



Peridigm: A New Paradigm in Computational Peridynamics

**SIAM Conference on
Mathematical Aspects of Materials Science**
**Mathematical and Computational Aspects of
Peridynamics and Related Nonlocal Models**

June 12, 2013

**Michael Parks, Dave Littlewood, John Mitchell,
Stewart Silling, John Foster, Dan Turner**

Computing Research Center
Sandia National Laboratories
Albuquerque, New Mexico

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

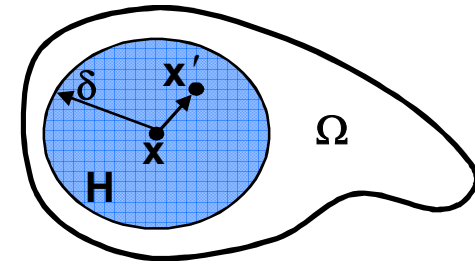
What is Peridynamics?

- ❑ Peridynamics is a nonlocal extension of classical solid mechanics that permits discontinuous solutions

- ❑ Peridynamic equation of motion (integral, nonlocal)

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

- ❑ Replace PDEs with integral equations
 - ❑ Utilize same equation everywhere; nothing “special” about cracks
 - ❑ No assumption of differentiable fields (admits fracture)
 - ❑ Damage incurred when deformation criteria satisfied (critical stretch, etc.)
 - ❑ No obstacle to integrating nonsmooth functions
 - ❑ Integrand is “force” function; contains constitutive model
 - ❑ Integrand = 0 for points \mathbf{x}, \mathbf{x}' more than δ apart (like cutoff radius in MD!)
 - ❑ PD is “continuum form of molecular dynamics”
- ❑ Impact
 - ❑ Nonlocality
 - ❑ Larger solution space than corresponding classical PDE-based models (fracture)
 - ❑ Account for material behavior at small & large length scales (multiscale material model)



Point \mathbf{x} interacts directly with all points \mathbf{x}' within H

“It can be said that all physical phenomena are nonlocal. Locality is a fiction invented by idealists.”



A. Cemal Eringen



Part I

Brief Overview of Peridynamics

Part II

Demonstration Computations

Part III

Peridigm: A Computational Peridynamics Code

Part IV

Peridigm: Recent Developments

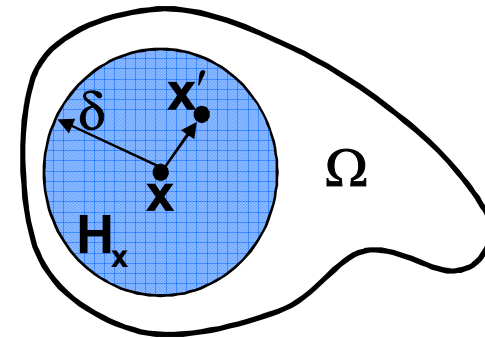
Part V

Peridigm: Tutorial and Example

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 H_x (*family of \mathbf{x}*)



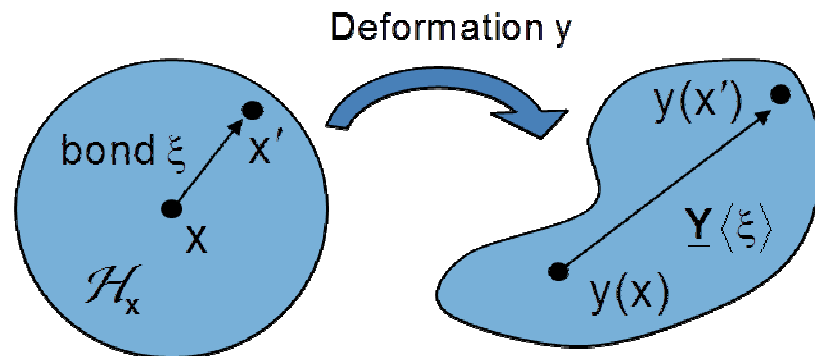
□ Bonds and bond forces

- Vector between \mathbf{x} and any point in its family is called a *bond*: $\xi = \mathbf{x}' - \mathbf{x}$
- 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 H_x and collective deformation of $H_{x'}$
- 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 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

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

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

- $\underline{\mathbf{T}}[\mathbf{x}]$ 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
- For elastic materials, $\underline{\mathbf{T}}[\mathbf{x}] = \mathbf{W}_{\underline{\mathbf{Y}}}$ (Fréchet derivative)

□ Peridynamics vs. standard equations

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

Relation	Peridynamic Theory	Standard Theory
Kinematics	$\underline{\mathbf{Y}} \langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$	$\mathbf{F} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear Momentum Balance	$\rho \ddot{\mathbf{u}}(\mathbf{x}) = \int_{\mathcal{H}_{\mathbf{x}}} \{ \underline{\mathbf{T}}[\mathbf{x}, \mathbf{t}] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', \mathbf{t}] \langle \mathbf{x} - \mathbf{x}' \rangle \} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x})$	$\rho \ddot{\mathbf{u}}(\mathbf{x}) = \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive Model	$\underline{\mathbf{T}} = \hat{\mathbf{T}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular Momentum Balance	$\int_{\mathcal{H}_{\mathbf{x}}} \{ \underline{\mathbf{Y}} \langle \mathbf{x}' - \mathbf{x} \rangle \times \underline{\mathbf{T}} \langle \mathbf{x}' - \mathbf{x} \rangle \} dV_{\mathbf{x}'} = 0$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$



Peridynamic Material Modeling

- **Linear Peridynamic Solid (LPS)***
- Nonlocal analog to linear isotropic elastic solid
- k is bulk modulus, μ is shear modulus

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

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

- Many other peridynamic material models available: elastic-plastic, viscoelastic, etc.
- Can wrap classical material models (existing material libraries) in peridynamic “skin”

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

Peridynamic Fracture Modeling

□ Fracture (“Critical Stretch”)

- Break bond if bond stretch s exceeds critical stretch s_0
- If work to break bond ξ is $w_0(\xi)$, then energy release rate found by summing this work per unit crack area

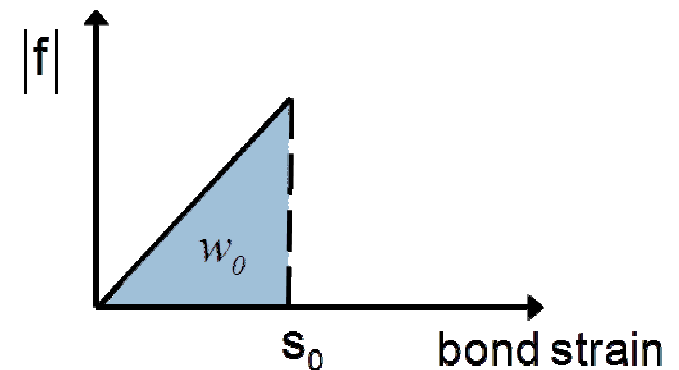
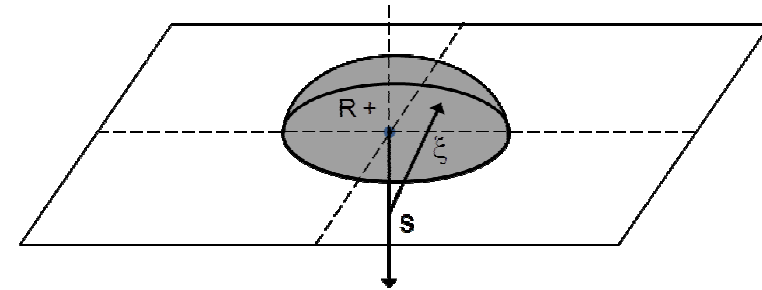
$$\mathbf{G} = \int_0^\delta \int_{R_+} \mathbf{w}_0(\xi) dV_\xi ds$$

- Can then get the critical strain s_0 for bond breakage in terms of \mathbf{G} (strain energy release rate), an experimentally measurable quantity

□ Fracture (“Critical Work”)*

- Break bond if work done on bond exceeds critical value*

- Many others possible...





Part I
Brief Overview of Peridynamics

Part II
Demonstration Computations

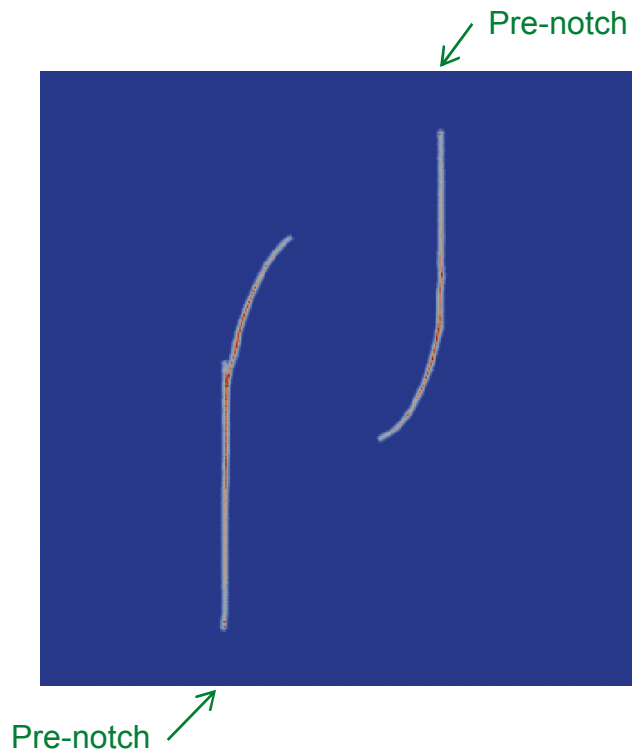
Part III
Peridigm: A Computational Peridynamics Code

Part IV
Peridigm: Recent Developments

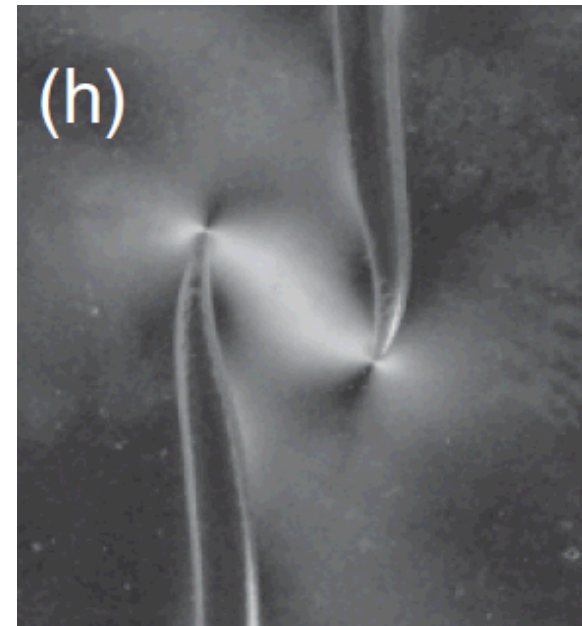
Part V
Peridigm: Tutorial and Example

Two Interacting Cracks

- ❑ Offset notches thin rectangular elastic plate
- ❑ Uniaxial strain applied from sides
- ❑ Approaching cracks produce “en passant” crack pattern



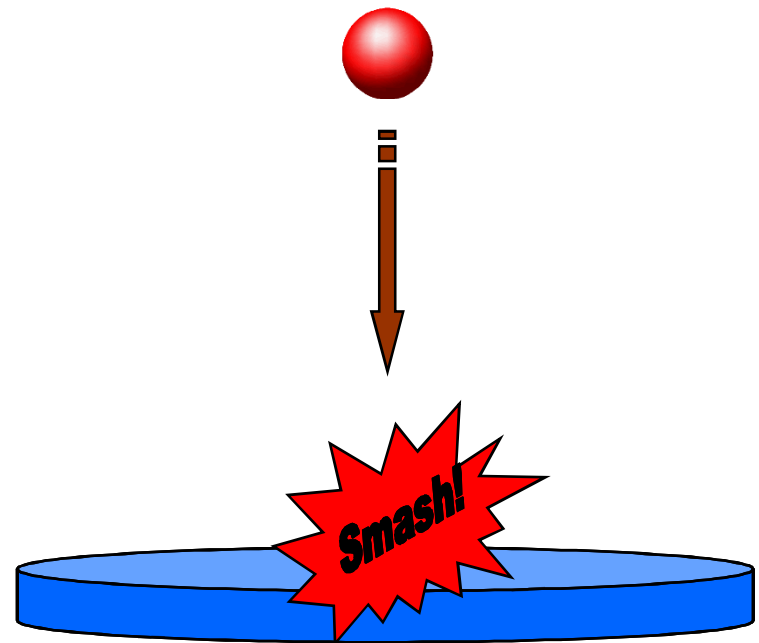
Peridynamics



Physical Experiment*

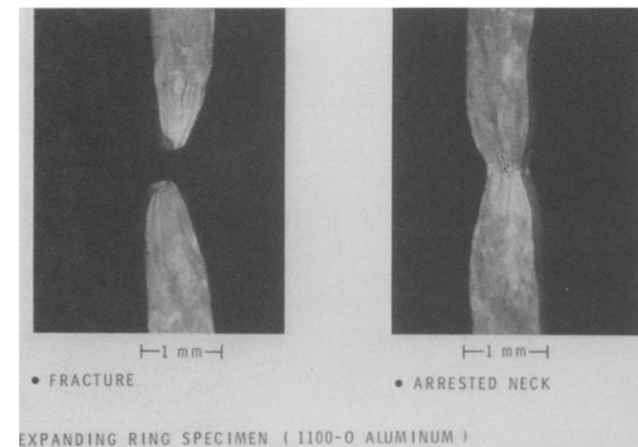
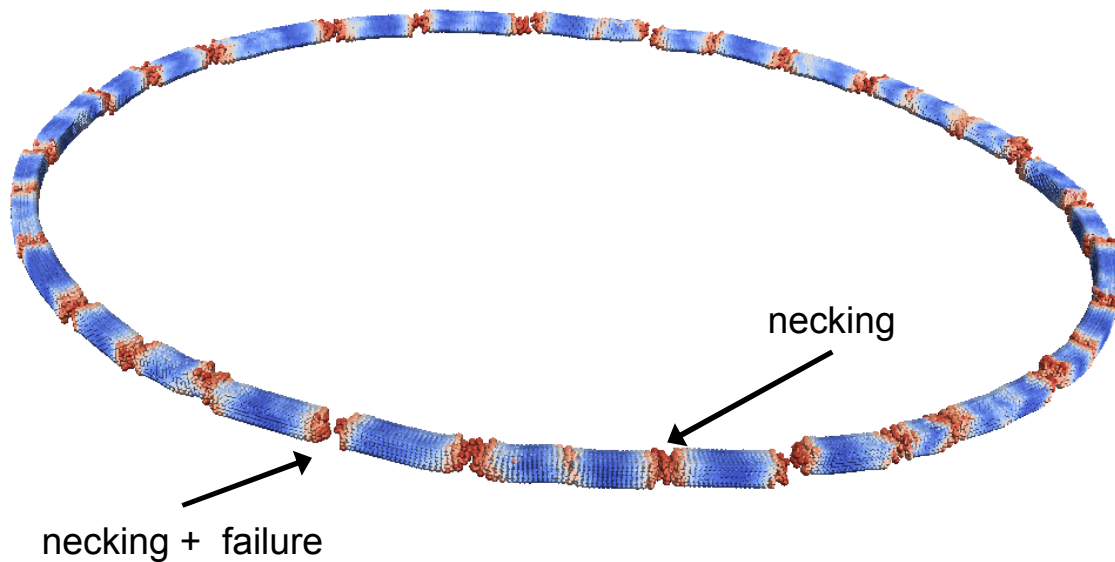
Hard Sphere Impact on Brittle Disk*

- ❑ Projectile
 - ❑ Sphere (diameter 0.01 m)
 - ❑ Velocity 100 m/s
- ❑ Target
 - ❑ Disk: diameter 0.074 m,
 - ❑ thickness 0.0025 m
- ❑ Elastic modulus 14.9 GPa
- ❑ Density 2200 kg/m³



Electromagnetically loaded ring

- ❑ 1100-0 aluminum ring (ductile)
- ❑ Motivated by ring fragmentation experiments of Grady & Benson*
- ❑ Used peridynamic elastic/plastic model**



Fracture and arrested neck region
from dynamic expansion of ring*

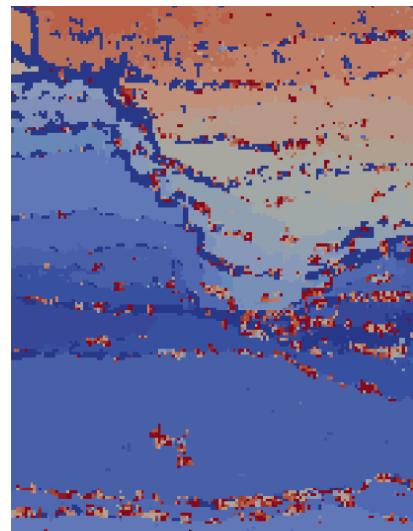
* D. Grady, D. Benson, Fragmentation of metal rings by electromagnetic loading, *Experimental Mechanics*, 23(4), pp. 393-400, 1983

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

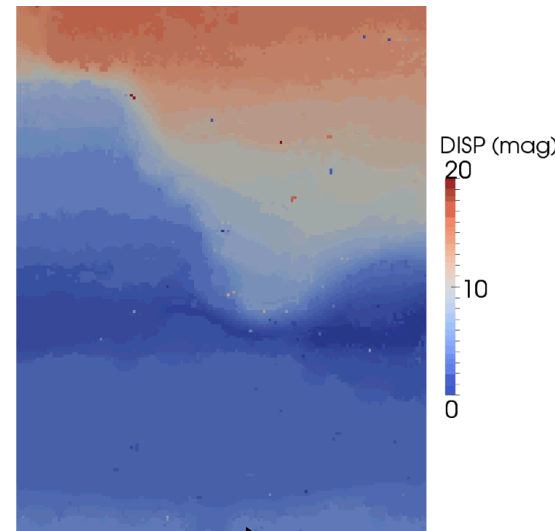
Improved Digital Image Correlation (DIC) Using Peridynamic Damage Modeling (Dan Turner)

- ❑ DIC often fails near cracks or discontinuities
- ❑ Displacements obtained by interpolation across a crack are highly inaccurate
- ❑ Use peridynamics to compute displacements in regions where DIC fails
- ❑ Treat the quality DIC displacements as a boundary condition and solve for rest of domain as if it were a peridynamic material

Failure of fiber-reinforced concrete tensile specimens



Standard DIC algorithm
(Dark blue regions represent failed correlation, spurious colors represent inaccurate displacements)



Peridynamics enhanced result

Improved Digital Image Correlation (DIC) Using Peridynamic Damage Modeling (Dan Turner)

- ❑ Computed damage profile closely matches experimental results
- ❑ Displacement (strain) accuracy is considerably improved

Failure of fiber-reinforced concrete tensile specimens

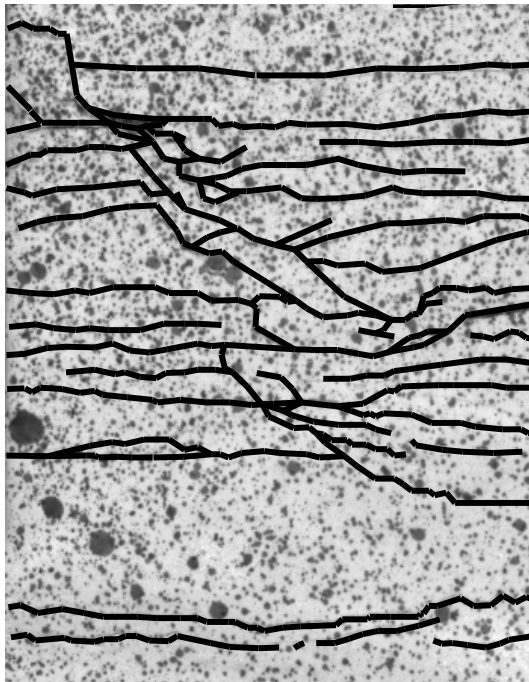
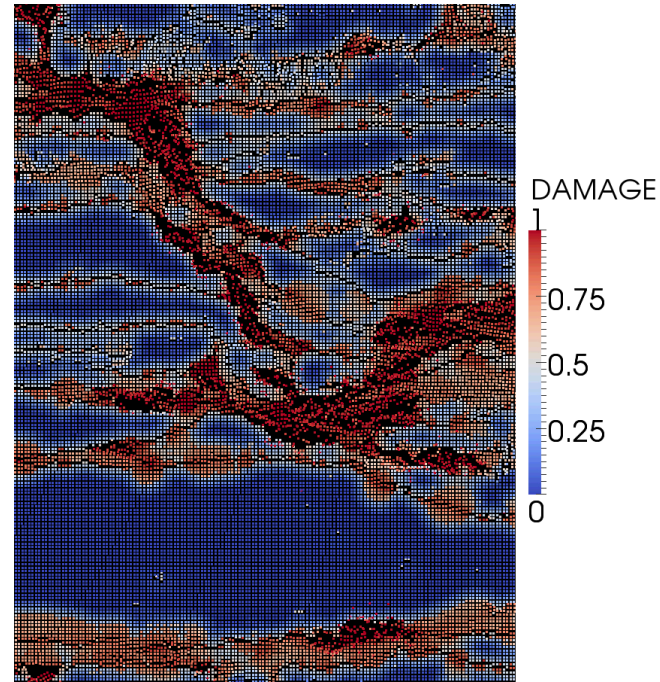


Photo of damaged concrete specimen (lines represent cracks)



Damage profile computed using peridynamics



Part I
Brief Overview of Peridynamics

Part II
Demonstration Computations

Part III
Peridigm: A Computational Peridynamics Code

Part IV
Peridigm: Recent Developments

Part V
Peridigm: Tutorial and Example

Peridigm

- ❑ **Peridigm** (Open Source, C++)
- ❑ Developers: Parks, Littlewood, Mitchell, Silling
- ❑ <https://software.sandia.gov/trac/peridigm>
- ❑ Intended as Sandia's primary open-source PD code
- ❑ Built upon Sandia's Trilinos Project (trilinos.sandia.gov)

- ❑ **Features/Capabilities**
- ❑ Massively parallel
- ❑ Exodus mesh input
- ❑ Multiple materials (only state based)
 - ❑ elastic, elastic-plastic, elastic-plastic with hardening, viscoelastic
- ❑ Explicit time integration (Velocity-Verlet)
- ❑ Implicit time integration (Newmark-beta method)
- ❑ Quasistatics (Nonlinear, via Newton/Krylov or nonlinear CG)
- ❑ Linear (preconditioned Krylov subspace methods)
- ❑ Automatic differentiation Jacobians
- ❑ DAKOTA interface for UQ/optimization/calibration, etc. (dakota.sandia.gov)



Peridigm: Peridynamics via Agile Components

Peridigm

Software Quality Tools



Mailing Lists



Version Control



Build System

Testing (CTest)



UQ

Optimization

Error Estimation

Calibration



Visualization



Project Management

Issue Tracking

Wiki



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)

Solver Tools

Iterative Solvers (Belos)

Direct Solvers (Amesos)

Nonlinear Solvers (NOX)

Eigensolvers (Anasazi)

Preconditioners (IFPack)

Multilevel (ML)

Peridynamic Codes

- ❑ **EMU** (Export controlled, F90)
 - ❑ Developer: Silling (www.sandia.gov/emu/emu.htm)
 - ❑ Research code
- ❑ **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 (lammmps.sandia.gov)
 - ❑ More info & user guide: www.sandia.gov/~mlparks
- ❑ **Peridigm** (Open Source, C++)
 - ❑ Developers: Parks, Littlewood, Mitchell, Silling
 - ❑ Intended as Sandia's primary open-source PD code
 - ❑ Built upon Sandia's Trilinos Project (trilinos.sandia.gov)
 - ❑ Massively parallel, Exodus mesh input, Multiple material blocks
 - ❑ Explicit, implicit time integration
 - ❑ State-based linear elastic, elastic-plasticity, viscoelastic models
 - ❑ DAKOTA interface for UQ/optimization/calibration, etc. (dakota.sandia.gov)
- ❑ **Peridynamics in Sierra/SolidMechanics** (Export controlled, C++)
 - ❑ Developer: Littlewood
 - ❑ Sandia engineering analysis code
- ❑ **Peridynamics is a capability that can be added to (almost) any analysis code!**



Peridigm Material Models

Linear Peridynamic Solid (LPS)*

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

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

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

- Many other peridynamic material models available:

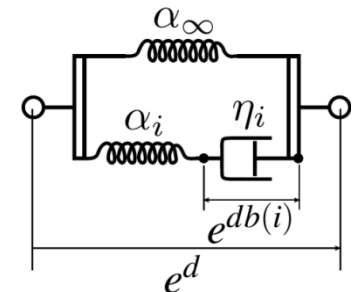
Elastic-Plastic Model**

- Nonlocal analogue to perfect plasticity model

Elastic-Plastic Model with Hardening (J. Foster, UTSA)

Viscoelastic Model***

- Nonlocal analog to standard linear solid



*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.

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

Peridigm: Structure & User Interface

- ❑ **Peridigm designed to be user extensible**
 - ❑ User defined material models, compute classes, etc.
- ❑ **Compute class: Compute any user-defined quantity**
 - ❑ Class must declare what data it needs allocated
 - ❑ Examples: per-element or per-node scalar, vector, tensor, etc.
 - ❑ Class must provide routine that computes user-defined quantity
 - ❑ **User writes only serial code -- parallel communication handled “auto-magically”**
- ❑ **Example: Compute Acceleration (for output)**

```
#!/ Fill the acceleration vector
int PeridigmNS::Compute_Acceleration::compute( Teuchos::RCP< std::vector<Block> > blocks ) const {
    int retval(0);

    Teuchos::RCP<Epetra_Vector> force, acceleration;
    std::vector<Block>::iterator blockIt;
    for(blockIt = blocks->begin() ; blockIt != blocks->end() ; blockIt++){
        force          = blockIt->getData(m_forceDensityFieldId, PeridigmField::STEP_NP1);
        acceleration   = blockIt->getData(m_accelerationFieldId, PeridigmField::STEP_NP1);
        *acceleration  = *force;
        double density = blockIt->getMaterialModel()->Density();
        // Report if any calls to Scale() failed.
        retval = retval || acceleration->Scale(1.0/density);
    }

    return retval;
}
```

- ❑ **Declare “acceleration” as output field in input deck**
 - ❑ Only specified fields are computed



Peridigm: Structure & User Interface

❑ Peridigm material models: Create your own!

```
//! Returns a vector of field specs that specify the variables associated with the material
virtual Teuchos::RCP< std::vector<Field_NS::FieldSpec> > VariableSpecs() const = 0;

//! Initialize the material model.
virtual void initialize(const double dt,
                      const int numOwnedPoints,
                      const int* ownedIDs,
                      const int* neighborhoodList,
                      PeridigmNS::DataManager& dataManager) const {}

//! Evaluate the forces on the cells
virtual void computeForce(const double dt,
                        const int numOwnedPoints,
                        const int* ownedIDs,
                        const int* neighborhoodList,
                        PeridigmNS::DataManager& dataManager) const = 0;

//! Evaluate the Jacobian
virtual void computeJacobian(const double dt,
                            const int numOwnedPoints,
                            const int* ownedIDs,
                            const int* neighborhoodList,
                            PeridigmNS::DataManager& dataManager,
                            PeridigmNS::SerialMatrix& jacobian) const;

// other routines
```



Part I
Brief Overview of Peridynamics

Part II
Demonstration Computations

Part III
Peridigm: A Computational Peridynamics Code

Part IV
Peridigm: Recent Developments

Part V
Peridigm: Tutorial and Example

Surface Correction Factor (John Mitchell)

- ❑ PD material models developed to get linear bulk response correct (i.e., match classical response).
 - ❑ In PD, points close to surface have fewer bonds than points in bulk
 - ❑ Model response is different near the surface!
 - ❑ **Surface effects conflict with engineering analyst expectations!**
 - ❑ Modify model near surface to correct for “missing” bonds
 - ❑ Introduce a “surface correction factor”
-
- ❑ Demonstration: Applied strain to dogbone

Axial Displacement



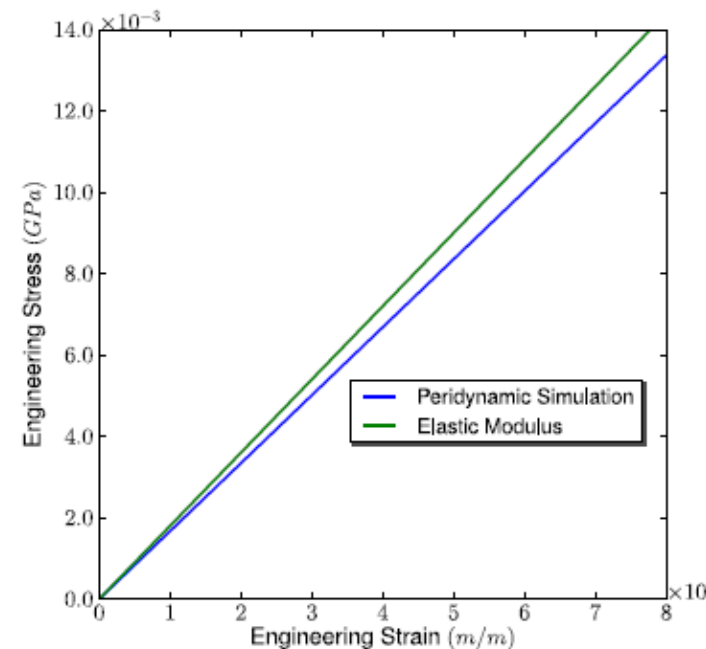
Stored Elastic Energy



Sources of Error:

- 1) Geometric surface effects
- 2) Nonlocal model (dilatation on surface) and related model properties
- 3) Discretization error

Stress versus Strain



Thermal Stress (Dave Littlewood)

- ❑ Introduce thermal stress due to specified temperature field
 - ❑ Modify bond extension to account for temperature change
 - ❑ Demonstration: Precracked plate clamped at top & bottom subjected to $-\Delta T$

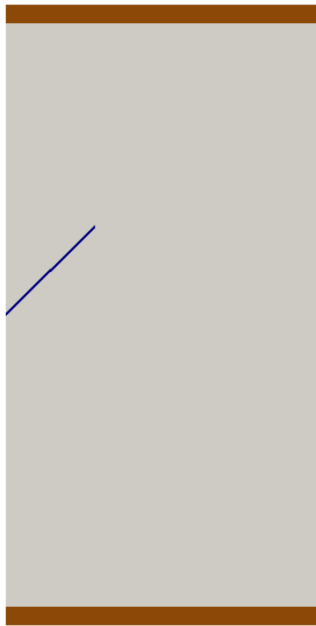
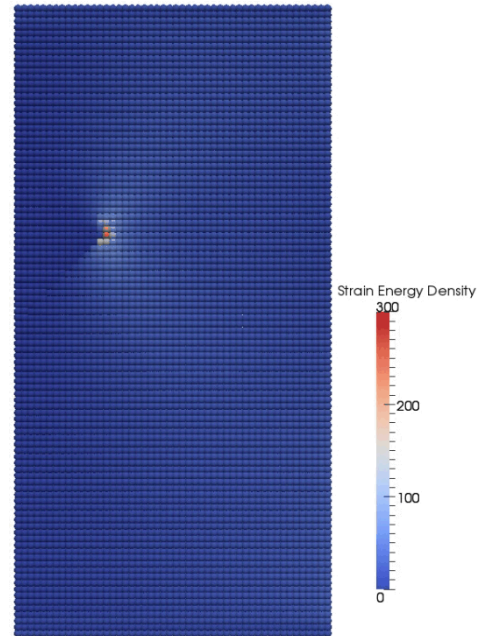


Plate with precrack



Strain energy density after temperature change

- ❑ Can simulate thermally driven fracture, etc.
- ❑ Required bond-cutting planes (John Mitchell, Dave Littlewood)
 - ❑ Break all bonds across a plane to introduce precrack

New Input Deck Format (John Foster)

- ❑ More readable input deck format (.peridigm format)
 - ❑ Use human-readable plain text instead of XML Teuchos ParameterList format
 - ❑ Sublists indicated by indentation, as in python

Old Format

```
<ParameterList>
  <Parameter name="Verbose" type="bool" value="false"/>

  <ParameterList name="Discretization">
    <Parameter name="Type" type="string" value="Exodus" />
    <Parameter name="Horizon" type="double" value="0.1900"/>
    <Parameter name="Input Mesh File" type="string" value="tensile_test.g"/>
  </ParameterList>

  <ParameterList name="Materials">
    <ParameterList name="My Material">
      <Parameter name="Material Model" type="string" value="Elastic"/>
      <Parameter name="Density" type="double" value="8.0"/>
      <Parameter name="Bulk Modulus" type="double" value="1.500e12"/>
      <Parameter name="Shear Modulus" type="double" value="6.923e11"/>
    </ParameterList>
  </ParameterList>

  <ParameterList name="Blocks">
    <ParameterList name="My Block">
      <Parameter name="Block Names" type="string" value="block_1 block_2
block_3"/>
      <Parameter name="Material" type="string" value="My Material"/>
    </ParameterList>
  </ParameterList>

  <ParameterList name="Boundary Conditions">
    <ParameterList name="Prescribed Displacement Bottom">
      <Parameter name="Type" type="string" value="Prescribed Displacement"/>
      <Parameter name="Node Set" type="string" value="nodelist_1"/>
      <Parameter name="Coordinate" type="string" value="y"/>
      <Parameter name="Value" type="string" value="y*0.01*t"/>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

New Format

```
Verbose "false"

Discretization
  Type "Exodus"
  Horizon {0.1900*2.0/2.0}
  Input Mesh File "tensile_test.g"

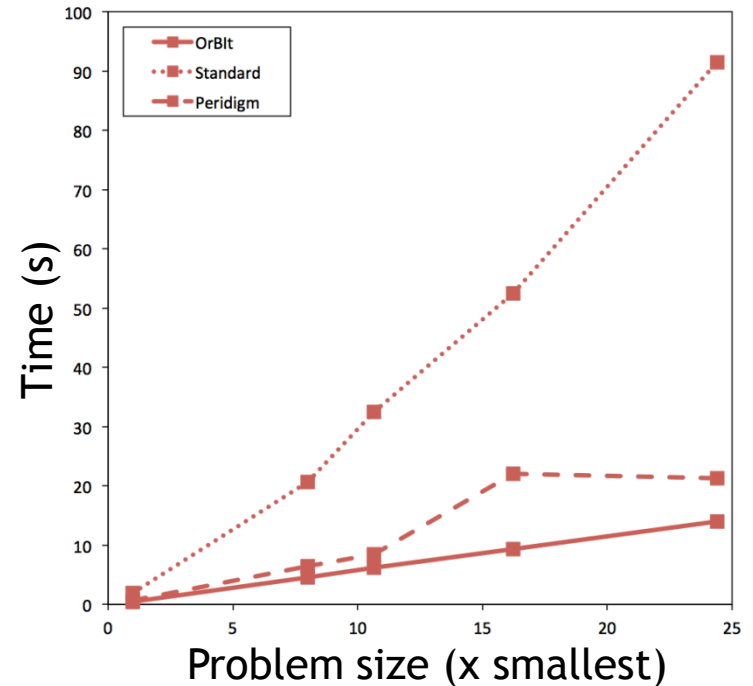
Materials
  My Material
    Material Model "Elastic"
    Density 8.0
    Bulk Modulus 1.500e12
    Shear Modulus 6.923e11

Blocks
  My Block
    Block Names "block_1 block_2 block_3"
    Material "My Material"

Boundary Conditions
  Prescribed Displacement Bottom
    Type "Prescribed Displacement"
    Node Set "nodelist_1"
    Coordinate "y"
    Value "y*0.01*t"
```

Matrix Assembly via Bond Iteration (Dan Turner)

- ❑ Ongoing algorithmic research into assembly of nonlocal tangent stiffness matrices
- ❑ Bond iteration provides 3-4 x speedup over cell iteration in assembly time
- ❑ Broken bonds can be removed from iteration loop
- ❑ Computes sensitivities for a single row at a time (saves on sparse matrix insertion)*
- ❑ Controlling damage propagation to achieve convergence is simpler
- ❑ Avoids repetitious computing of contributions from neighbors that share a bond
- ❑ Can be done using standard cell based fields



Serial Assembly Time Comparison

*This provides the greatest performance improvement



Part I
Brief Overview of Peridynamics

Part II
Demonstration Computations

Part III
Peridigm: A Computational Peridynamics Code

Part IV
Peridigm: Recent Developments

Part V
Peridigm: Tutorial and Example

Fragmenting Cylinder

❑ Fragmenting Brittle Cylinder

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

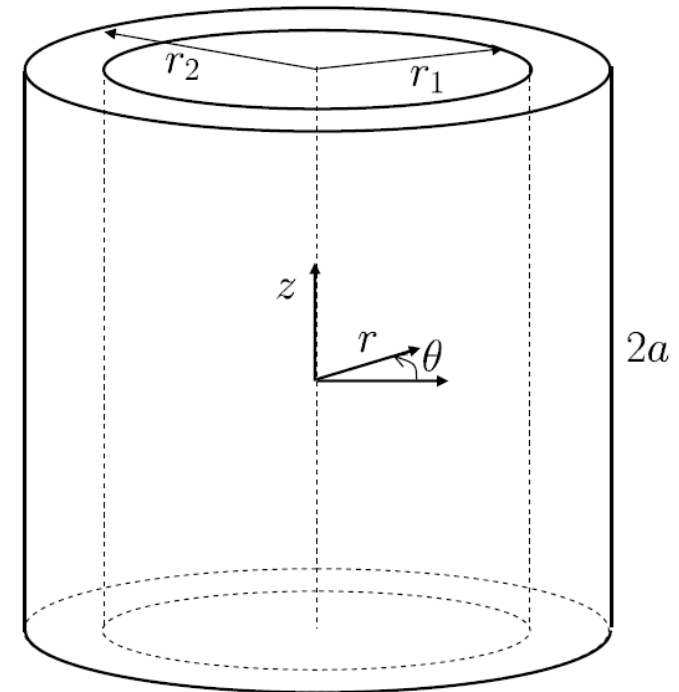
❑ Material properties

- ❑ Inner radius $r_1 = 0.020$ m
- ❑ Outer radius $r_2 = 0.025$ m
- ❑ Length $2a = 0.1$ m
- ❑ Density $\rho = 7800$ kg/m³
- ❑ Bulk modulus $k = 130$ GPa
- ❑ Shear modulus $\mu = 78$ GPa
- ❑ Yield stress $Y = 500$ GPa
- ❑ Ultimate stress $\sigma = 700$ GPa
- ❑ Elongation at failure $\varepsilon = 0.02$

❑ Initial Velocity

- ❑ $v(r) = V_{r0} - V_{r1}(a/z)^2$
- ❑ $v(z) = V_{z0}(a/z)$
- ❑ $v(\theta) = 0$

where $V_{r0} = 200$ m/s, $V_{r1} = 50$ m/s, $V_{z0} = 100$ m/s





Running Peridigm

❑ Usage:

```
Peridigm input.peridigm
```

where `input.peridigm` is a properly formatted input deck.

❑ An input deck contains these sections:

```
[Discretization Section]  
[Materials Section]  
[Damage Models Section]  
[Blocks Section]  
[Contact Section]  
[Boundary Conditions Section]  
[Solver Section]  
[Output Sections]
```


Running Peridigm

□ Input Deck

Discretization

```
Type "PdQuickGrid"  
Horizon "0.00417462"  
NeighborhoodType "Spherical"  
TensorProductCylinderMeshGenerator  
  Type "PdQuickGrid"  
  Inner Radius 0.020  
  Outer Radius 0.025  
  Cylinder Length 0.100  
  Ring Center x 0.0  
  Ring Center y 0.0  
  Z Origin 0.0  
  Number Points Radius 5
```

Alternative: Read
from
Exodus/Genesis
mesh generated by
meshing tool
(example: CUBIT)



Materials

```
My Linear Elastic Material  
  Material Model "Elastic"  
  Density 7800.0  
  Bulk Modulus 130.0e9  
  Shear Modulus 78.0e9
```

← Material properties

Damage Models

```
My Critical Stretch Damage Model  
  Damage Model "Critical Stretch"  
  Critical Stretch 0.02
```

← Damage model
properties

Running Peridigm

Blocks

```
My Group of Block
  Block Names "block_1"
  Material "My Linear Elastic Material"
  Damage Model "My Critical Stretch Damage Model"
```

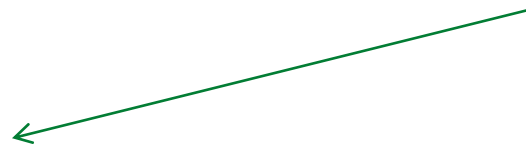
Used to associate blocks of elements with specific material models



Boundary Conditions

```
Initial Velocity X
  Type "Initial Velocity"
  Node Set "All"
  Coordinate "x"
  Value "(200 - 50*((z/0.05)-1)^2)*cos(atan2(y,x)) + rnd(5) "
```

Function parser: Enter any mathematical function to specify initial velocities or boundary conditions as a function of space & time



```
Initial Velocity Y
  Type "Initial Velocity"
  Node Set "All"
  Coordinate "y"
  Value "(200 - 50*((z/0.05)-1)^2)*sin(atan2(y,x)) + rnd(5) "
```

```
Initial Velocity Z
  Type "Initial Velocity"
  Node Set "All"
  Coordinate "z"
  Value "(100*((z/0.05)-1)) + rnd(5) "
```

Alternative: Specify nodesets in exodus/genesis database



Running Peridigm

Solver

```
Verbose "false"  
Initial Time 0.0  
Final Time 2.5e-4  
Verlet ←  
    Fixed dt 1.0e-8
```

Alternative: Implicit time
integrator (Newmark-Beta)
or quasistatic solver
(damped Newton)

Output

```
Output File Type "ExodusII"  
Output Format "BINARY"  
Output Filename "fragmenting_cylinder"  
Output Frequency 250  
Parallel Write "true"  
Output Variables  
    Proc_Num  
    Displacement  
    Velocity  
    Acceleration  
    Force_Density ←  
    Element_Id  
    Dilatation  
    Damage  
    Weighted_Volume
```

Output from
compute class
defined earlier

The Results...

❑ Fragmenting Brittle Cylinder



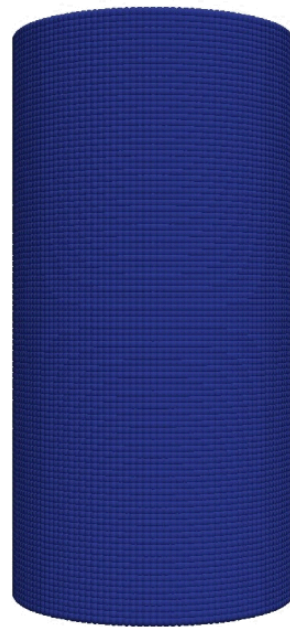
Before



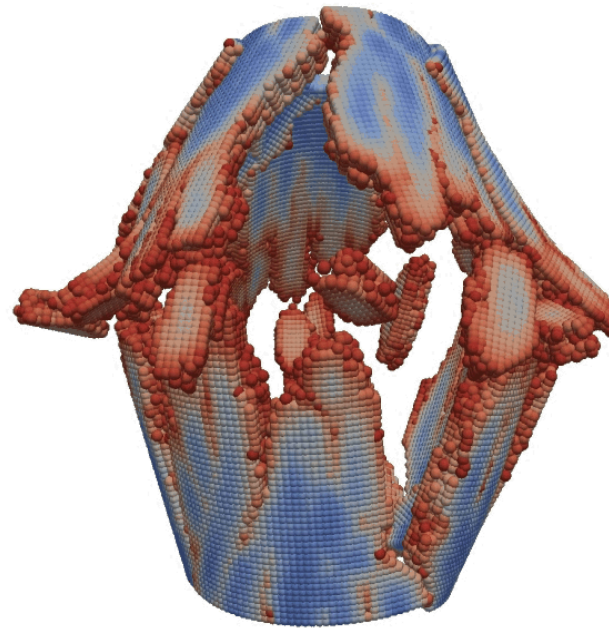
After
(brittle)

The Results...

Fragmenting Brittle Cylinder



Before



After
(brittle)

What about ductile failure?

Running Peridigm

❑ Modify the material section and damage model

Materials

```
My Elastic Plastic Material
Material Model "Elastic Plastic"
Density 7800.0
Bulk Modulus 130.0e9
Shear Modulus 78.0e9
```

Change material
type and
parameters

Damage Models

```
My Critical Stretch Damage Model
Damage Model "Critical Stretch"
Critical Stretch 0.12
```

Increase critical stretch to be consistent with
elongation at failure for material.

Allows material to yield plastically before
failure.

The Results...

❑ Fragmenting Ductile Cylinder



Before



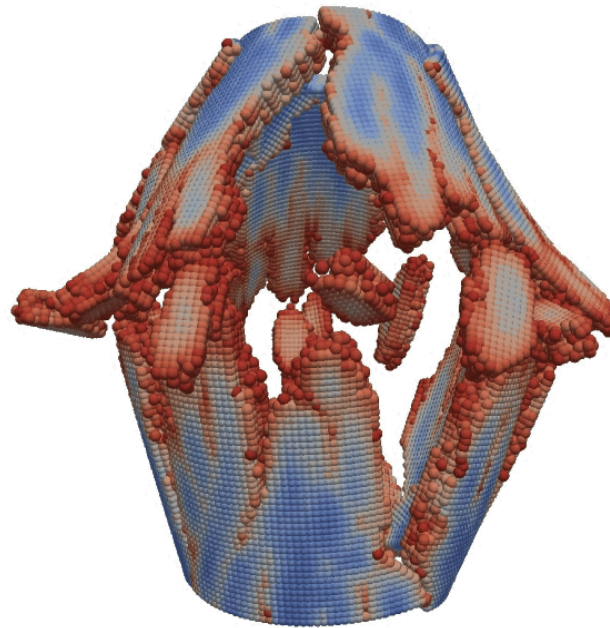
After
(ductile)

The Results...

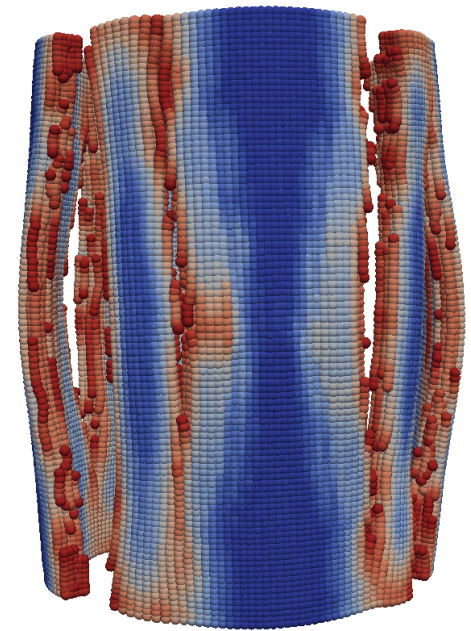
- ❑ Fragmenting Cylinders
 - ❑ Brittle fracture characteristically different from ductile fracture



Before



After
(brittle)



After
(ductile)



Summary

- Peridynamics overview
- Example computations
- Peridigm overview
- Peridigm fragmenting cylinder demonstration
 - Input deck distributed with Peridigm...
 - Other interesting examples (disk impact, tensile test)

- Peridigm
 - <https://software.sandia.gov/trac/peridigm>

- Contact me for more info: mlparks@sandia.gov

- Papers, etc.: www.sandia.gov/~mlparks

- Thank you!

Tensile Test

- ❑ Stainless steel dogbone specimen.
- ❑ Apply displacement boundary conditions until dogbone yields.
- ❑ Quasistatic solve

before



after

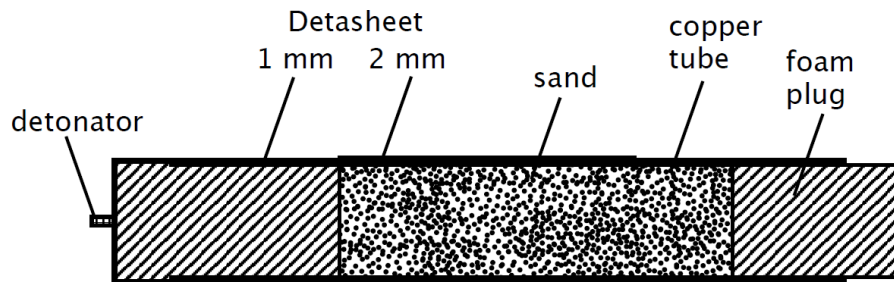


Color proportional to yield.

Displacement exaggerated 10 \times

Explosively Compressed Cylinder*

- ❑ Motivated by experiments of Vogler & Lappo*
 - ❑ Commonly used for consolidation of powders
 - ❑ Copper cylinders filled with granular material and wrapped with Detasheet explosive
 - ❑ Polyurethane foam plugs used to keep granular sample in tube.
-
- ❑ Geometry and Material Properties
 - ❑ Copper tubes 305 mm long, ID 50.8 mm, wall thickness of 1.52 mm
 - ❑ PETN based Detasheet with thicknesses of 1, 2, 4, or 6 mm were used, and a
 - ❑ Detonation traveled down length of tube, compressing both tube and sand fill



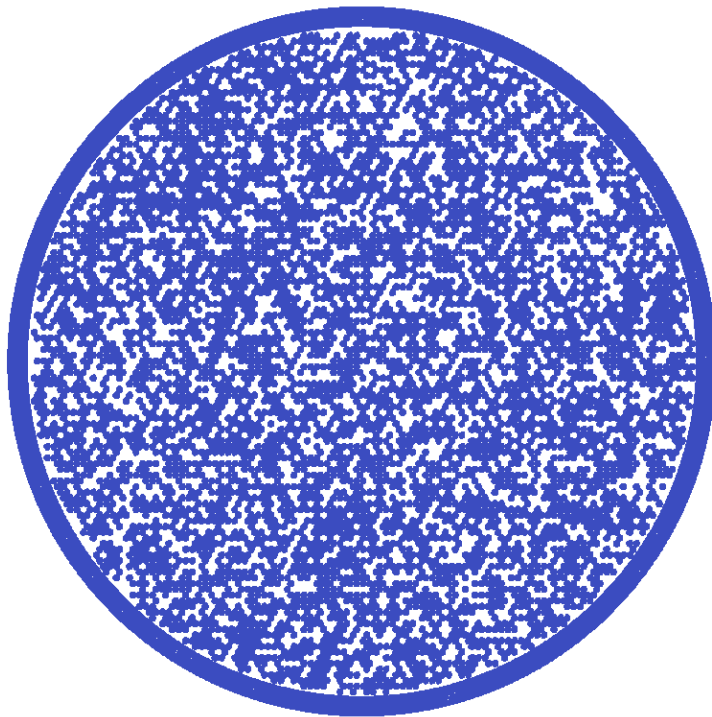
Cylinder schematic



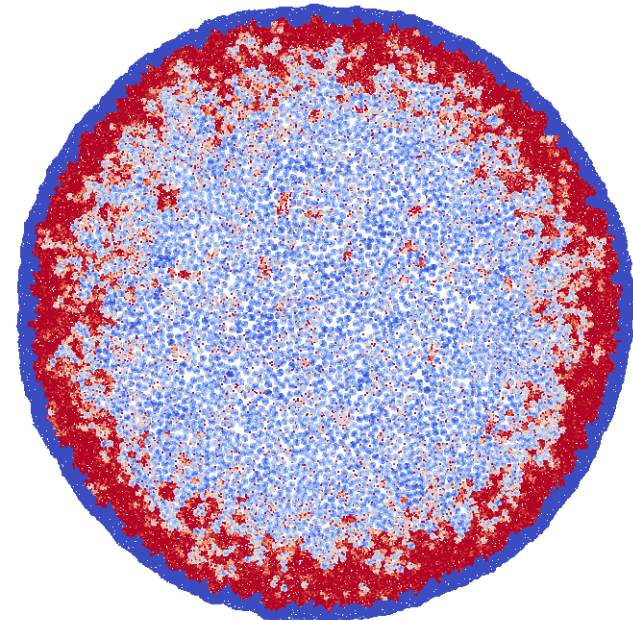
Cylinder after compression

Explosively Compressed Cylinder

- ❑ Peridigm computational results (with C. Hoffarth (ASU), D. Littlewood (SNL))
 - ❑ Color indicates damage (blue = undamaged, red = damaged)



Before



After