

Computational Peridynamics

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15th U.S. Nation Congress on Computational Mechanics

July 28th, 2019



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Short Course
Peridynamic Theory of Solid Mechanics

Computational Peridynamics

Outline

- Ingredients of a peridynamics simulation
 - Governing equations
 - Constitutive model, bond failure law
 - Contact model
 - Discretization
 - Time integrator
- Surface effect in peridynamic simulations
- Estimation of the maximum stable time step for dynamic simulations
- Convergence of peridynamic models
- Demonstration of meshfree peridynamics for model analysis
- Modeling damage and failure



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1. Ingredients of a peridynamic simulation

Ingredients for computational peridynamics

- Governing equations
 - Continuum form of the balance of linear momentum

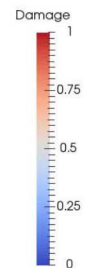
$$\rho(\mathbf{x}) \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{B}} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}'[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t)$$

- Semi-discrete form: meshless discretization of the strong form

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

- | | |
|-----------------------------------|----------------------------|
| ■ Boundary and initial conditions | ■ Discretization |
| ■ Constitutive model | ■ Time integration |
| ■ Bond failure law | ■ Explicit |
| ■ Contact model | ■ Implicit |
| | ■ Pre- and post-processing |

Meshfree peridynamic model of an expanding, fragmenting cylinder



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.

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

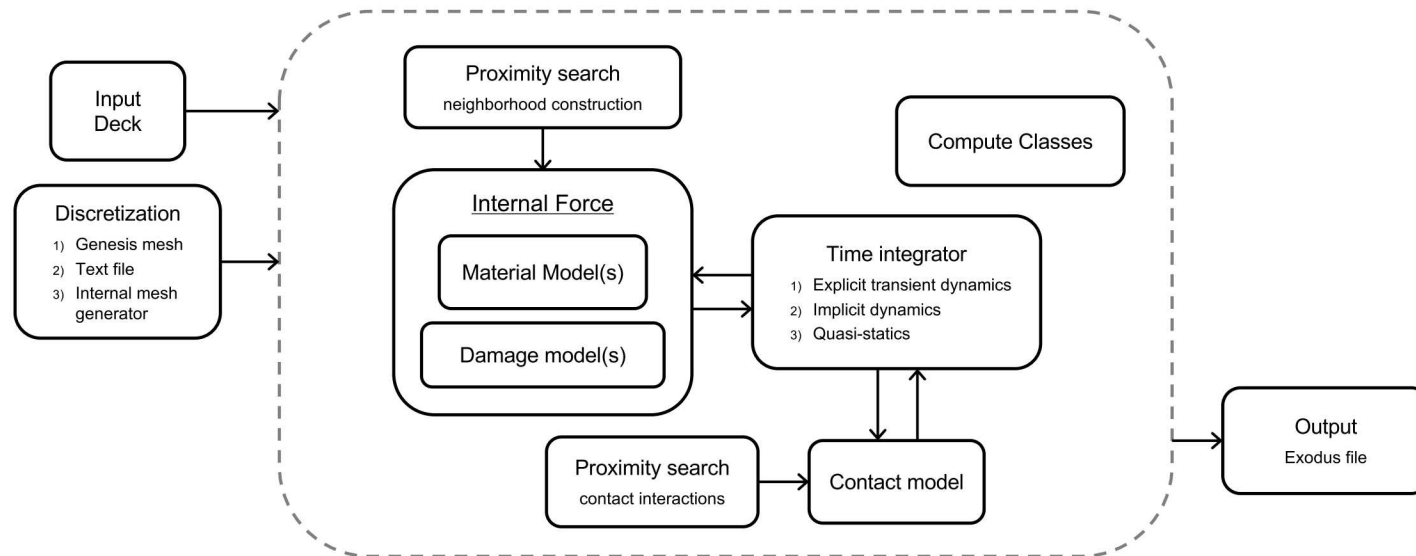


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1. Ingredients of a peridynamic simulation

Model for a peridynamics simulation code



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1. Ingredients of a peridynamic simulation

Constitutive models

- Bond-based models
 - Direct pairwise interactions
- State-based models
 - Multi-point interactions
- Correspondence models
 - Wrapper for classic stress-strain models

Example: Linear peridynamic solid [Silling]

- State-based model
- Deformation decomposed into deviatoric and dilatational components

$$\theta = \frac{3}{m} \int_{\mathcal{H}} (\underline{\omega} \underline{x}) \cdot \underline{e} dV \qquad \underline{e}^d = \underline{e} - \frac{\theta \underline{x}}{3}$$

- Magnitude of pairwise force density given by

$$\underline{t} = \frac{3k\theta}{m} \underline{\omega} \underline{x} + \frac{15\mu}{m} \underline{\omega} \underline{e}^d$$

S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.



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1. Ingredients of a peridynamic simulation

Software implementation of the Linear Peridynamic Solid

Algorithm 1 The initialization routine for a *linear peridynamic solid* material with a Gaussian influence function.

```

1: procedure LINEAR PERIDYNAMIC SOLID INITIALIZATION
2:   ▷ Compute the weighted volume for each node.
3:   for each node  $i$  do
4:      $m_i \leftarrow 0$ 
5:     for each node  $j$  in neighbor list for node  $i$  do
6:        $\xi \leftarrow \mathbf{x}_j - \mathbf{x}_i$ 
7:        $\underline{\omega} \leftarrow \exp\left(-\frac{|\xi|^2}{\delta^2}\right)$ 
8:        $m_i \leftarrow m_i + \underline{\omega} |\xi|^2 \Delta V_j$ 
9:     end for
10:  end for
11: end procedure

```

Algorithm 2 Routine for calculation of the internal force density for a *linear peridynamic solid* material with a Gaussian influence function.

```

1: procedure LINEAR PERIDYNAMIC SOLID INTERNAL FORCE
2:   ▷ Initialize the global force density vector to zero.
3:   for each node  $i$  do
4:      $\mathbf{f}_i \leftarrow 0$ 
5:   end for
6:   ▷ Compute the dilatation for each node.
7:   for each node  $i$  do
8:      $\theta_i \leftarrow 0$ 
9:     for each node  $j$  in neighbor list for node  $i$  do
10:       $\xi \leftarrow \mathbf{x}_j - \mathbf{x}_i$ 
11:       $\eta \leftarrow \mathbf{u}_j - \mathbf{u}_i$ 
12:       $\underline{\omega} \leftarrow \exp\left(-\frac{|\xi|^2}{\delta^2}\right)$ 
13:       $e \leftarrow |\xi + \eta| - |\xi|$ 
14:       $\theta_i \leftarrow \theta_i + \frac{3}{m_i} \underline{\omega} |\xi| e \Delta V_j$ 
15:    end for
16:  end for
17:  ▷ Compute the pairwise contributions to the global force density vector.
18:  for each node  $i$  do
19:    for each node  $j$  in neighbor list for node  $i$  do
20:       $\xi \leftarrow \mathbf{x}_j - \mathbf{x}_i$ 
21:       $\eta \leftarrow \mathbf{u}_j - \mathbf{u}_i$ 
22:       $\underline{\omega} \leftarrow \exp\left(-\frac{|\xi|^2}{\delta^2}\right)$ 
23:       $e \leftarrow |\xi + \eta| - |\xi|$ 
24:       $\underline{e}^d \leftarrow e - \frac{\theta_i}{3} \underline{\omega} |\xi|$ 
25:       $\underline{t} \leftarrow \frac{3}{m_i} k \theta_i \underline{\omega} |\xi| + \frac{15\mu}{m_i} \underline{\omega} e^d$ 
26:       $\underline{\mathbf{M}} \leftarrow \frac{\xi + \eta}{|\xi + \eta|}$ 
27:       $\mathbf{f}_i \leftarrow \mathbf{f}_i + \underline{t} \underline{\mathbf{M}} \Delta V_j$ 
28:       $\mathbf{f}_j \leftarrow \mathbf{f}_j - \underline{t} \underline{\mathbf{M}} \Delta V_i$ 
29:    end for
30:  end for
31: end procedure

```

David J. Littlewood. Roadmap for Peridynamic Software Implementation. SAND Report 2015-9013. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2015.



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1. Ingredients of a peridynamic simulation

Bond failure law

- Critical stretch [Silling]
 - Brittle failure
 - Critical stretch value determined from the material's energy release rate
- Energy-based approach [Foster]
- Ductile failure models [Silling]

Example: Critical stretch law

- Bond fails irreversibly when critical stretch is exceeded

$$s_{\max} = \frac{y_{\max} - x}{x}$$

$$d = \begin{cases} 0 & \text{if } s_{\max} < s_0 \\ 1 & \text{if } s_{\max} \geq s_0 \end{cases}$$

S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, Peridynamic states and constitutive modeling, *Journal of Elasticity*, 88, 2007.



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1. Ingredients of a peridynamic simulation

Software implementation of the Critical Stretch Bond Failure Law

Algorithm 3 Routine for evaluation of the *critical stretch* bond failure law. Bond damage values, d_{ij} , are initialized to zero at the beginning of the simulation and set to a value of one if the bond stretch exceeds the specified critical value.

```
1: procedure CRITICAL STRETCH BOND FAILURE
2:   for each node  $i$  do
3:      $\triangleright$  Evaluate the stretch of each bond.
4:     for each node  $j$  in neighbor list for node  $i$  do
5:        $\xi \leftarrow \mathbf{x}_j - \mathbf{x}_i$ 
6:        $\eta \leftarrow \mathbf{u}_j - \mathbf{u}_i$ 
7:        $s = \frac{|\xi + \eta| - |\xi|}{|\xi|}$ 
8:        $\triangleright$  Check the bond stretch against the critical value.
9:       if  $s \geq s_o$  then
10:         $d_{ij} = 1.0$ 
11:      end if
12:    end for
13:  end for
14: end procedure
```



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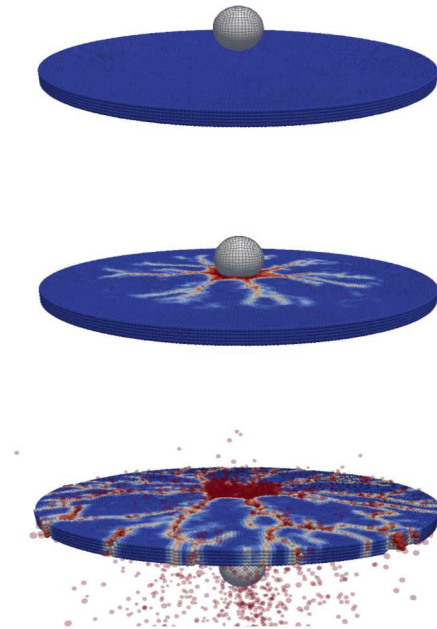
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1. Ingredients of a peridynamic simulation

Modeling contact

- Contact algorithms involve two distinct steps:
 - Proximity search
 - Enforcement
- The majority of meshfree peridynamic simulations to date have utilized the short-range force approach of Silling
- Local contact models have also been applied to peridynamic simulations
 - Iterative penalty approach to disallow interpenetration and minimize contact gap
- Contact modeling remains an open research topic in peridynamics



Simulation of brittle fracture

1. Silling, S.A. and Askari, E. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures* 83:1526-1535, 2005.
2. SIERRA Solid Mechanics Team, Sierra/SolidMechanics 4.22 user's guide, SAND Report 2011-7597, Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2011.



Computational Peridynamics

1. Ingredients of a peridynamic simulation

Short-range force contact models

- Spring-like repulsive force
- Active when relative distance is smaller than the prescribed contact radius
- Does not require explicit definition of contact surfaces
- Interpenetration is possible (high velocity, node misalignment)
- Friction may be incorporated by decomposing relative motion into normal and tangential components

Example of a short-range force contact model

Force is zero if distance between nodes is greater than d_{ij}

$$d_{ij} = \min \{ \beta |\mathbf{x}_j - \mathbf{x}_i|, \alpha (r_i + r_j) \}$$

Short-range force includes static and dynamic components

$$\mathbf{f}_{\text{static}} = A C_{ij} \left(\frac{d - |\mathbf{y}_j - \mathbf{y}_i|}{d} \right) \Delta V_i \Delta V_j \mathbf{M}_{ij}$$

$$C_{ij} = \frac{18k}{\pi \delta^4} \quad \mathbf{M}_{ij} = \frac{\mathbf{y}_j - \mathbf{y}_i}{|\mathbf{y}_j - \mathbf{y}_i|}$$

$$\mathbf{f}_{\text{damping}} = \epsilon \gamma_c v_{ij} \mathbf{M}_{ij}$$

$$v_{ij} = (\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{M}_{ij}$$

$$\gamma_c = 2 \sqrt{A C_{ij} \Delta V_i \Delta V_j \bar{m}}$$



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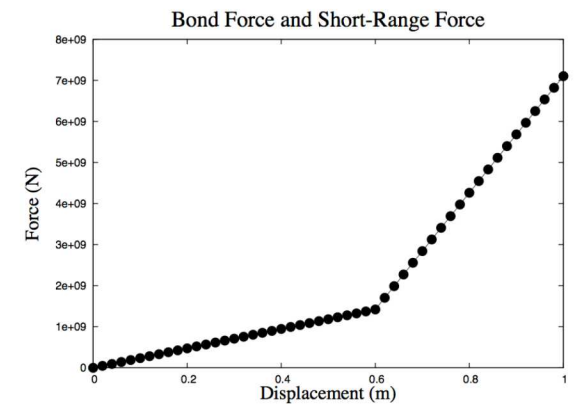
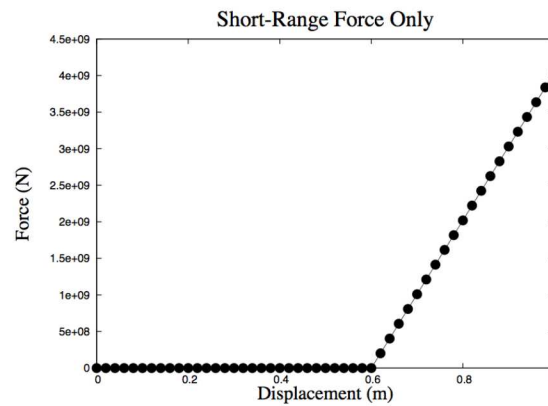
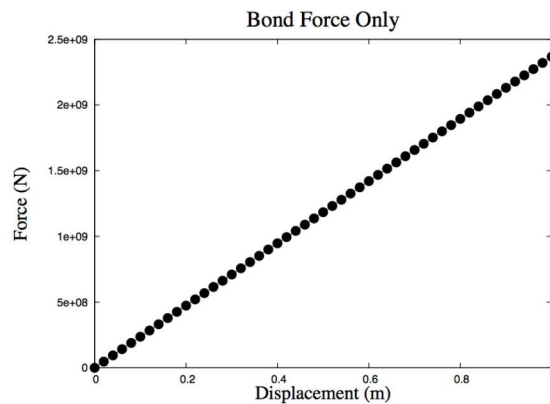
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1. Ingredients of a peridynamic simulation

Illustration of short range force and standard bond force



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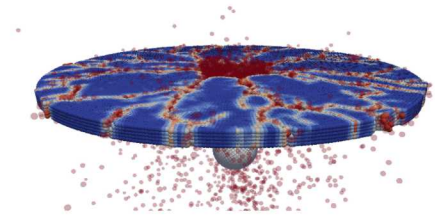
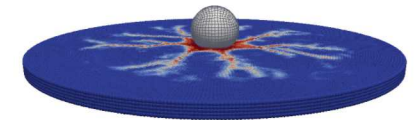
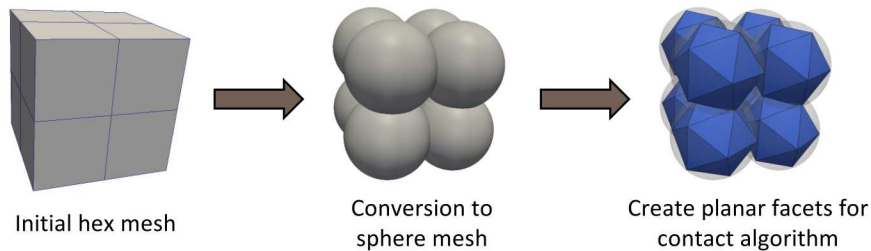
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1. Ingredients of a peridynamic simulation

Applying a traditional (local) contact model to peridynamics

- Contact algorithm operates on planar facets
- Peridynamics algorithm operates on sphere elements
- Lofted geometry allows for coupling of peridynamics and contact algorithm



Simulation of brittle fracture

D. J. Littlewood. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. In *Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition (IMECE)*, Vancouver, British Columbia, Canada, 2010.

SIERRA Solid Mechanics Team. Sierra/SolidMechanics 4.36 user's guide. SAND Report 2015-2199, Sandia National Laboratories, Albuquerque, NM and Livermore, CA.



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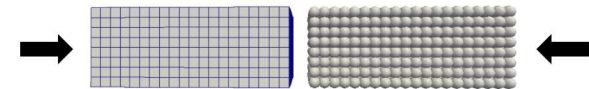
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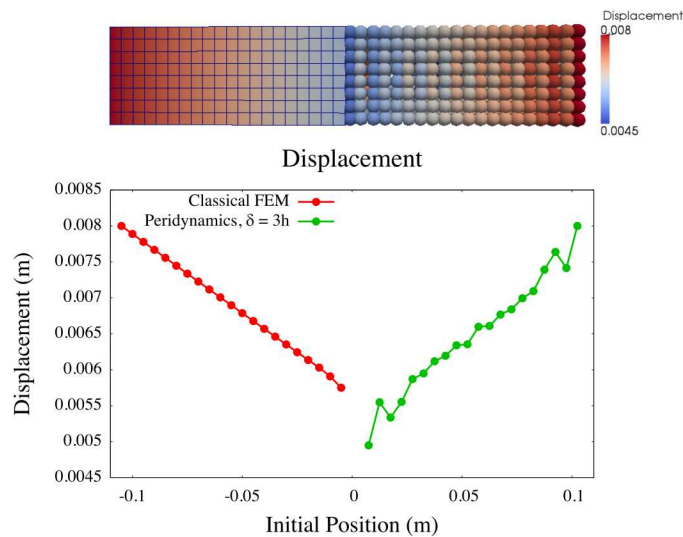
1. Ingredients of a peridynamic simulation

Challenges with contact and nonlocal models

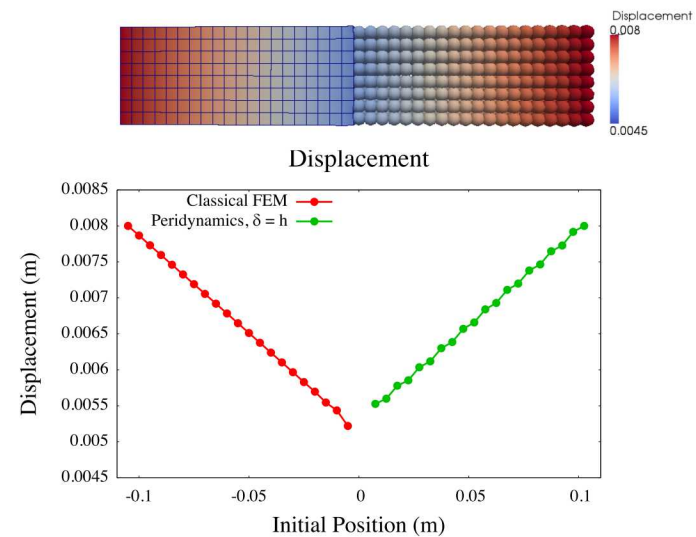
Simple test: To bars in contact and under compression



Horizon = 3 * Mesh Spacing



Horizon = Mesh Spacing



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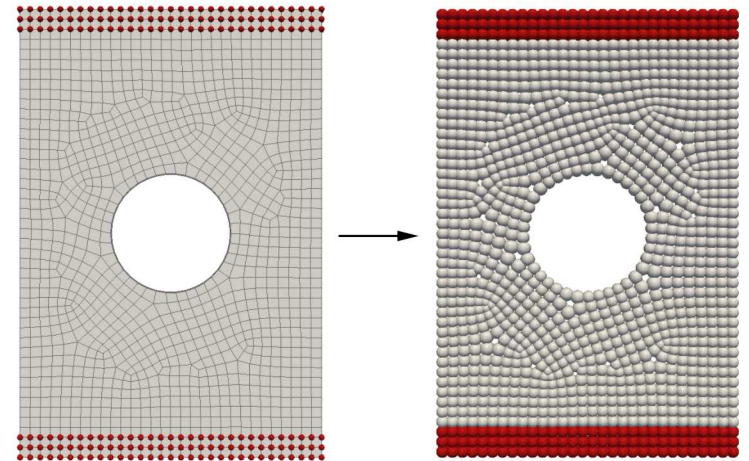
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Computational Peridynamics

1. Ingredients of a peridynamic simulation

Meshfree discretizations for peridynamics

- Meshfree discretization is defined by nodal volumes: (x, y, z, V)
- Each nodal volumes is assigned a material model, etc.
 - Nodal volumes may be grouped into "blocks" to simplify bookkeeping
- Example approaches for generating a meshfree discretization:
 - Simulation code internal mesh generator
 - Pre-processing script to generate (x, y, z, V) data
 - Conversion of a FEM hex/tet mesh to nodal volumes
- Concerns specific to peridynamics:
 - A variable horizon is generally not supported in peridynamics
 - Discretization can be nonuniform, but large variations in V can produce undesirable results
 - Boundary conditions are generally applied over a volumetric region; bookkeeping can be challenging, thin layers can cause difficulty



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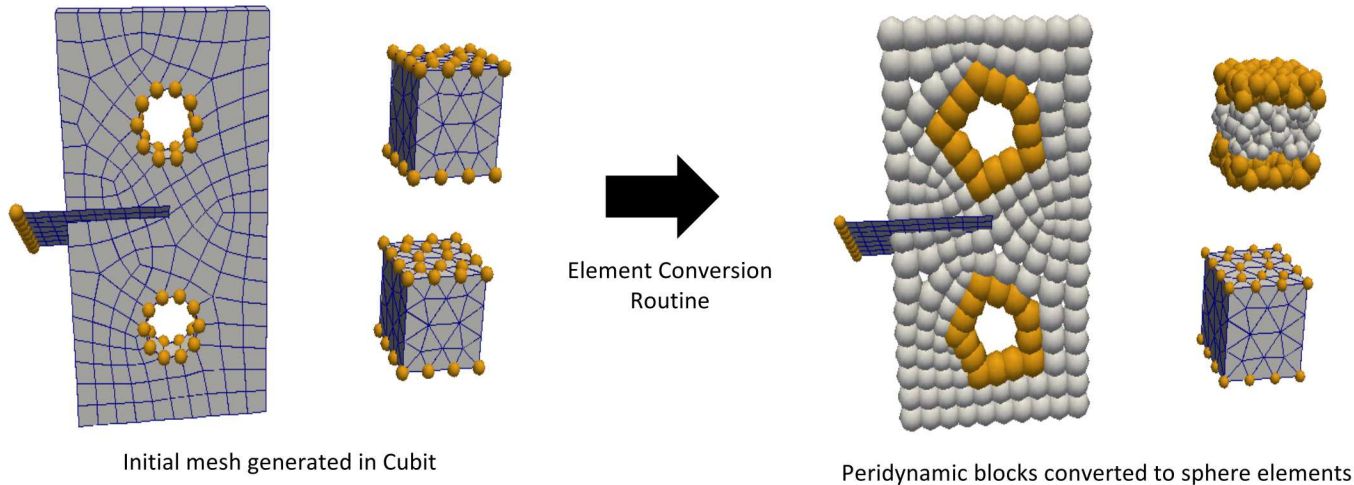
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1. Ingredients of a peridynamic simulation

Conversion of a FEM mesh to a meshfree discretization

- Node sets defined in the original hex/tet mesh must be transferred to meshless discretization
 - Elements are preserved (one-to-one map) but nodes in the FEM mesh are not preserved
- A mechanism is required for treating small features, controlling visibility between material points
 - A so-called bond filter may be used to disallow pairwise interactions



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1. Ingredients of a peridynamic simulation

Time integration for computational solid mechanics

- Explicit integration (dynamics): Velocity-Verlet, a.k.a. leapfrog
 - Well suited for modeling pervasive damage
 - Does not require the solution of a global system of equations
 - Conditionally stable, requires small time step
 - Equivalent to Newmark Beta with $\beta = 0$, $\gamma = 0.5$
- Implicit integration for quasi-statics
 - Assumes that acceleration is zero everywhere, solve for equilibrium
 - Wave propagation is neglected
 - Requires solution of a global system of equations
 - Care must be taken w.r.t. rigid body modes
- Implicit integration for dynamics
 - Newmark Beta
 - Requires solution of a global system of equations



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1. Ingredients of a peridynamic simulation

Explicit time integration

- Appropriate for dynamic problems and those with pervasive material failure

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

- Conditionally stable
- Requires estimate of the critical time step
- Requires many small time steps
- Easy to implement
- Does not require solution of global system of equations

Algorithm 1 Velocity Verlet

$$1: \mathbf{v}^{n+1/2} = \mathbf{v}^n + \frac{\Delta t}{2} \mathbf{M}^{-1}(\mathbf{f}^n + \mathbf{b}^n)$$

$$2: \mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \mathbf{v}^{n+1/2}$$

$$3: \mathbf{v}^{n+1} = \mathbf{v}^{n+1/2} + \frac{\Delta t}{2} \mathbf{M}^{-1}(\mathbf{f}^{n+1} + \mathbf{b}^{n+1})$$



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1. Ingredients of a peridynamic simulation

Implicit time integration

- Unconditionally stable
- Allows for large time steps
- Suitable for solution of static and quasi-static problems
- Suitable for implicit dynamics
- Requires solution of system of equations involving current and future configurations
 - Generally nonlinear
 - Newton-like methods require tangent stiffness matrix
 - Matrix-free schemes offer a promising alternative approach (e.g., Jacobian-Free Newton-Krylov)

S. A. Silling. Linearized theory of peridynamic states. *Journal of Elasticity*, 99:85–111, 2010.

J. A. Mitchell. A nonlocal, ordinary, state-based plasticity model for peridynamics. SAND Report 2011-3166, Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2011.

M.L. Parks, D.J. Littlewood, J.A. Mitchell, and S.A. Silling, Peridigm Users' Guide v1.0.0. Sandia Report SAND2012-7800, 2012.

Brothers, M.D., Foster, J.T., and Millwater, H.R. A comparison of different methods for calculating tangent-stiffness matrices in a massively parallel computational peridynamics code. *Computer Methods in Applied Mechanics and Engineering* 279:247-267, 2014.

David J. Littlewood. Roadmap for Peridynamic Software Implementation. SAND Report 2015-9013. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2015.



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1. Ingredients of a peridynamic simulation

The tangent stiffness matrix

- Approaches for construction:
 - Analytic (i.e., peridynamic modulus state)
 - Finite difference
 - Automatic differentiation
- Tangent is expensive
 - Expensive to construct
 - Expensive to store
 - Expensive to apply
- Number of nonzeros is directly related to the number of peridynamic bonds
 - Nonzero entry for all bonded nodes
 - Nonzero entry for all nodes that are bonded to a common node (state based)

Algorithm 1 Construction of the tangent stiffness matrix by central finite difference.

```
1: procedure TANGENT STIFFNESS MATRIX
2:   ▷ Initialize the tangent stiffness matrix to zero.
3:    $\mathbf{K} \leftarrow \mathbf{0}$ 
4:   ▷ Traverse each node in the discretization.
5:   for each node  $i$  do
6:      $\{\text{traversal list}\} \leftarrow$  node  $i$  and all neighbors of node  $i$ 
7:     for each node  $j$  in  $\{\text{traversal list}\}$  do
8:       ▷ Evaluate the force state at  $\mathbf{x}_i$  under perturbations of displacement.
9:       for each displacement degree of freedom  $r$  at node  $j$  do
10:         $\underline{\mathbf{T}}^{\epsilon+} \leftarrow \underline{\mathbf{T}}[\mathbf{x}_i](\mathbf{u} + \epsilon^r)$ 
11:         $\underline{\mathbf{T}}^{\epsilon-} \leftarrow \underline{\mathbf{T}}[\mathbf{x}_i](\mathbf{u} - \epsilon^r)$ 
12:        ▷ Evaluate pairwise forces under perturbations of displacement.
13:        for each node  $k$  in neighbor list of node  $i$  do
14:           $\mathbf{f}^{\epsilon+} \leftarrow \underline{\mathbf{T}}^{\epsilon+} \langle \mathbf{x}_k - \mathbf{x}_i \rangle \Delta V_i \Delta V_k$ 
15:           $\mathbf{f}^{\epsilon-} \leftarrow \underline{\mathbf{T}}^{\epsilon-} \langle \mathbf{x}_k - \mathbf{x}_i \rangle \Delta V_i \Delta V_k$ 
16:           $\mathbf{f}^{\text{diff}} \leftarrow \mathbf{f}^{\epsilon+} - \mathbf{f}^{\epsilon-}$ 
17:          for each degree of freedom  $s$  at node  $k$  do
18:             $K_{sr} \leftarrow K_{sr} + \frac{f_s^{\text{diff}}}{2\epsilon}$ 
19:          end for
20:        end for
21:      end for
22:    end for
23:  end for
24: end procedure
```



Computational Peridynamics

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- Ingredients of a peridynamics simulation
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 - Time integrator
- **Surface effect in peridynamic simulations**
- Estimation of the maximum stable time step for dynamic simulations
- Convergence of peridynamic models
- Demonstration of meshfree peridynamics for model analysis
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2. Surface effect

The peridynamic surface effect is a significant concern for engineering applications

- The majority of peridynamic material models were derived based on bulk response
- Material points close to the surface have a reduced nonlocal region (fewer bonds) relative to material points in the bulk
- Ordinary peridynamic material models exhibit inconsistencies at the surface

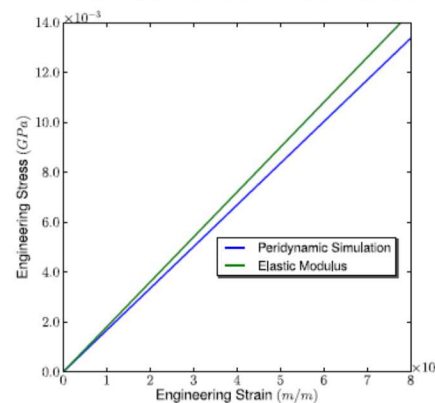
Axial Displacement



Stored Elastic Energy

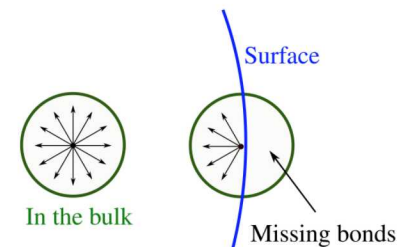


Stress versus Strain



Root problem

An important subset of peridynamic models assumes that a full neighborhood of bonds is present



[Images courtesy John Mitchell]



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2. Surface effect

One possible approach to mitigating the surface effect

- **Position-Aware Linear Solid (PALS)** constitutive model takes proximity to free surfaces into account

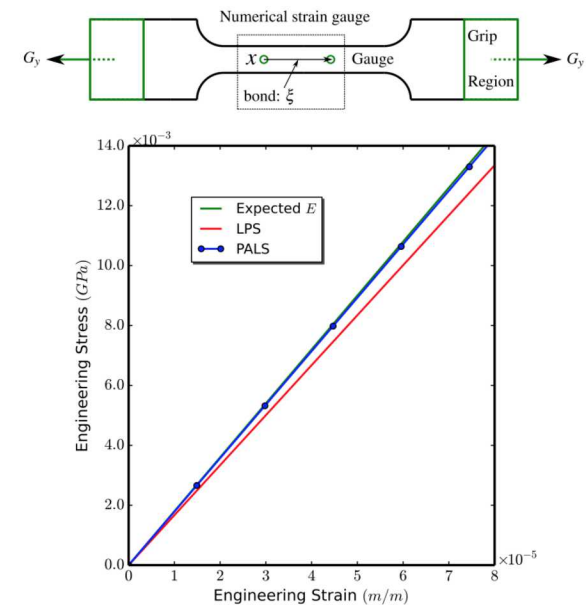
$$W = \frac{1}{2} K \theta^2 + \mu (\underline{\sigma} \underline{\varepsilon}) \bullet \underline{\varepsilon}, \quad \theta = (\underline{\omega} |X|) \bullet \underline{e}$$

- Coefficients σ and ω are determined for each point in the discretized model
- Calculation of σ and ω ensures that the expected strain energy is recovered for a set of *matching deformations*

J. Mitchell, S. Silling, and D. Littlewood. A position-aware linear solid (PALS) model for isotropic elastic materials. *Journal of Mechanics of Materials and Structures* 10(5):539-557, 2015.

Example calculation

PALS model accurately recovers elastic modulus in tensile test



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3. Estimation of the maximum stable time step

Candidate approaches for estimating the maximum stable time step

- Courant-Friedrichs-Lewy (CFL) condition

$$c = \sqrt{\frac{k}{\rho}} \quad \Delta t \leq \frac{\Delta x}{c}$$

- Approach of Silling and Askari for microelastic materials (von Neumann analysis)

$$\Delta t_c = \sqrt{\frac{2\rho}{\sum_p V_p C_{ip}}} \quad C_{ip} = |\mathbf{C}(x_p - x_i)| = \left| \frac{\partial \mathbf{f}}{\partial \boldsymbol{\eta}} \right|$$

- Global estimate using eigenvalue analysis (via Lanczos method)

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f} \quad (\mathbf{K} - \lambda\mathbf{M})\mathbf{x} = 0 \quad \Delta t_c = \frac{2}{\sqrt{\lambda}}$$

Littlewood, D.J., Thomas, J.D., and Shelton, T.R. Estimation of the critical time step for peridynamic models. Presented at the SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, Pennsylvania, 2013.

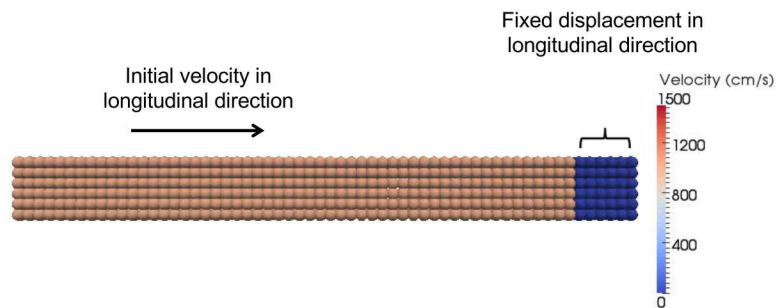


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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

3. Estimation of the maximum stable time step

- Critical time step for simulation of wave propagation
 - Compared approaches for estimating the maximum stable time step against empirical observations
 - CFL limit with element size as the length scale, and the method of Silling & Askari were conservative
 - Lanczos method was very accurate (but expensive)
 - CFL limit with the horizon as the length scale was unstable



Time Step	Kinetic Energy
0.1 μ s	3.51 J
0.2 μ s	3.51 J
0.3 μ s	3.51 J
0.4 μ s	3.51 J
0.5 μ s	14.1 J
0.6 μ s	NaN
0.7 μ s	NaN
0.8 μ s	NaN
0.9 μ s	NaN
1.0 μ s	1.75e+299 J

Silling and Askari

max. time step = 0.241 μ s
max. kinetic energy = 3.51 J

CFL Limit (element size)

max. time step = 0.329 μ s
max. kinetic energy = 3.51 J

Empirical Observation

max. time step = 0.499 μ s
max. kinetic energy = 3.51 J

Global Lanczos

max. time step = 0.500 μ s
max. kinetic energy = 3.51 J

CFL Limit (horizon)

max. time step = 1.00 μ s
max. kinetic energy = **unstable**



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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

3. Estimation of the maximum stable time step

Time Step	Percentage of Broken Bonds	Maximum Kinetic Energy ($t > 10 \mu s$)
0.01 μs	44.3 %	3.83 kJ
0.1 μs	44.5 %	3.82 kJ
0.2 μs	44.7 %	3.82 kJ
0.3 μs	45.3 %	3.82 kJ
0.4 μs	45.3 %	3.82 kJ
0.5 μs	45.4 %	3.82 kJ
0.6 μs	46.7 %	3.81 kJ
0.7 μs	49.1 %	3.83 kJ
0.8 μs	73.5 %	3.82 kJ
0.9 μs	95.3 %	4.39 kJ
1.0 μs	99.1 %	6.40 kJ

Silling and Askari

max. time step = 0.290 μs
percentage of broken bonds = 44.7 %
max. kinetic energy = 3.82 kJ

CFL Limit (element size)

max. time step = 0.395 μs
percentage of broken bonds = 45.3 %
max. kinetic energy = 3.51 J

Global Lanczos

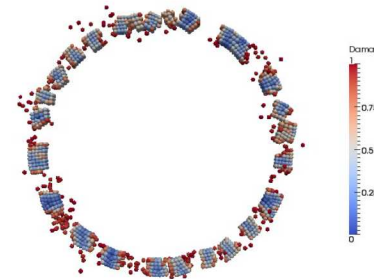
max. time step = 0.682 μs
percentage of broken bonds = 46.0 %
max. kinetic energy = 3.83 kJ

Empirical Observation

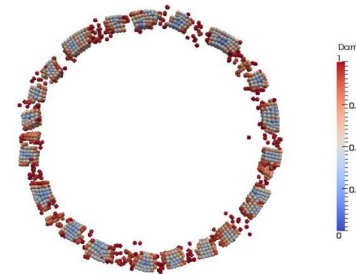
max. time step = 0.707 μs
percentage of broken bonds = 50.0 %
max. kinetic energy = 3.83 kJ

CFL Limit (horizon)

max. time step = 1.19 μs
percentage of broken bonds = 99.1 %
max. kinetic energy = **unstable**



Time step = 5.0 μs
46.7% of bonds broken



Time step = 7.5 μs
62.7 % of bonds broken



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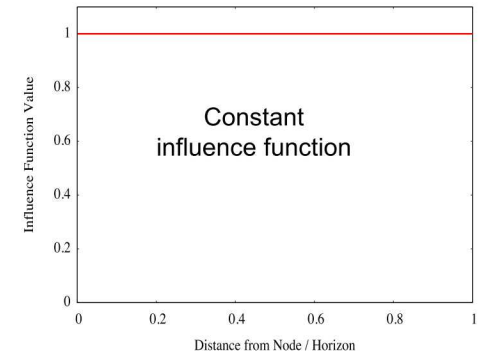
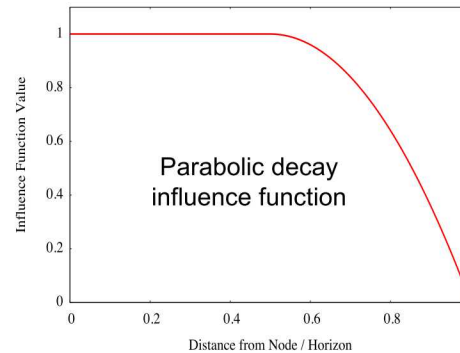
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Computational Peridynamics

3. Estimation of the maximum stable time step

- Choice of influence function affects critical time step
- Lanczos algorithm successfully detects changes in critical time step
- Observation: Influence function that decays with increasing bond length results in reduced critical time step



Peridynamic Linear Solid

	Parabolic decay influence function	Constant influence function
Max. Lanczos time step	0.381 μ s	0.434 μ s
Empirical result	0.381 μ s	0.434 μ s

14% Increase

Correspondence Material Model

	Parabolic decay influence function	Constant influence function
Max. Lanczos time step	0.490 μ s	0.549 μ s
Empirical result	0.490 μ s	0.549 μ s

12% Increase



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Short Course
Peridynamic Theory of Solid Mechanics

Computational Peridynamics

Outline

- Ingredients of a peridynamics simulation
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- Surface effect in peridynamic simulations
- Estimation of the maximum stable time step for dynamic simulations
- **Convergence of peridynamic models**
- Demonstration of meshfree peridynamics for model analysis
- Modeling damage and failure



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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

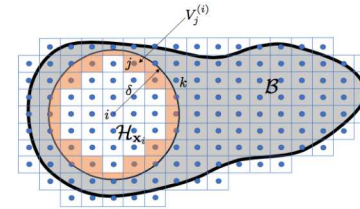
5. Convergence of meshfree models

Convergence of meshfree peridynamics

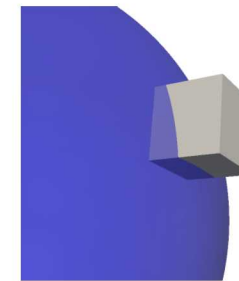
- Two forms of convergence: horizon and mesh spacing
 - Convergence to a local solution as horizon approaches zero
 - Convergence to a nonlocal solution under mesh refinement with horizon held constant
- Current practice introduces errors and spoils convergence
 - Quadrature, poor treatment of neighbor-horizon intersections

Approaches for improving convergence behavior

- Improved treatment of neighbor-horizon intersections
 - Variety of correction techniques (scalar multiplier):
 - PD-LAMMPS, Hu-Ha-Bobaru, analytic partial area (2D)
 - Application of smoothly-decaying influence functions
 - Approximate calculation of partial volumes (3D)
 - Geometry, quadrature



Neighbor-horizon intersection in 2D



Neighbor-horizon intersection in 3D

Seleson, P. Improved one-point quadrature algorithms for two-dimensional peridynamic models based on analytical calculations, *CMAME*, 282, pp. 184-217, 2014.

Seleson, P., and Littlewood, D.J. Convergence studies in meshfree peridynamic simulations. *Computers and Mathematics with Applications* 71:2432-2448, 2016.

Seleson, P., and David J. Littlewood, D.J. Numerical tools for effective meshfree discretizations of peridynamic models. In George Z. Voyiadjis, editor, *Handbook of Nonlocal Continuum Mechanics for Materials and Structures*. Springer. Accepted.



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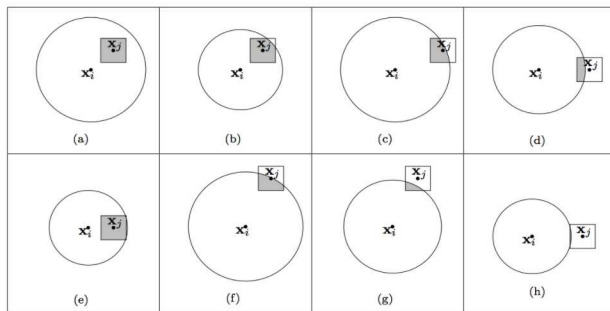
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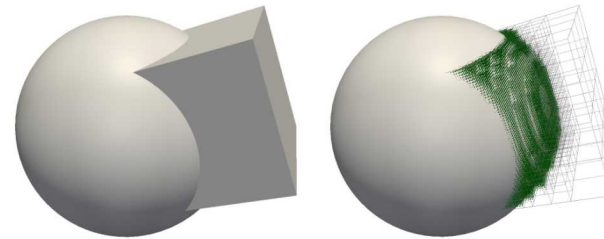
Computational Peridynamics

5. Convergence of meshfree models

Explicit calculation of partial areas (2D) and volumes (3D)



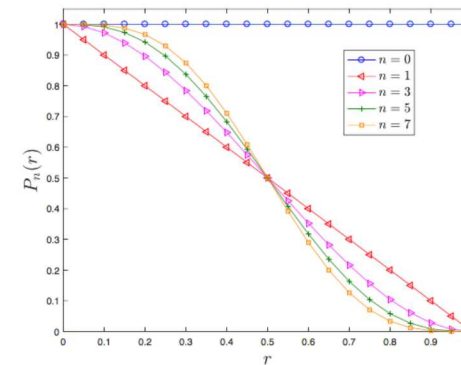
Analytic calculation of partial areas (2D)



Numerical approximation of partial volumes (3D)

Application of smoothly-decaying influence functions

- Mitigates numerical difficulties at neighbor-horizon interface
- Changes the underlying model (physics)



Candidate influence functions



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5. Convergence of meshfree models

Numerical experiments: Solution of statics problem with known solution

- Linearized LPS material model equates to classical local model under assumption of a quadratic displacement field

Peridynamic equation of static elasticity, linearized LPS model

$$\begin{aligned}
 - \int_{\mathcal{H}_{\mathbf{x}}} \frac{\omega(|\boldsymbol{\xi}|)}{m} \left\{ (3K - 5G) (\vartheta^{\text{lin}}[\mathbf{x}] + \vartheta^{\text{lin}}[\mathbf{x} + \boldsymbol{\xi}]) \boldsymbol{\xi} \right. \\
 \left. + 30G \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} (\mathbf{u}(\mathbf{x} + \boldsymbol{\xi}) - \mathbf{u}(\mathbf{x})) \right\} dV_{\boldsymbol{\xi}} = \mathbf{b}(\mathbf{x}) \quad \mathbf{x} \in \Omega, \\
 \mathbf{u}(\mathbf{x}) = \mathbf{g}(\mathbf{x}) \quad \mathbf{x} \in \mathcal{B} \setminus \Omega.
 \end{aligned}$$

Classical Navier-Cauchy equation
of static elasticity

$$- \left[G \nabla^2 \mathbf{u}(\mathbf{x}) + \left(K + \frac{1}{3} G \right) \nabla (\nabla \cdot \mathbf{u})(\mathbf{x}) \right] = \mathbf{b}(\mathbf{x}).$$

- Permits verification via method of manufactured solutions

Quadratic displacement field

$$\begin{aligned}
 u(\mathbf{x}) &= U_{11}x^2 + U_{22}y^2 + U_{33}z^2 + U_{12}xy + U_{13}xz + U_{23}yz, \\
 v(\mathbf{x}) &= V_{11}x^2 + V_{22}y^2 + V_{33}z^2 + V_{12}xy + V_{13}xz + V_{23}yz, \\
 w(\mathbf{x}) &= W_{11}x^2 + W_{22}y^2 + W_{33}z^2 + W_{12}xy + W_{13}xz + W_{23}yz,
 \end{aligned}$$

Body force density for static equilibrium

$$\begin{aligned}
 b_1 &= - \left[2G (U_{11} + U_{22} + U_{33}) + \left(K + \frac{1}{3} G \right) (2U_{11} + V_{12} + W_{13}) \right], \\
 b_2 &= - \left[2G (V_{11} + V_{22} + V_{33}) + \left(K + \frac{1}{3} G \right) (U_{12} + 2V_{22} + W_{23}) \right], \\
 b_3 &= - \left[2G (W_{11} + W_{22} + W_{33}) + \left(K + \frac{1}{3} G \right) (U_{13} + V_{23} + 2W_{33}) \right].
 \end{aligned}$$



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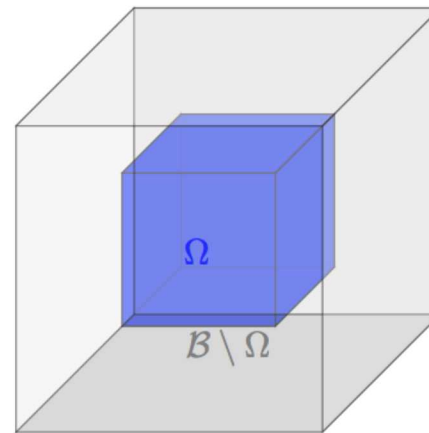
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Computational Peridynamics

5. Convergence of meshfree models

Numerical experiments: Solution of statics problem with known solution

- Cubic computational domain
- U_{11} nonzero, all other components of quadratic displacement field set to zero
- Displacement prescribed over boundary layer
- Body force applied to inner region
- Solution for inner region should converge to the analytic solution under mesh refinement (horizon fixed)



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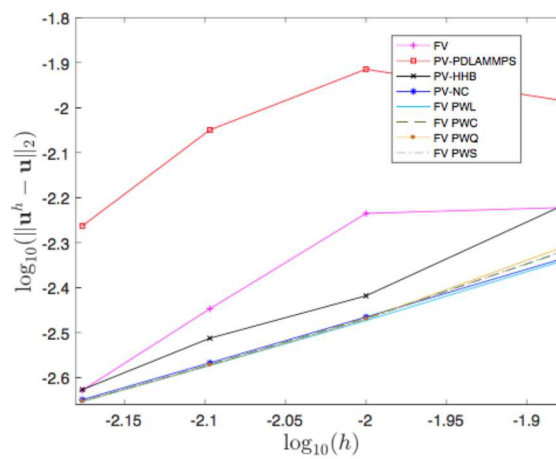
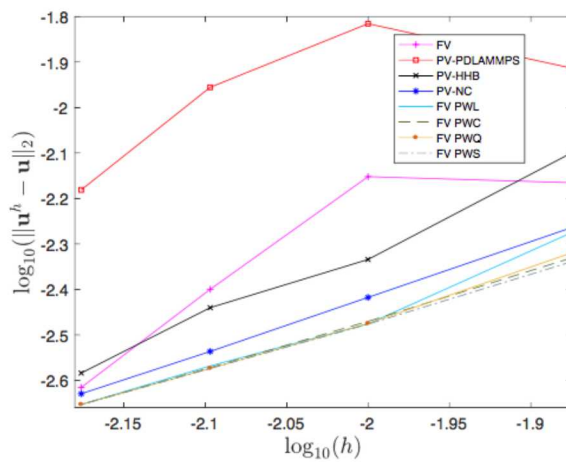
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Computational Peridynamics

5. Convergence of meshfree models

Convergence results for different partial-volume schemes and different influence functions



Algorithm	$\alpha = 0$		$\alpha = 1$	
	\bar{r}	R	\bar{r}	R
FV	1.53	0.165	1.38	0.128
PV-PDLAMMPS	0.86	0.186	0.89	0.167
PV-HHB	1.56	0.035	1.34	0.030
PV-NC	1.22	0.003	1.05	0.001
FV PWL	1.24	0.036	1.05	0.004
FV PWC	1.07	0.005	1.11	0.009
FV PWQ	1.10	0.014	1.15	0.016
FV PWS	1.04	0.006	1.12	0.012



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Computational Peridynamics

5. Convergence of meshfree models

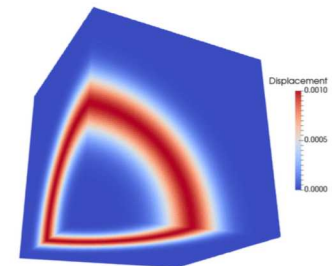
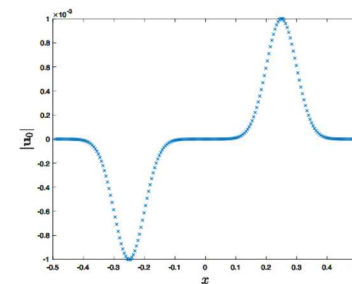
Numerical experiments: Solution of dynamics problem

- Cubic computational domain
- Initial displacement applied to shell of internal nodes
- Wave allowed to propagate freely through domain
- Solutions compared against highly-refined benchmark solution

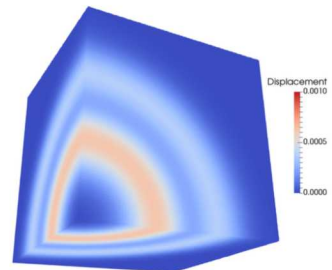
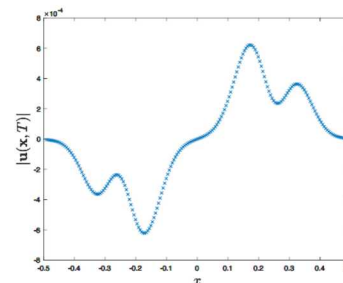
Initial conditions

$$\mathbf{u}_0(\mathbf{x}) = \begin{cases} ae^{-\frac{(|\mathbf{x}|-r_0)^2}{\ell^2}} \frac{\mathbf{x}}{|\mathbf{x}|} & \text{if } (r_0 - 3\ell) \leq |\mathbf{x}| \leq (r_0 + 3\ell) \\ 0 & \text{otherwise,} \end{cases}$$
$$\mathbf{v}_0(\mathbf{x}) = \mathbf{0},$$

Initial displacement



Final displacement



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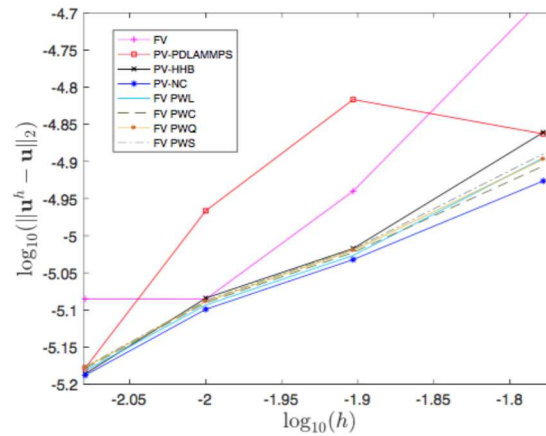
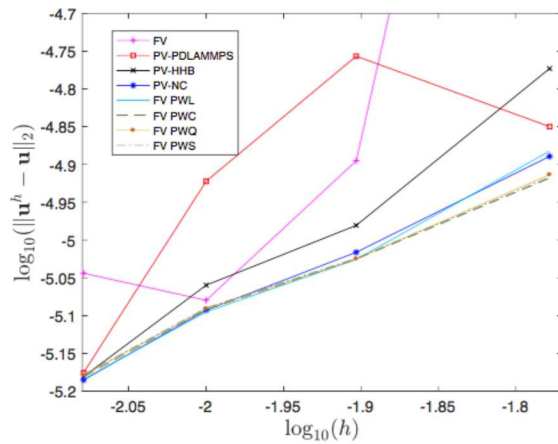
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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

5. Convergence of meshfree models

Convergence results for different partial-volume schemes and different influence functions



Algorithm	$\alpha = 0$		$\alpha = 1$	
	\bar{r}	R	\bar{r}	R
FV	4.27	0.514	1.41	0.099
PV-PDLAMMPS	1.05	0.202	1.02	0.157
PV-HHB	1.31	0.038	1.04	0.026
PV-NC	0.96	0.013	0.85	0.016
FV PWL	0.98	0.019	0.93	0.017
FV PWC	0.85	0.016	0.88	0.015
FV PWQ	0.86	0.015	0.91	0.015
FV PWS	0.85	0.016	0.93	0.015



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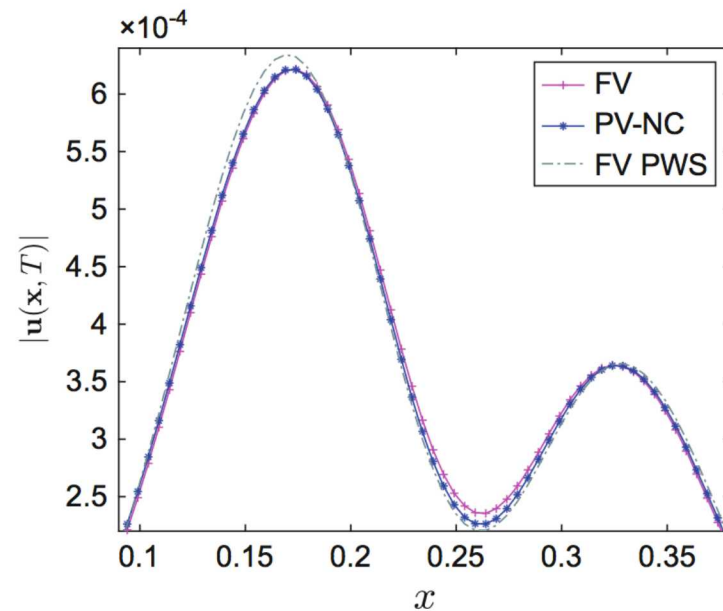
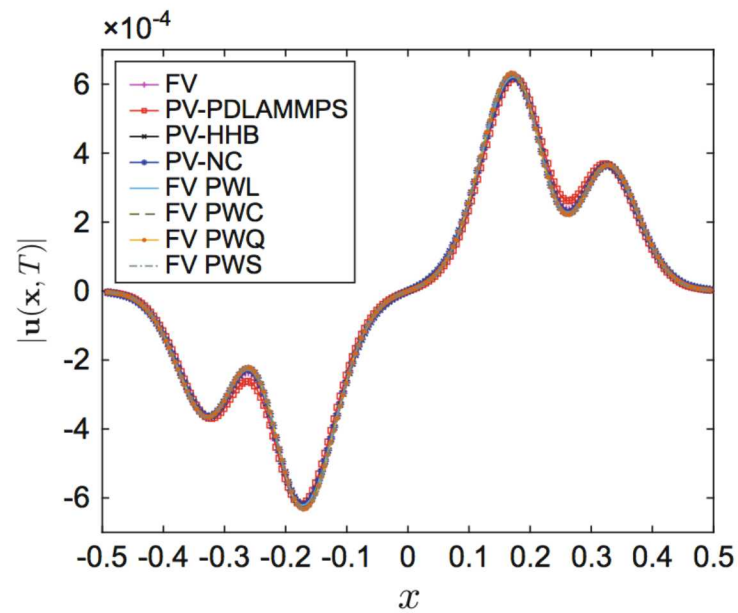
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5. Convergence of meshfree models

Changing the influence function changes the underlying model (physics)



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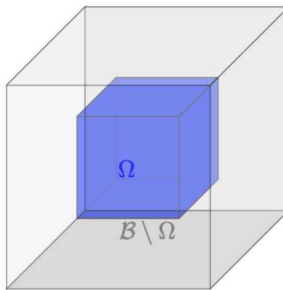
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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

5. Convergence of meshfree models

Convergence studies with peridynamic are inherently difficult / expensive

- Volumetric region for prescribed displacement becomes large as horizon increases
- Number of nodes / bonds becomes large as horizon decreases
- Number of bonds becomes huge as the ratio of the horizon to the node spacing becomes large



δ/L	0.000	0.001	0.005	0.010	0.050	0.100
$ B \setminus \Omega / \Omega $	0.000	0.012	0.062	0.130	0.953	3.630

N_{neig} (δ/h)	Number of PD bonds	
	FV	PV-NC
3	12,433,244	25,077,672
4	62,022,592	110,046,364
5	242,986,412	384,681,876
6	753,964,092	1,040,684,328
7	1,838,660,296	2,552,461,732
8	4,080,378,204	5,479,353,788
9	8,456,684,628	10,782,968,496
10	15,752,838,172	19,683,573,672



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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

Outline

- Ingredients of a peridynamics simulation
 - Governing equations
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 - Discretization
 - Time integrator
- Surface effect in peridynamic simulations
- Estimation of the maximum stable time step for dynamic simulations
- Convergence of peridynamic models
- **Demonstration of meshfree peridynamics for model analysis**
- Modeling damage and failure



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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

7. Demonstration of meshfree peridynamics for modal analysis

Why modal analysis?

- Modal analysis is used to determine the dominant structural modes and natural frequencies of a given system
- Peridynamic models containing material damage can be used in the analysis of experimentally-measured frequency responses (nondestructive testing of bridges, etc.)

How does it work?

- Modal analysis is achieved by solving for the dominant eigenvalues and eigenvectors of the tangent stiffness matrix

Test case

One-dimensional analysis of simply-supported beam with square cross section

Classical (local) analytic solution

E	Elastic modulus
h	Height and depth of beam
m	Mass of beam
l	Length of beam
n	Positive integer
f_n	Characteristic linear frequency (mode n)

$$f_n = \frac{n^2 \pi}{2} \sqrt{\frac{E h^4}{12 m l^4}}$$



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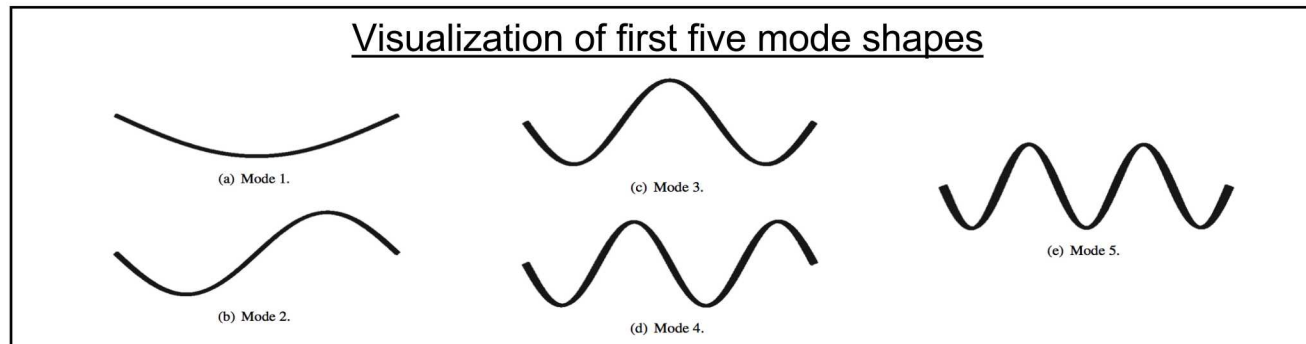
Computational Peridynamics

7. Modal analysis of peridynamic models

Results from peridynamic simulation

- Beam dimensions: 1m x 0.01m x 0.01m
- Material: steel ($E = 206.8$ GPa)
- Peridynamic horizon: 0.000713m
- Correspondence elastic material model
- Beam discretized with 840K elements

Mode	Classical Theory	Peridynamic Simulation	Percent Difference
1	23.30 Hz	23.26 Hz	0.17 %
2	93.22 Hz	93.02 Hz	0.21 %
3	209.73 Hz	209.06 Hz	0.32 %
4	372.86 Hz	371.29 Hz	0.43 %
5	582.59 Hz	579.39 Hz	0.55 %



David J. Littlewood, Kyran Mish, and Kendall Pierson. 2012. Peridynamic simulation of damage evolution for structural health monitoring. Proceedings of the ASME 2012 International Mechanical Engineering Congress and Exposition (IMECE2012), Houston, TX.



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Peridynamic Theory of Solid Mechanics

Computational Peridynamics

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- **Modeling damage and failure**



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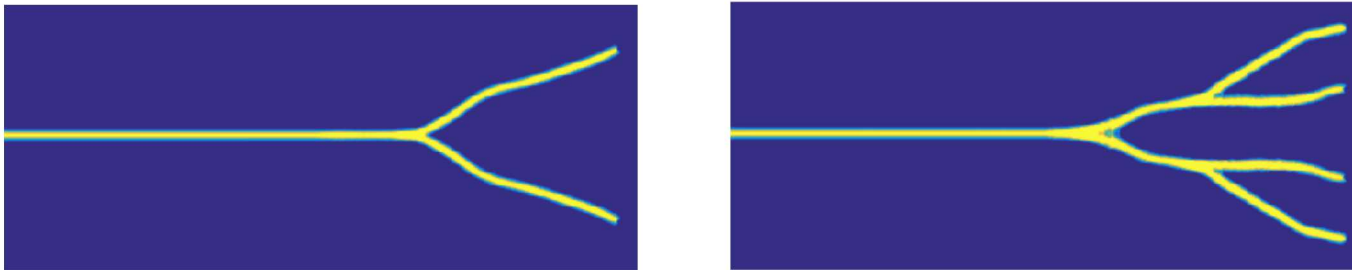
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Computational Peridynamics

7. Modeling failure and damage

Modeling failure and damage with peridynamics

- Modeling pervasive damage is a primary advantage of peridynamics
- Nonlocality separates the length scale (horizon) from the mesh, which **relieves mesh dependence**
- **Convergent solutions** to material failure problems (localizing phenomenon) are possible with peridynamics, impossible with a local model
- Cracks develop / grow / branch in peridynamic simulations based primarily on energetics



[Images courtesy Seleson]



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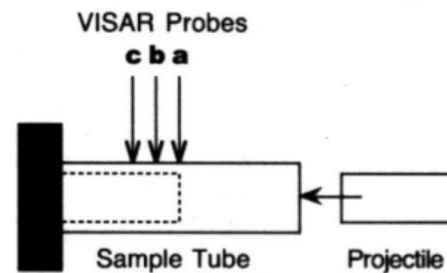
7. Modeling failure and damage

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-plastic material model with linear hardening
- Lexan plugs modeled with traditional FEM, EOS-enabled Johnson-Cook material model



Experimental setup
[Vogler, et al.]



Computational model

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.

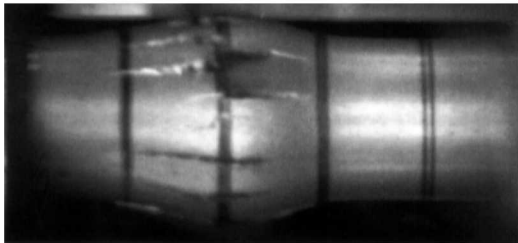
D. J. Littlewood. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. In *Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition (IMECE)*, Vancouver, British Columbia, Canada, 2010.



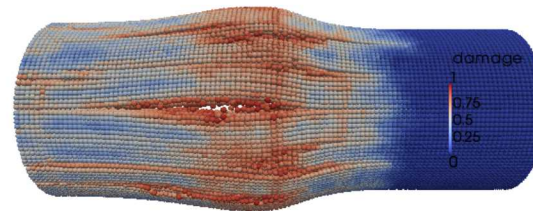
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Computational Peridynamics

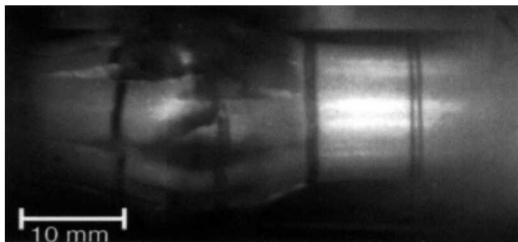
7. Modeling failure and damage



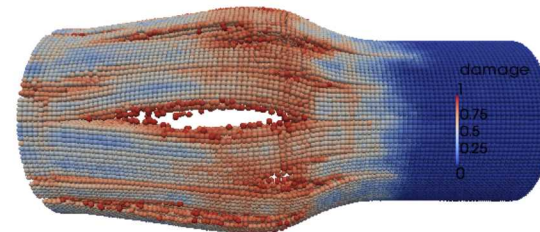
Experimental image at 15.4
microseconds [Vogler et. al]



Simulation at 15.4 microseconds



Experimental image at 23.4
microseconds [Vogler et. al]



Simulation at 23.4 microseconds



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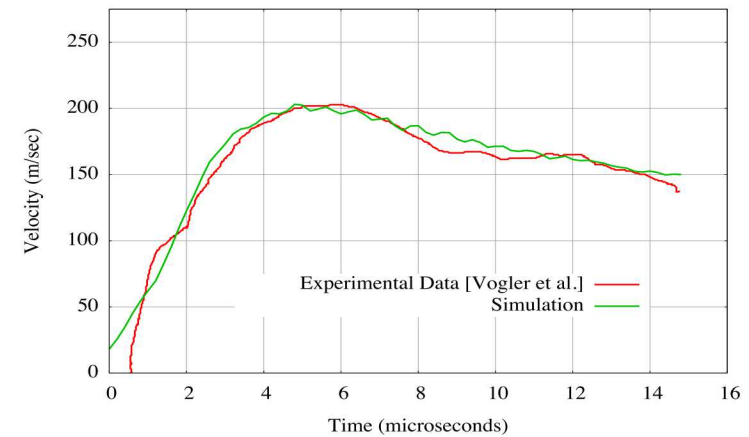
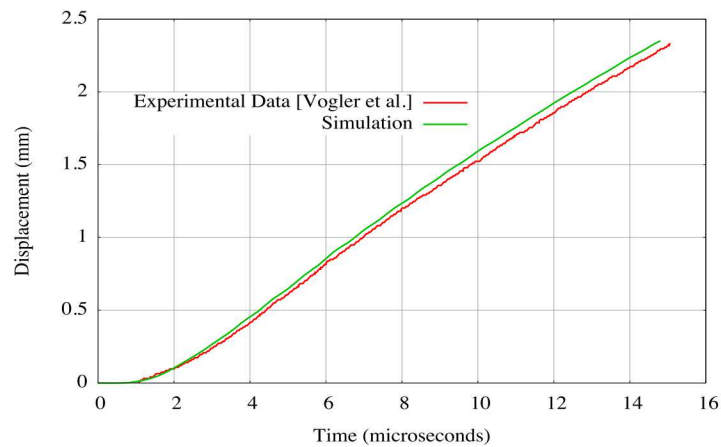
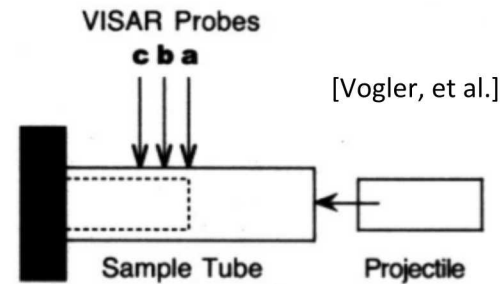


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7. Modeling failure and damage

Displacement and velocity
on tube surface
at probe position A



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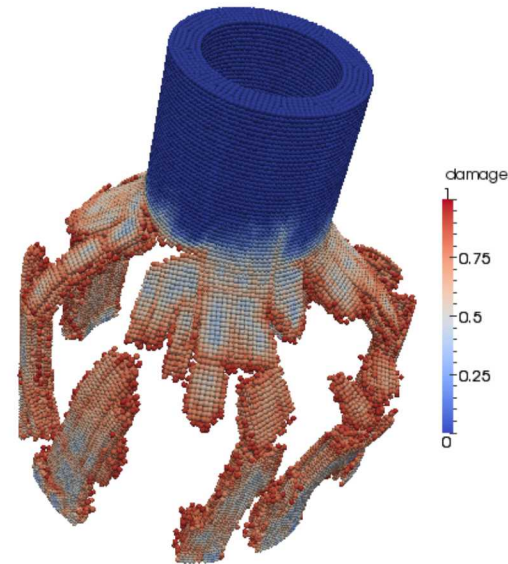
Short Course
Peridynamic Theory of Solid Mechanics

Computational Peridynamics

7. Modeling failure and damage

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



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Computational Peridynamics

7. Modeling failure and damage

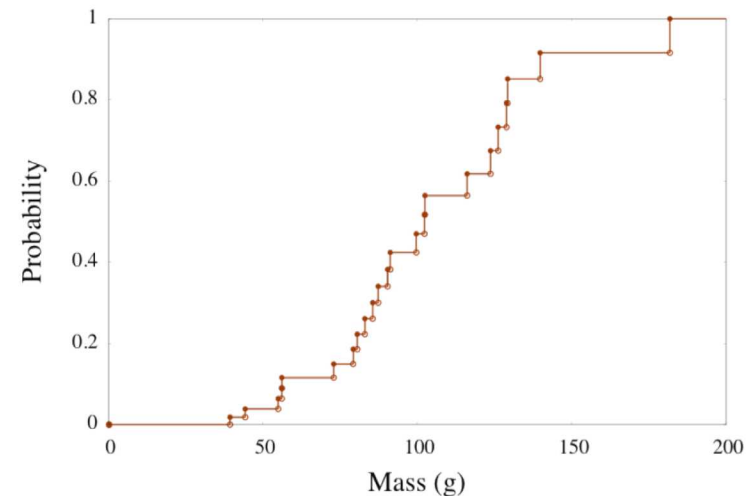
Characterizing fragment data with a Cumulative Distribution Function

- A CDF can be created for any quantity of interest
- Provides insight into the fragmentation process
- Allows for comparison with experimental data

$$P(X) = \frac{1}{M} \sum_{\substack{i=1 \\ X_i \leq X}}^{N_{\text{frag}}} m_i \quad M = \sum_{i=1}^{N_{\text{frag}}} m_i$$

$P(X)$ is the probability that a given material point belongs to a fragment whose property value X_i is less than X

Example: CDF for fragment mass



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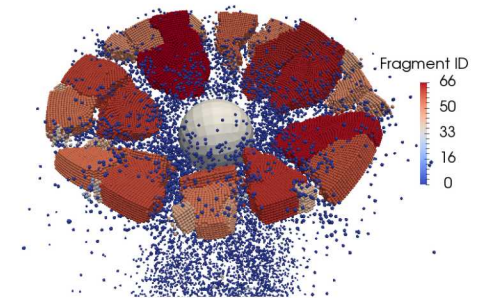
7. Modeling failure and damage

Fragments identification in a meshfree peridynamic simulation

- Provide post-processing capability for characterizing fragmentation process

Approach

- Computational domain is traversed to identify networks of unbroken bonds
- Process is iterative, converges when fragment numbers are no longer changing
- A fragment number is assigned to every node in the model
- Tiny fragments are (optionally) combined and assigned a common fragment number
- Related quantities of interest are computed for each fragment
 - Mass, center of mass, linear and angular momentum, moments of inertia, block names



Identification of
disk fragments

```
DO initialize fragment numbers to node ids
REPEAT until fragment numbers stop changing
  FOR every node  $i$ 
    FOR all neighbors  $j$  of node  $i$ 
      IF the bond between nodes  $i$  and  $j$  is unbroken
        DO assign  $\max(F_i, F_j)$  to nodes  $i$  and  $j$ 
```

David Littlewood, Stewart Silling, Paul Demmie. 2016. Identification of Fragments in a Meshfree Peridynamic Simulation. Proceedings of the ASME 2016 International Mechanical Engineering Congress and Exposition, Phoenix, Arizona.

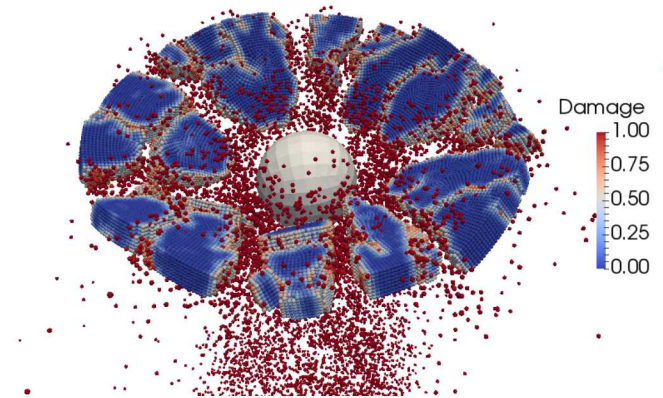


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7. Modeling failure and damage

- Elastic sphere impacting a brittle elastic disk
- Projectile modeled with classical FEM
 - Elastic material model
 - Radius 5.0 mm,
 - Initial velocity 35.0 m/s
- Target modeled with peridynamics
 - Bond-based microelastic material model
 - Critical stretch bond failure rule
 - Radius 17.0 mm, height 2.5 mm



Material parameters
for projectile

Parameter	Value
Density ρ	993.1 kg/m ³
Bulk modulus k	1.0 GPa
Poisson's ratio ν	0.3

Material parameters
for target

Parameter	Value
Density ρ	2200.0 kg/m ³
Bulk modulus k	14.9 GPa
Horizon δ	1.0 mm
Critical stretch s_{crit}	0.0005

Parameters for
fragment identification

output file = frag_data.csv
increment = 4.0e-5
minimum fragment size = 5



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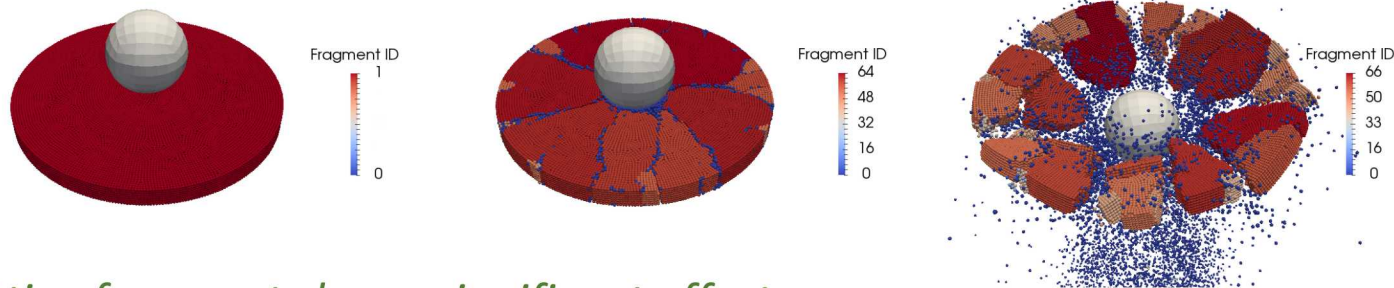
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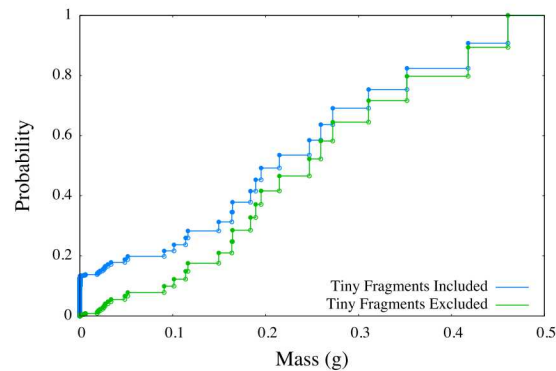
Computational Peridynamics

7. Modeling failure and damage

Algorithm captures evolution of fragmentation process



Exclusion of tiny fragments has a significant effect



Threshold Fragment Size	Total Mass of Tiny Fragments
1	0.000 g
2	0.531 g
3	0.613 g
4	0.641 g
5	0.651 g



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Computational Peridynamics

7. Modeling failure and damage

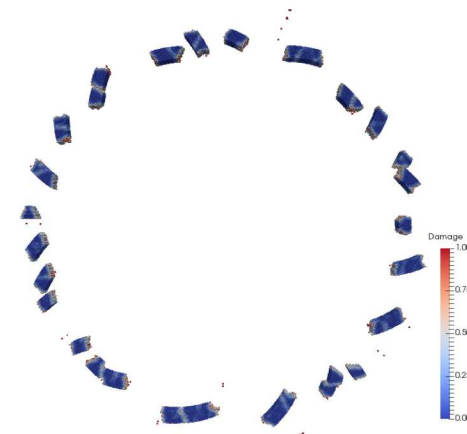
- Fragmentation of an expanding ductile ring
- Bond-based microplastic material model
- Critical stretch bond failure rule
- Inner radius 110.0 mm, outer radius 125.0 mm, height 25.0 mm
- Initial outward radial velocity 100.0 m/s
- ~60,000 nodal volumes

Discretization of ring



Material parameters

Parameter	Value
Density ρ	7850.0 kg/m ³
Bulk modulus k	140.0 GPa
Horizon δ	5.025 mm
Yield stretch s_Y	0.000988
Critical stretch s_{crit}	0.02



Parameters for
fragment identification

output file = frag_data.csv
increment = 2.4e-5
minimum fragment size = 0



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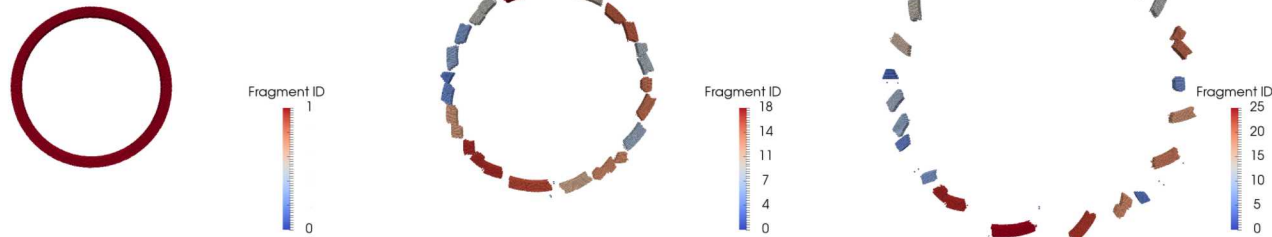
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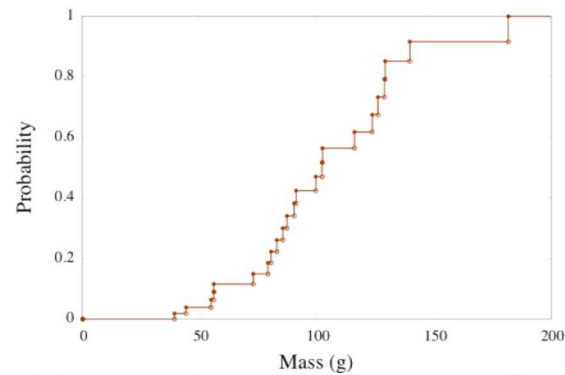
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7. Modeling failure and damage

Algorithm captures evolution of fragmentation process



Exclusion of tiny fragments does not affect results



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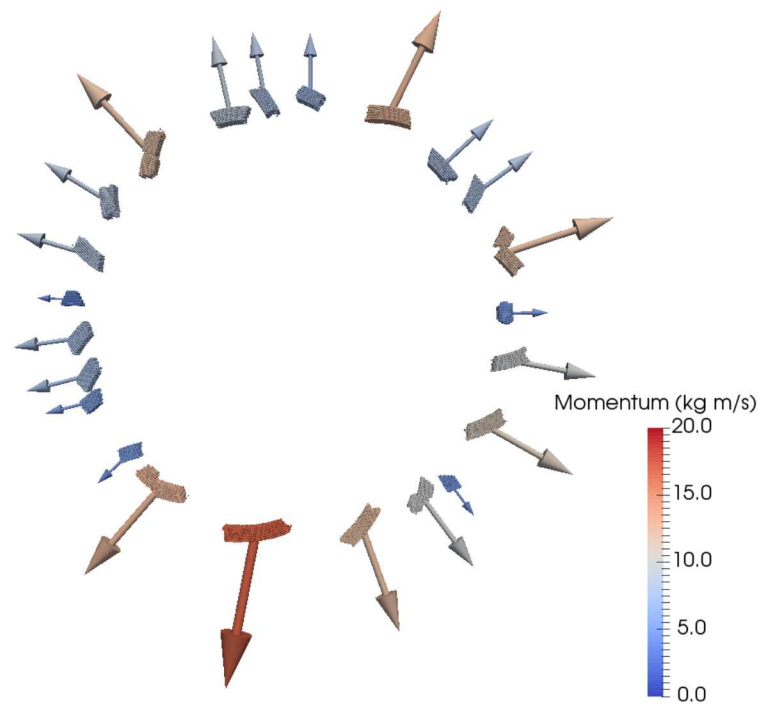
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Computational Peridynamics

7. Modeling failure and damage

Visualization of
fragment momentum



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The Peridigm Peridynamics Code



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The Peridigm Peridynamics Code

Outline

- Introduction
- Example simulations
 - Tensile test
 - Disk impact
- Hands-on examples



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Short Course
Peridynamic Theory of Solid Mechanics

Peridigm Tutorial

1. Introduction

What is Peridigm?

- Open-source software developed at Sandia National Laboratories
- C++ code based on Sandia's *Trilinos* project
- Platform for multi-physics peridynamic simulations
- Capabilities:
 - State-based constitutive models
 - Implicit and explicit time integration
 - Contact for transient dynamics
 - Large-scale parallel simulations
- Compatible with pre- and post-processing tools
 - Cubit mesh generation
 - Paraview visualization tools
 - SEACAS utilities
- Designed for extensibility



<https://peridigm.sandia.gov>



<https://trilinos.org>



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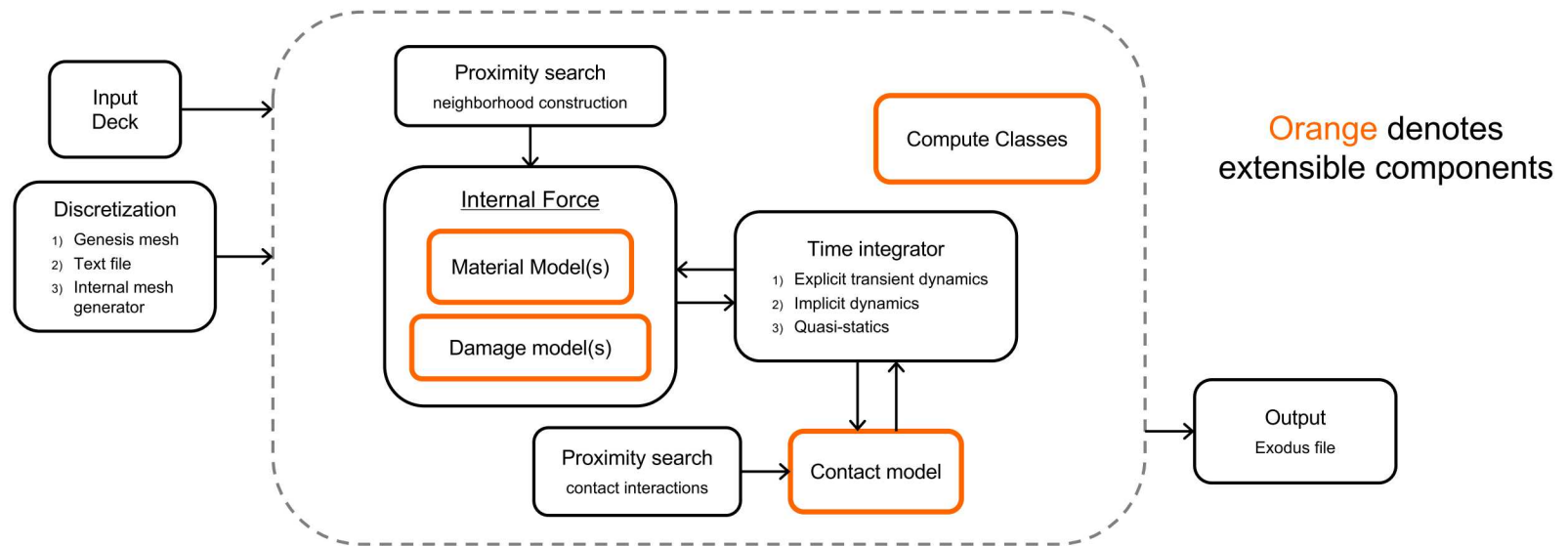
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Peridigm Tutorial

1. Introduction

Design goals

- State-based peridynamics
- Explicit and Implicit time integration
- Contact
- Massively parallel
- Performance
- Extensibility



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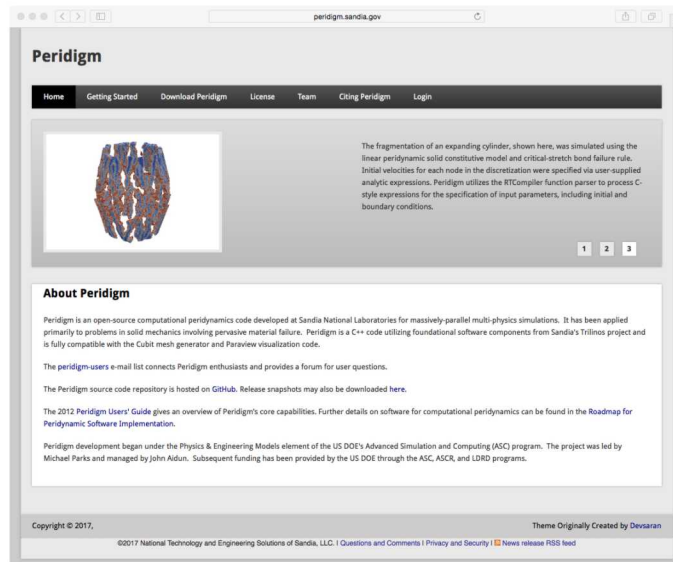
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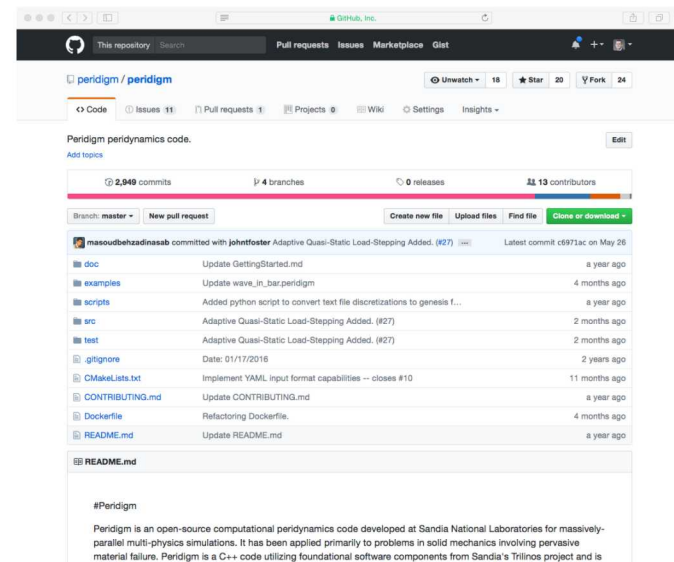
1. Introduction

Obtaining the Peridigm source code

<http://peridigm.sandia.gov>



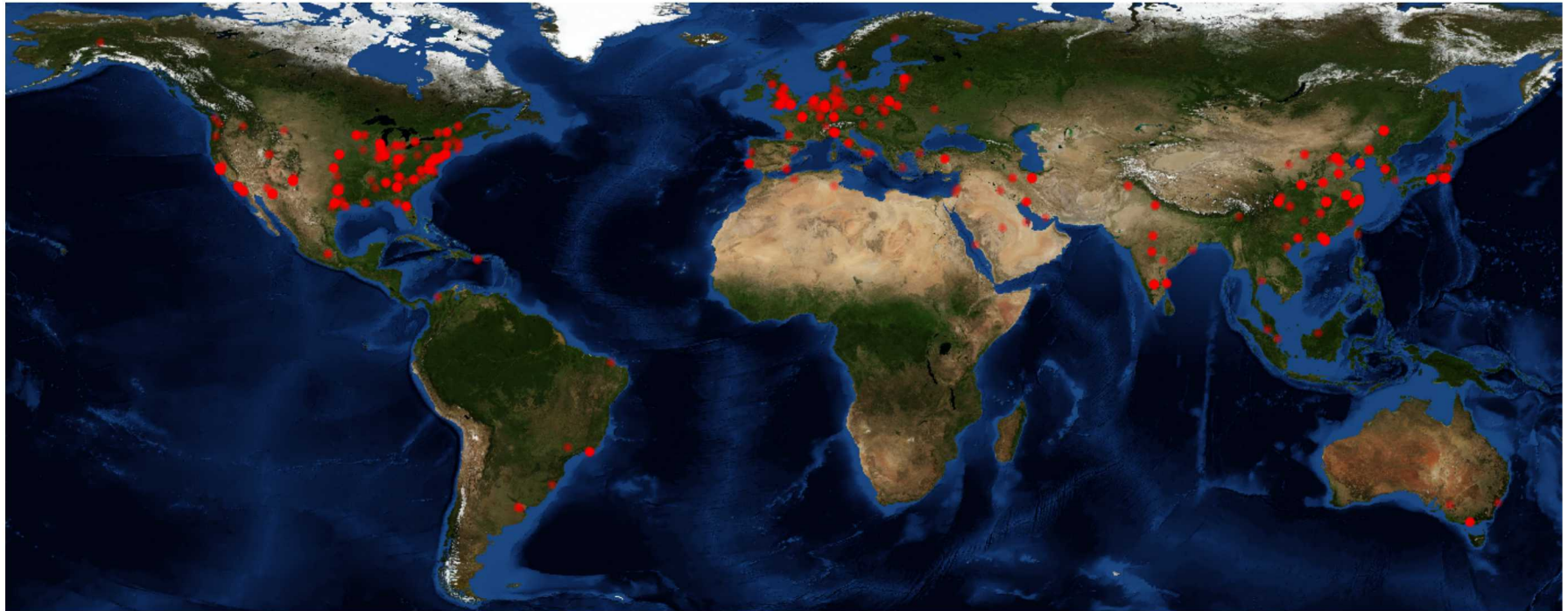
<https://github.com/peridigm/peridigm>



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Peridigm Tutorial

1. Introduction



Peridigm Downloads from <http://peridigm.sandia.gov> (July 2014 – June 2017)



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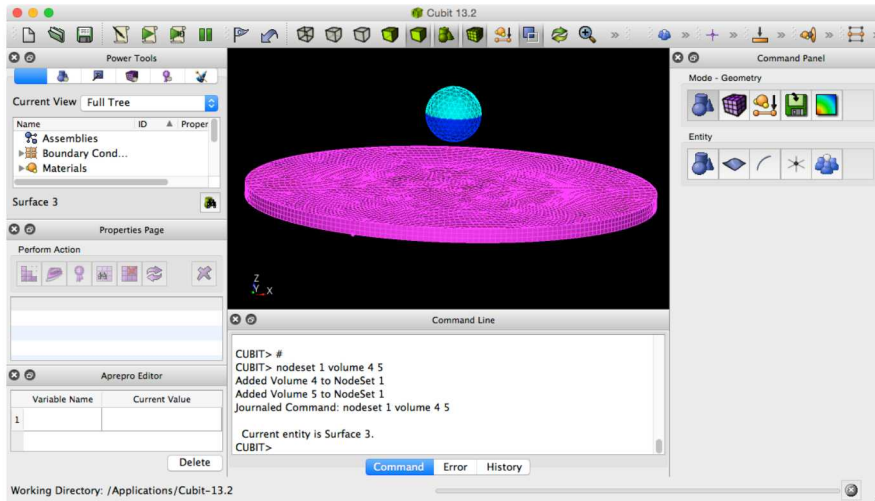
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1. Introduction

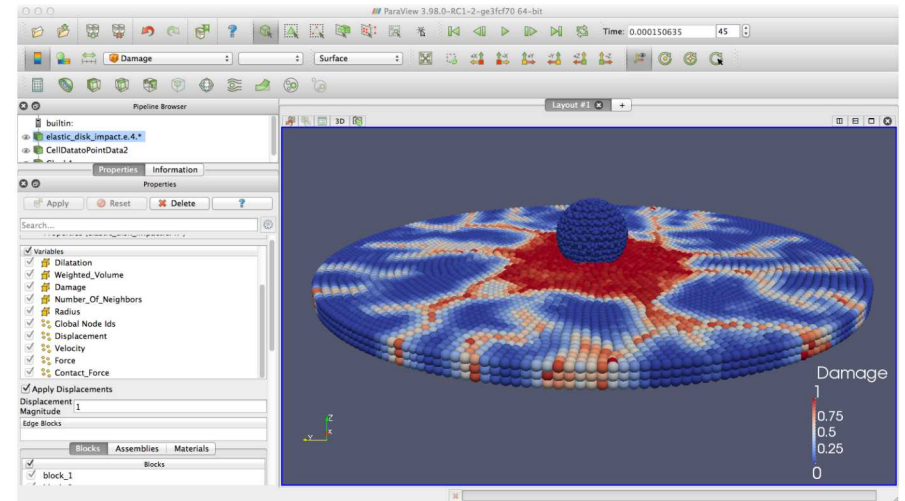
Peridigm Input

- Input deck (text file)
- Discretization (mesh, can be text file or genesis file)



Peridigm Output

- Genesis file



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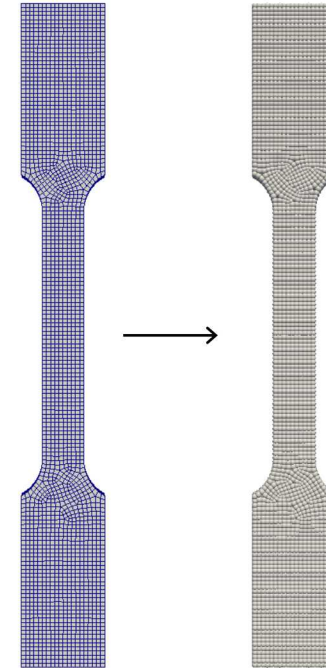
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2. Example simulation: Tensile test

Simulation of a standard displacement-controlled tensile test

- Meshless discretization created from genesis hexahedral mesh (Cubit)
- Elastic correspondence model (classic stress-strain model)
- Prescribed displacement boundary conditions
- Quasi-static time integration
 - Newton solver
 - Construction of tangent stiffness matrix
- Compute classes for computing engineering stress and strain
 - Track ends of virtual strain gauge
 - Compute net reaction forces



Discretization created by converting a hexahedral mesh to nodal volumes



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2. Example simulation: Tensile test

Input deck (1 of 4)

```
Discretization
  Type "Exodus"
  Input Mesh File "tensile_test.g"

Materials
  My Material
    Material Model "Elastic Correspondence"
    Density 8.0
    Bulk Modulus 1.500e12
    Shear Modulus 6.923e11
    Hourglass Coefficient 0.02

Blocks
  My Block
    Block Names "block_1 block_2 block_3"
    Material "My Material"
    Horizon 0.16

Solver
  Initial Time 0.0
  Final Time 1.0
  QuasiStatic
    Number of Load Steps 4
    Absolute Tolerance 1.0
    Maximum Solver Iterations 10
```



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2. Example simulation: Tensile test

Input deck (2 of 4)

```
Boundary Conditions
  Prescribed Displacement Bottom
    Type "Prescribed Displacement"
    Node Set "nodelist_1"
    Coordinate "y"
    Value "y*0.005*t"
  Prescribed Displacement Top
    Type "Prescribed Displacement"
    Node Set "nodelist_2"
    Coordinate "y"
    Value "y*0.005*t"
  Prescribed Displacement Fix Bottom Rigid Body Motion In X
    Type "Prescribed Displacement"
    Node Set "nodelist_3"
    Coordinate "x"
    Value "0.0"
  Prescribed Displacement Fix Bottom Rigid Body Motion In Z
    Type "Prescribed Displacement"
    Node Set "nodelist_4"
    Coordinate "z"
    Value "0.0"
  Prescribed Displacement Fix Top Rigid Body Motion In X
    Type "Prescribed Displacement"
    Node Set "nodelist_5"
    Coordinate "x"
    Value "0.0"
  Prescribed Displacement Fix Top Rigid Body Motion In Z
    Type "Prescribed Displacement"
    Node Set "nodelist_6"
    Coordinate "z"
    Value "0.0"
```



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2. Example simulation: Tensile test

Input deck (3 of 4)

Compute Class Parameters

Strain Gage Top Initial Position

Compute Class "Nearest_Point_Data"

X 0.0317

Y 1.238

Z 0.0

Variable "Model_Coordinates"

Output Label "Gage_Top_Initial_Position"

Verbose "True"

Strain Gage Bottom Initial Position

Compute Class "Nearest_Point_Data"

X 0.0317

Y -1.238

Z 0.0

Variable "Model_Coordinates"

Output Label "Gage_Bottom_Initial_Position"

Verbose "True"

Strain Gage Top Displacement

Compute Class "Nearest_Point_Data"

X 0.0317

Y 1.238

Z 0.0

Variable "Displacement"

Output Label "Gage_Top_Displacement"

Verbose "True"

Strain Gage Bottom Displacement

Compute Class "Nearest_Point_Data"

X 0.0317

Y -1.238

Z 0.0

Variable "Displacement"

Output Label "Gage_Bottom_Displacement"

Verbose "True"

Top Reaction Force

Compute Class "Block_Data"

Calculation Type "Sum"

Block "block_3"

Variable "Force"

Output Label "Top_Reaction_Force"

Bottom Reaction Force

Compute Class "Block_Data"

Calculation Type "Sum"

Block "block_1"

Variable "Force"

Output Label "Bottom_Reaction_Force"



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2. Example simulation: Tensile test

Input deck (4 of 4)

Output

```
Output File Type "ExodusII"
Output Filename "tensile_test"
Output Frequency 1
Output Variables
  Displacement "true"
  Velocity "true"
  Element_Id "true"
  Proc_Num "true"
  Force_Density "true"
  Hourglass_Force_Density "true"
  Force "true"
  Volume "true"
  Gage_Top_Initial_Position "true"
  Gage_Bottom_Initial_Position "true"
  Gage_Top_Displacement "true"
  Gage_Bottom_Displacement "true"
  Top_Reaction_Force "true"
  Bottom_Reaction_Force "true"
  Deformation_Gradient "true"
  Cauchy_Stress "true"
  Radius "true"
  Number_Of_Neighbors "true"
  Neighborhood_Volume "true"
```



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2. Example simulation: Tensile test

Output (1 of 3)

```
-- Peridigm
-- version 1.5.0 (Dev)

MPI initialized on 8 processors.

Nearest Point Data Compute Class:
  Requested variable: Model_Coordinates
  Requested location: 0.0317, 1.238, 0
  Closest Element Id: 6715
  Closest Element Position: 0.0317576, 1.23833, 8.35356e-17

Nearest Point Data Compute Class:
  Requested variable: Model_Coordinates
  Requested location: 0.0317, -1.238, 0
  Closest Element Id: 6676
  Closest Element Position: 0.0317605, -1.23854, 8.38424e-17

Nearest Point Data Compute Class:
  Requested variable: Displacement
  Requested location: 0.0317, 1.238, 0
  Closest Element Id: 6715
  Closest Element Position: 0.0317576, 1.23833, 8.35356e-17

Nearest Point Data Compute Class:
  Requested variable: Displacement
  Requested location: 0.0317, -1.238, 0
  Closest Element Id: 6676
  Closest Element Position: 0.0317605, -1.23854, 8.38424e-17

Allocating global tangent matrix...
  number of rows = 37875
  number of nonzeros = 30378033
```



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2. Example simulation: Tensile test

Output (2 of 3)

```
Load step 1, initial time = 0, final time = 0.25, convergence criterion = 1
iteration 1: residual = 6.15e+09
iteration 2: residual = 1.46418e+08
iteration 3: residual = 326680
iteration 4: residual = 42.3547
iteration 5: residual = 0.00403217
cpu time for load step = 1.2e+02 sec., cumulative cpu time = 1.2e+02 sec.
```

```
Load step 2, initial time = 0.25, final time = 0.5, convergence criterion = 1
iteration 1: residual = 6.1e+09
iteration 2: residual = 1.4e+06
iteration 3: residual = 2.8e+02
iteration 4: residual = 0.042
cpu time for load step = 65 sec., cumulative cpu time = 1.9e+02 sec.
```

```
Load step 3, initial time = 0.5, final time = 0.75, convergence criterion = 1
iteration 1: residual = 6.1e+09
iteration 2: residual = 1.4e+06
iteration 3: residual = 2.3e+02
iteration 4: residual = 0.035
cpu time for load step = 64 sec., cumulative cpu time = 2.5e+02 sec.
```

```
Load step 4, initial time = 0.75, final time = 1, convergence criterion = 1
iteration 1: residual = 6.1e+09
iteration 2: residual = 1.4e+06
iteration 3: residual = 1.9e+02
iteration 4: residual = 0.029
cpu time for load step = 63 sec., cumulative cpu time = 3.1e+02 sec.
```



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2. Example simulation: Tensile test

Output (3 of 3)

Memory Usage (Heap Alloc MB):

	Min	Max	Ave
Zoltan Search Tree	12	12	12
Post Execute	70	88	79
Allocated Jacobian	1.2e+02	1.4e+02	1.3e+02

Wallclock Time (seconds):

	Min	Max	Ave
Total	3.2e+02	3.2e+02	3.2e+02
Solve Linear System	1.7e+02	1.7e+02	1.7e+02
Output	0.086	0.14	0.12
Line Search	2.5	2.5	2.5
Internal Force	1.8	1.9	1.8
Gather/Scatter	1	1.1	1.1
Evaluate Jacobian	1.4e+02	1.4e+02	1.4e+02
Compute Residual	2.8	2.9	2.9
Apply Kinematic B.C.	0.0011	0.016	0.0044
Apply Initial Conditions	0	1.2e-06	5.1e-07
Apply Boundary Conditions	0.17	6.9	1.8
Apply Body Forces	1.5e-05	3.4e-05	1.9e-05
Allocate Global Tangent	7	7	7



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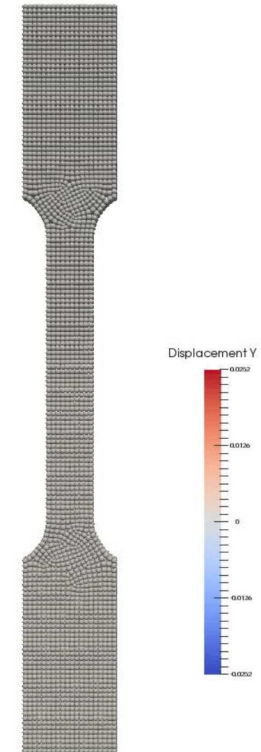
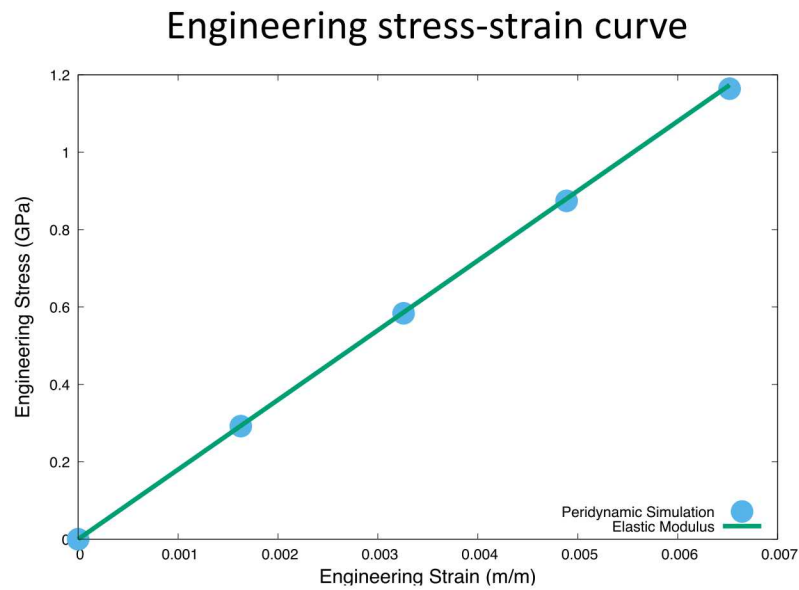
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2. Example simulation: Tensile test

Results



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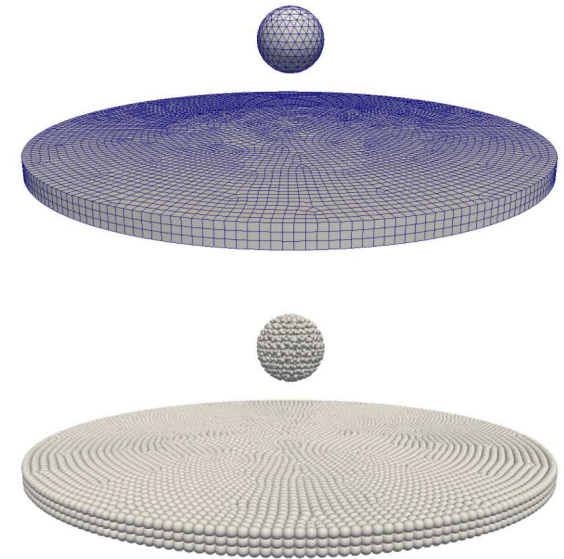
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3. Example simulation: Disk impact

Simulation of impact / brittle fracture

- Meshless discretization created from genesis hex/tet mesh (Cubit)
- Linear Peridynamic Solid material model
- Critical stretch bond failure rule applied to target
- Multiple material blocks (projectile, target)
- Explicit transient dynamics
- Short-range force contact model
- Initial velocity applied to projectile
- Standard exodus output, plus history output for global data



Discretization created by converting a hex/tet mesh to nodal volumes



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3. Example simulation: Disk impact

Input deck (1 of 4)

```
Discretization
  Type "Exodus"
  Input Mesh File "disk_impact.g"

Materials
  Disk Material
    Material Model "Elastic"
    Density 2200.0
    Bulk Modulus 14.90e9
    Shear Modulus 8.94e9
  Ball Material
    Material Model "Elastic"
    Density 7700.0
    Bulk Modulus 160.00e9
    Shear Modulus 78.30e9

Damage Models
  Disk Damage Model
    Damage Model "Critical Stretch"
    Critical Stretch 0.0005
```



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3. Example simulation: Disk impact

Input deck (2 of 4)

```
Blocks
  Disk Block
    Block Names "block_1"
    Material "Disk Material"
    Damage Model "Disk Damage Model"
    Horizon 0.0031
  Ball Block
    Block Names "block_2"
    Material "Ball Material"
    Horizon 0.0031

Contact
  Search Radius 0.01
  Search Frequency 100
Models
  My Contact Model
    Contact Model "Short Range Force"
    Contact Radius 0.000775
    Spring Constant 1.0e12
Interactions
  Interaction Disk with Ball
    First Block "block_1"
    Second Block "block_2"
    Contact Model "My Contact Model"
```



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3. Example simulation: Disk impact

Input deck (3 of 4)

```
Boundary Conditions
  Sphere Initial Velocity
    Type "Initial Velocity"
    Node Set "odelist_1"
    Coordinate "z"
    Value "-100.0"
```

```
Solver
  Initial Time 0.0
  Final Time 0.0008
  Verlet
    Safety Factor 0.7
```



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3. Example simulation: Disk impact

Input deck (4 of 4)

```
# Output file for full data set, disk_impact.e
Output_1
  Output File Type "ExodusII"
  Output Filename "disk_impact"
  Output Frequency 350
  Output Variables
    Displacement "true"
    Velocity "true"
    Element_Id "true"
    Proc_Num "true"
    Dilatation "true"
    Weighted_Volume "true"
    Force "true"
    Contact_Force "true"
    Damage "true"
    Number_Of_Neighbors "true"
    Radius "true"

# Output file for history data (global data), disk_impact.h
Output_2
  Output File Type "ExodusII"
  Output Filename "disk_impact"
  Output Frequency 35
  Output Variables
    Global_Kinetic_Energy "true"
    Global_Linear_Momentum "true"
    Global_Angular_Momentum "true"
```



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3. Example simulation: Disk impact

Output

```
-- Peridigm
-- version 1.5.0 (Dev)

MPI initialized on 8 processors.

** Warning: the selected contact search radius, 0.01, is large
** relative to the maximum element diameter (0.000735518).
** This may lead to the memory capacity being exceeded.

Time step (seconds):
  Stable time step  1.59402e-07
  User time step   not provided
  Safety factor    0.7
  Time step        1.11581e-07

Total number of time steps 7169

Explicit time integration [=====100% Complete]

Memory Usage (Heap Alloc MB):
```

	Min	Max	Ave
Zoltan Search Tree	73.8654	117.254	95.4224
Post Execute	38.5572	63.4641	50.5217
Contact Initialized	17.7726	26.7634	21.5481

```
Wallclock Time (seconds):
```

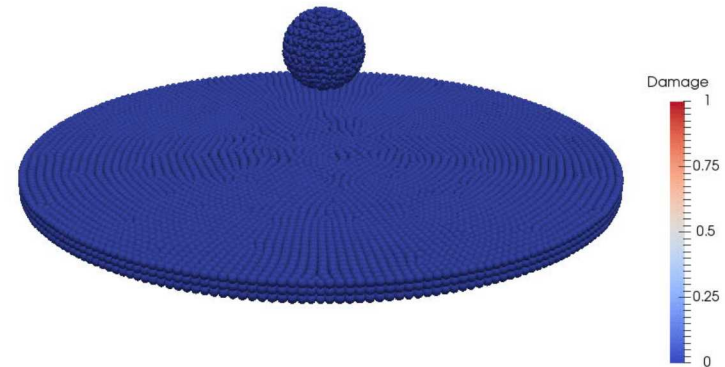
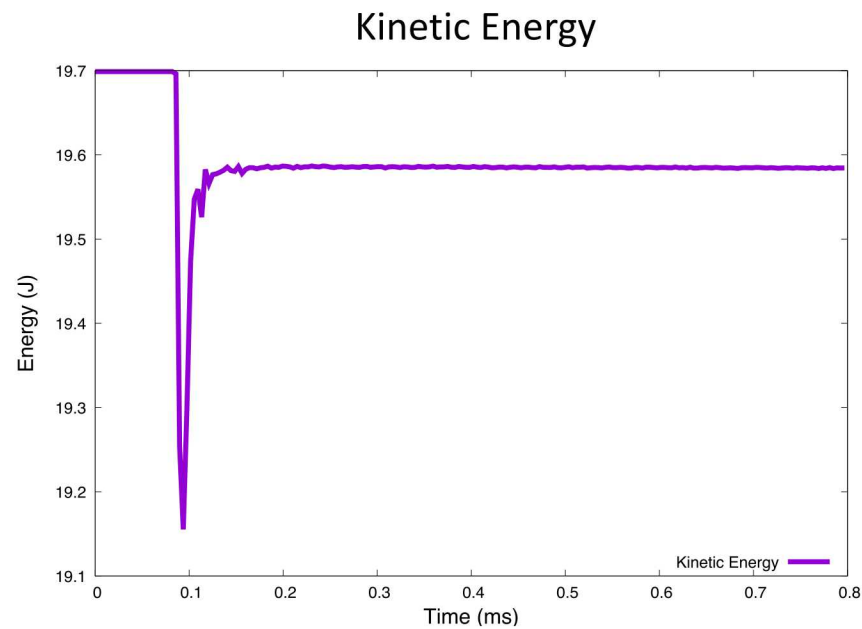
	Min	Max	Ave
Total	6.4e+02	6.4e+02	6.4e+02
Rebalance	1.8e+02	1.8e+02	1.8e+02
Output	16	17	17
Internal Force	2.1e+02	3.8e+02	2.9e+02
Initialize Contact Maps	0.00083	0.0022	0.0014
Gather/Scatter	64	2.4e+02	1.5e+02
Apply Kinematic B.C.	0.0051	0.011	0.0078
Apply Initial Conditions	3.9e-05	0.0012	0.00052
Apply Body Forces	0.047	0.078	0.062



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3. Example simulation: Disk impact

Results



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4. Hands-on example problems

Hands-on Examples



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