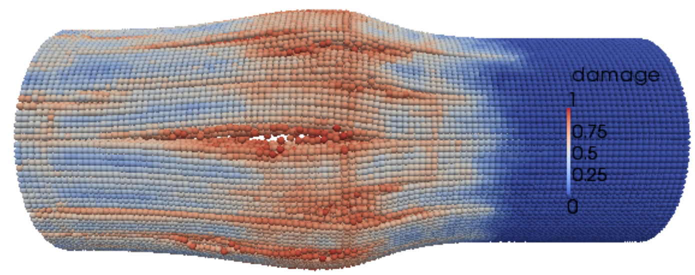


Model Discretization

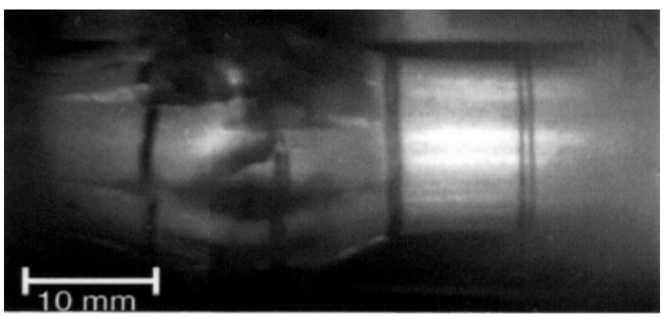
Predicted Damage Profiles



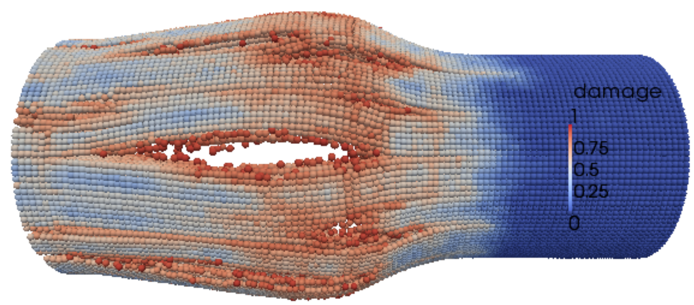
Experimental image at 15.4 microseconds [Vogler et. al]



Simulation at 15.4 microseconds



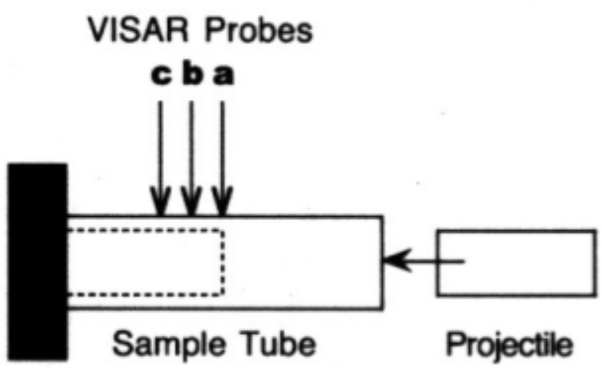
Experimental image at 23.4 microseconds [Vogler et. al]



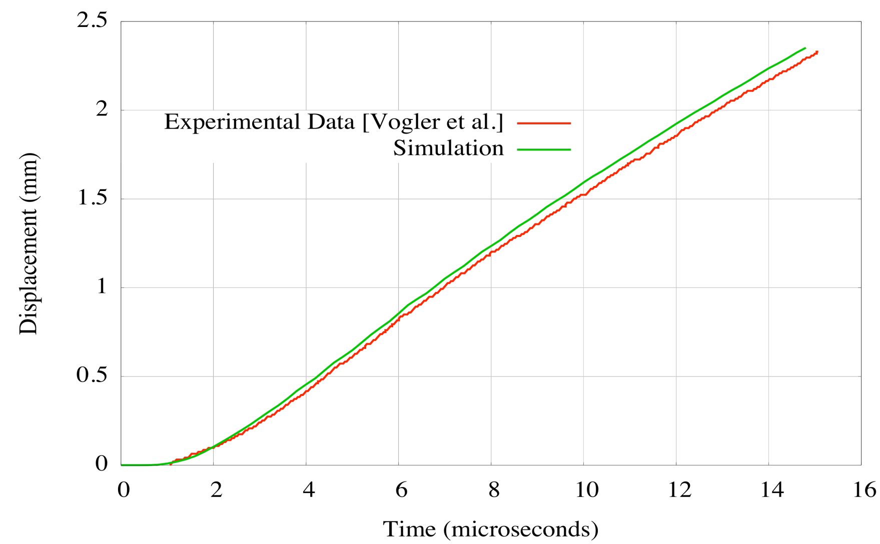
Simulation at 23.4 microseconds

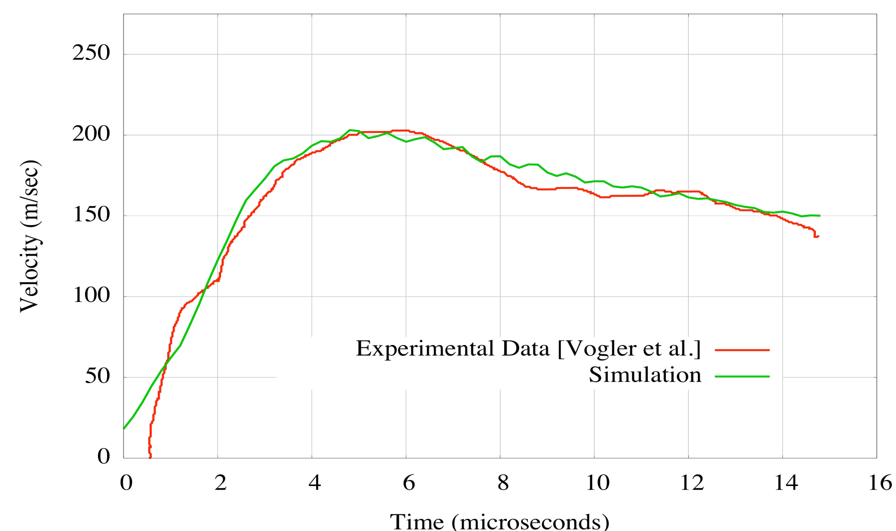
Predicted Displacement and Velocity on Tube Surface

Displacement and velocity
on tube surface
at probe position A



[Vogler et. al]

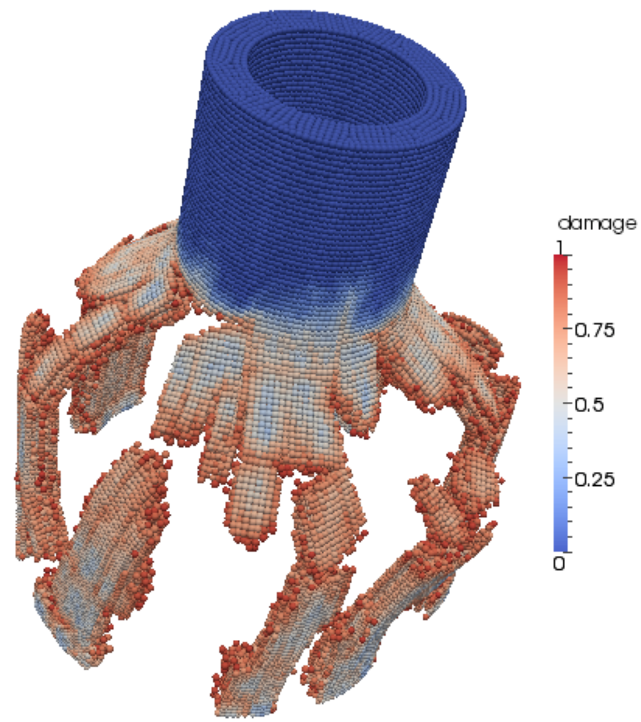




Fragmentation Pattern

<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

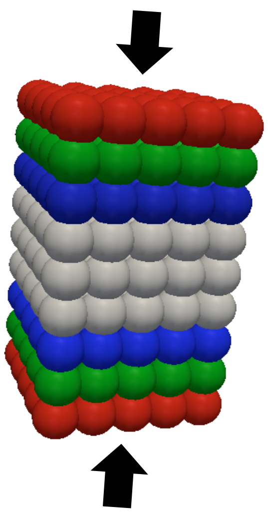


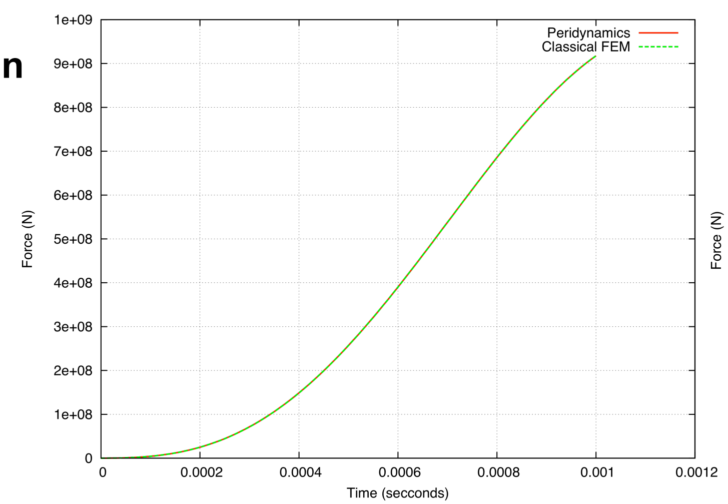
Simulation at 84.8 microseconds

Current Work:
Verification of Peridynamics Interface to LAME

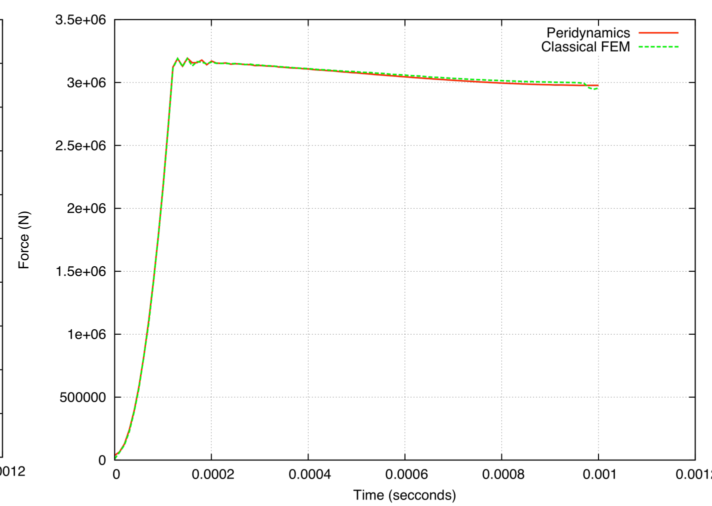
- Goal: Verify peridynamics interface to LAME
  - LAME contains 40+ material models suitable for peridynamics
- Strategy: Test against classical FEM solution
  - Construct test problems that yield equivalent peridynamic and FEM solutions
  - Automated test suite run for all applicable LAME material models

Example:
Uniaxial Compression





Thermo-elastic material model



Elastic-fracture material model

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Summary of Strengths and Weaknesses

Strengths

- Governing equations well posed at displacement discontinuities
- Robust framework for modeling crack growth (3D, scalable)
- Sound mathematical / mechanics foundation

Weaknesses

- Application of boundary conditions complex
- Additional research on constitutive relations required
- Complex underlying failure mechanisms
  - What are the relevant physics?
  - What is the best representation within mathematical / computational framework?

Timeline for Future Work

One-year goals

- Quasi-statics, implicit dynamics
- Elastic-plastic constitutive model, work-based damage law
- Code verification

Five-year goals

- Advanced material models (e.g. crystal plasticity, concrete)
- Direct coupling of peridynamics and classical finite elements
- Scalable solvers for nonlocal mechanics
- Multithreading / GPU implementations
- Code validation

Recent Advancements in Peridynamics with Applications to Failure Modeling

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Adaptation of Classical Material Models for Peridynamics

1) Approximate deformation gradient based on positions and deformations of all elements in the neighborhood

Approximate Deformation Gradient

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

Shape Tensor

$$\mathbf{K} = \sum_{i=0}^{N} \underline{\omega}_i \, \underline{\mathbf{X}}_i \otimes \underline{\mathbf{X}}_i \, \Delta V_{\mathbf{x}_i}$$

2) Deformation gradient (or strain, or strain rate) passed to classical material model, which computes stress

3) Stress converted to pairwise forces

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

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