

# Computational Peridynamics

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**Short Course**  
**Peridynamic Theory of Solid Mechanics**

# Computational Peridynamics

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## *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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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

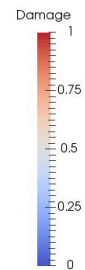
### *Ingredients for computational peridynamics*

- Governing equations
  - Continuum form of the balance of linear momentum
- Semi-discrete form: meshless discretization of the strong form

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

- |                                   |                            |
|-----------------------------------|----------------------------|
| ■ 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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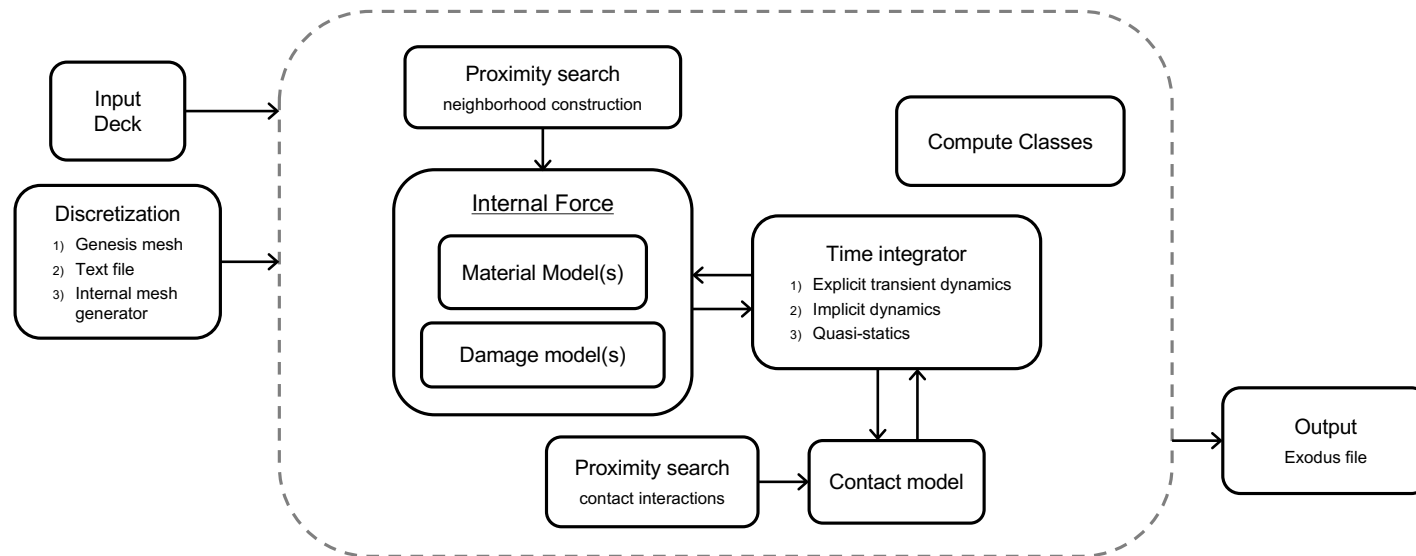
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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

### *Model for a peridynamics simulation code*



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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

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### *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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# Computational Peridynamics

## 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:       $\underline{e}^d \leftarrow e - \frac{\theta_i |\xi|}{3}$ 
25:       $\underline{t} \leftarrow \frac{3}{m_i} k \theta_i \underline{\omega} |\xi| + \frac{15\mu}{m_i} \underline{\omega} \underline{e}^d$ 
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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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

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### *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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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

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### *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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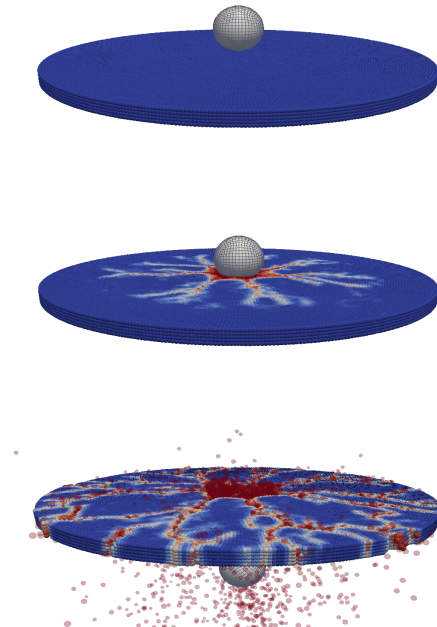
# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

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### *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.



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## 1. Ingredients of a peridynamic simulation

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### *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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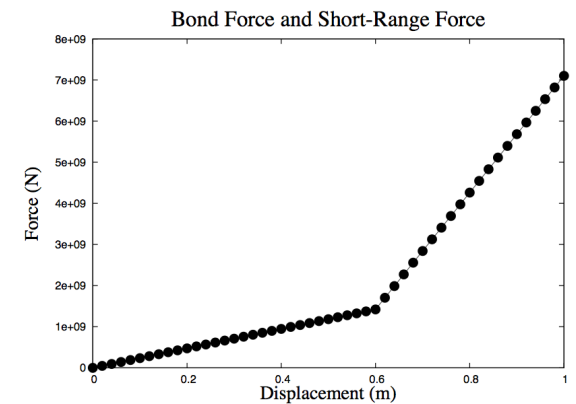
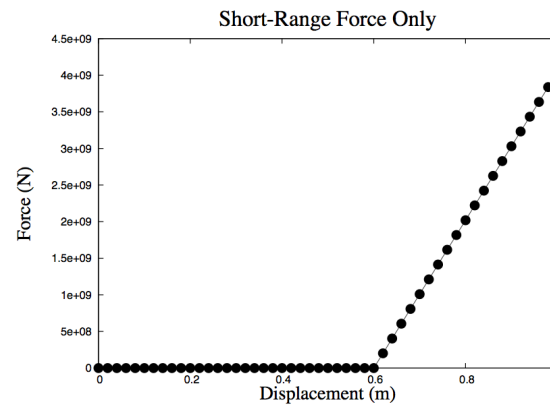
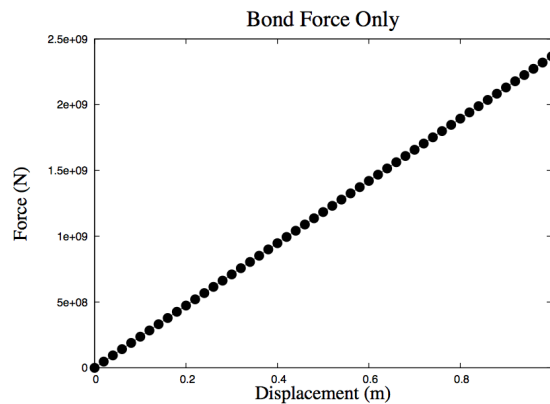
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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

### *Illustration of short range force and standard bond force*



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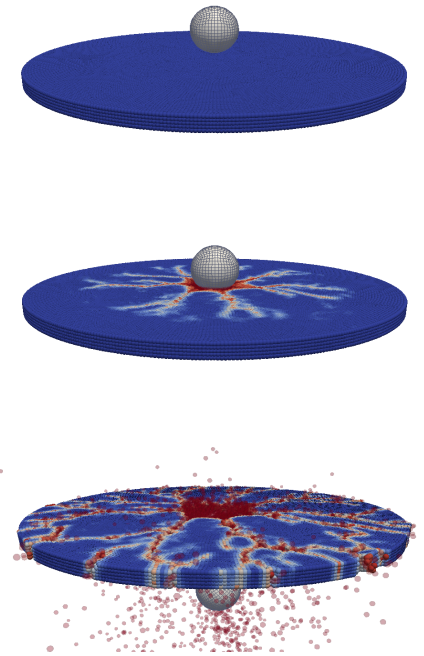
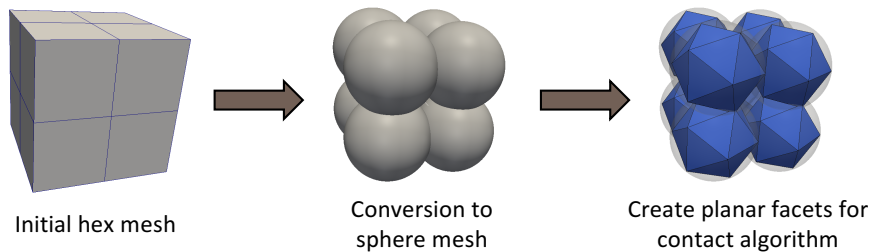
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# Computational Peridynamics

## 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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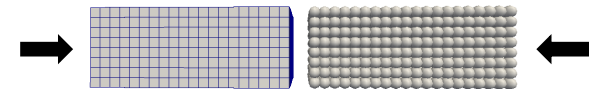


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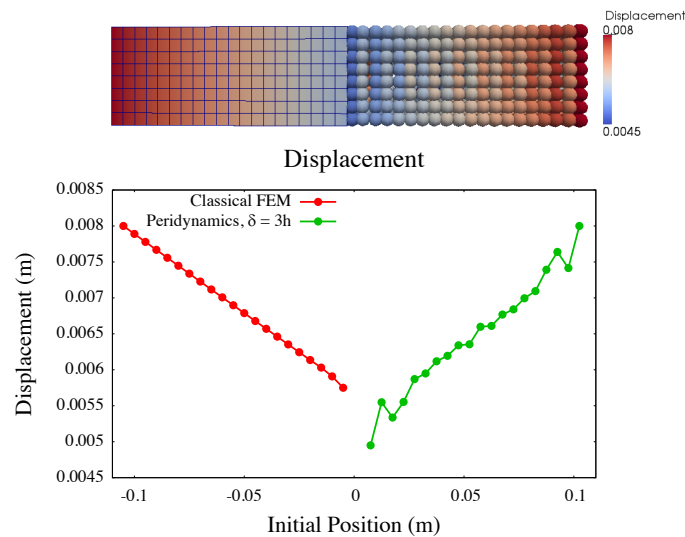
## 1. Ingredients of a peridynamic simulation

### *Challenges with contact and nonlocal models*

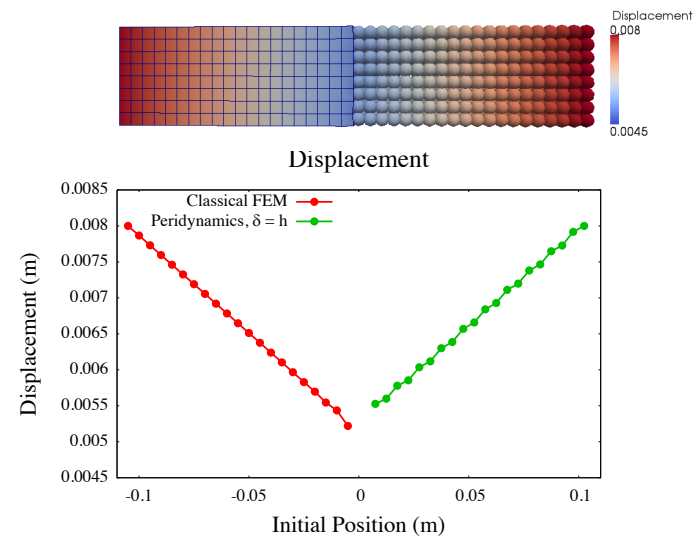
Simple test: Two bars in contact and under compression



Horizon = 3 \* Mesh Spacing



Horizon = Mesh Spacing



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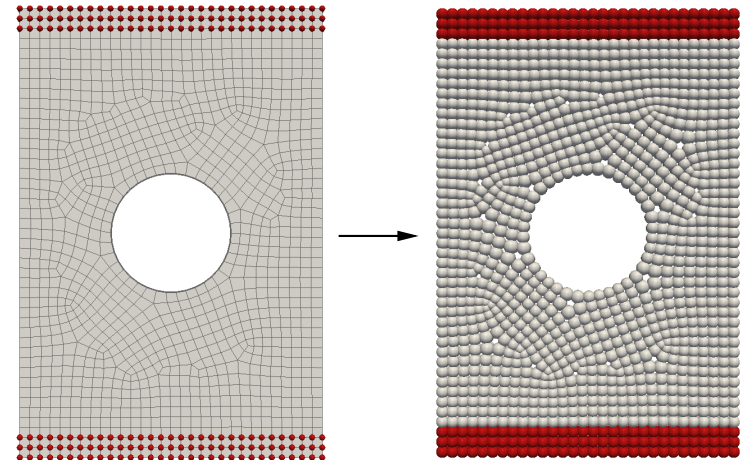
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# Computational Peridynamics

## 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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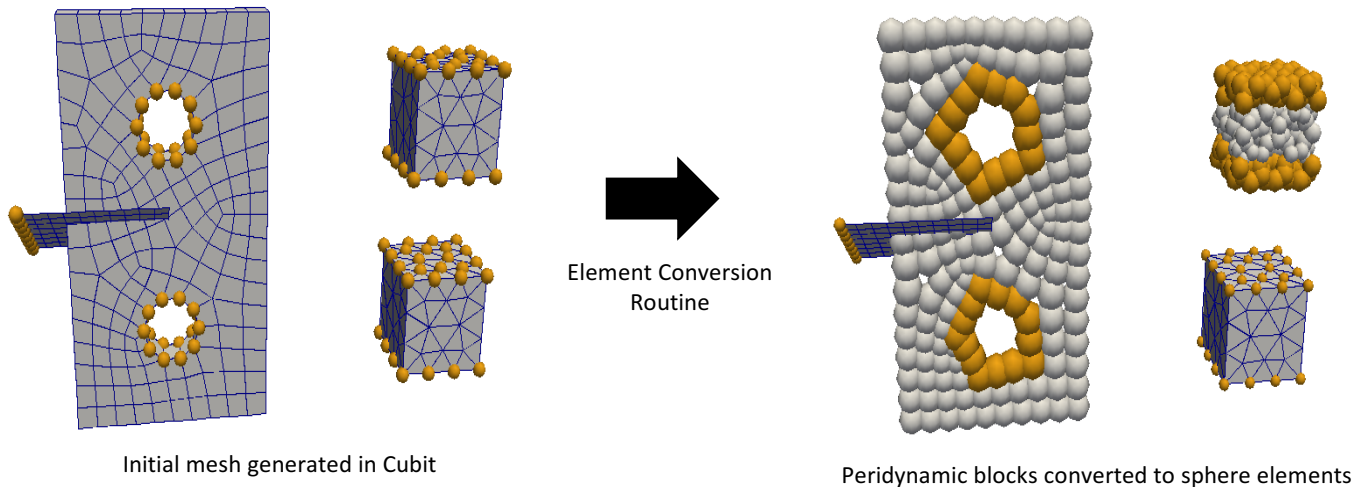
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## 1. Ingredients of a peridynamic simulation

### *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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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

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### *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



# Computational Peridynamics

## 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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# Computational Peridynamics

## 1. Ingredients of a peridynamic simulation

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### *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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# Computational Peridynamics

## 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:      $\{traversal\ list\} \leftarrow$  node  $i$  and all neighbors of node  $i$ 
7:     for each node  $j$  in  $\{traversal\ list\}$  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:           $\mathbf{f}^{diff} \leftarrow \mathbf{f}^{\epsilon+} - \mathbf{f}^{\epsilon-}$ 
17:          for each degree of freedom  $s$  at node  $k$  do
18:             $K_{sr} \leftarrow K_{sr} + \frac{f_s^{diff}}{2\epsilon}$ 
19:          end for
20:        end for
21:      end for
22:    end for
23:  end for
24: end procedure
```



# Computational Peridynamics

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## Outline

- Ingredients of a peridynamics simulation
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  - Discretization
  - Time integrator
- **Surface effect in peridynamic simulations**
- Estimation of the maximum stable time step for dynamic simulations
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# Computational Peridynamics

## 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

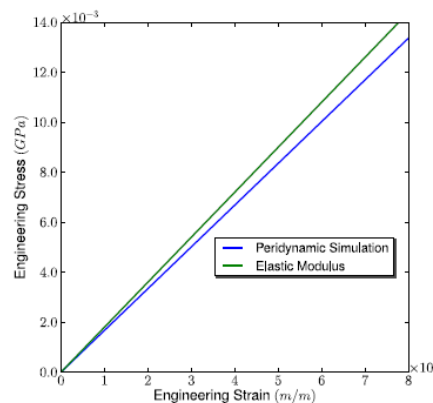
Axial Displacement



Stored Elastic Energy

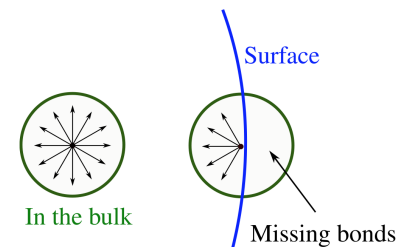


Stress versus Strain



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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# Computational Peridynamics

## 2. Surface effect

### *One possible approach to mitigating the surface effect*

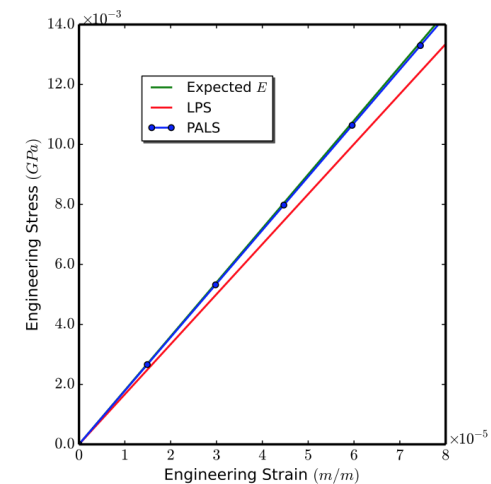
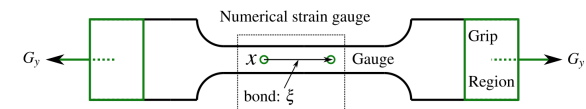
- **Position-Aware Linear Solid (PALS)** constitutive model takes proximity to free surfaces into account

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

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

### Example calculation

PALS model accurately recovers elastic modulus in tensile test



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.



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- Modeling damage and failure



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Peridynamic Theory of Solid Mechanics

# Computational Peridynamics

## 3. Estimation of the maximum stable time step

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### *Candidate approaches*

- Courant-Friedrichs-Lewy (CFL) condition
- Approach of Silling and Askari for microelastic materials (von Neumann analysis)
- Generalized Silling and Askari approach incorporating bond angles
- Global estimate using the Lanczos method
- Largest eigenvalue of 3x3 nodal stiffness matrix

Collaborators

Jesse Thomas

Timothy Shelton

### *Measures of success*

- Accuracy of estimate
  - Comparison against empirical result (numerical experiment)
- Computational expense

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.

Hughes, T.J.R. *The Finite Element Method: Linear Static and Dynamic Finite Element Analysis*. Prentice-Hall, Inc., Englewood Cliffs, NJ, 1987.

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

Koterias, J.R. and Lehoucq, R.B. Estimating the critical time-step in explicit dynamics using the Lanczos method. *International Journal for Numerical Methods in Engineering* 69:2780-2788, 2007.

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## Computational Peridynamics

### 3. Estimation of the maximum stable time step

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#### *Approach of Silling and Askari*

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

- Derived for one-dimensional problems with bond-based Prototype Microelastic Brittle material model
- Anecdotal evidence suggests time step estimate is conservative for other materials

#### *CFL limit*

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

- What is the proper characteristic length for peridynamic models?
- Anecdotal evidence suggests node spacing yields conservative estimate, horizon yields non-conservative estimate

#### *Eigenvalue analysis*

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f}$$

$$(\mathbf{K} - \lambda \mathbf{M}) \mathbf{x} = 0$$

$$\Delta t_c = \frac{2}{\sqrt{\lambda}}$$

- Requires an efficient algorithm to find the maximum global eigenvalue
  - E.g., Lanczos algorithm



# Computational Peridynamics

## 3. Estimation of the maximum stable time step

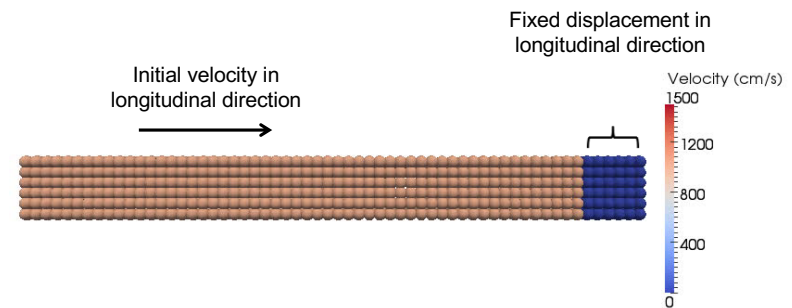
- Investigate material models
  - Microelastic bond-based
  - Linear peridynamic solid state-based
  - Wrapped classical elastic model
- Investigate critical time step estimates
  - Empirical (numerical experiment)
  - 1D approach of Silling and Askari
  - Generalized Silling and Askari
  - Element time step (3x3 stiffness probe)
  - Lanczos global estimate

### Simulation

|                  |              |
|------------------|--------------|
| Bar Length       | 10.0 cm      |
| Bar Width        | 1.0 cm       |
| Initial Velocity | 10.0 m/s     |
| Time Step        | 0.48 $\mu$ s |

### Material Parameters

|                 |                       |
|-----------------|-----------------------|
| Density         | 7.8 g/cm <sup>3</sup> |
| Young's Modulus | 300.0 GPa             |
| Poisson's Ratio | 0.25                  |
| Horizon         | 0.5075 cm             |



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# Computational Peridynamics

## 3. Estimation of the maximum stable time step

| Time Step   | Kinetic Energy |
|-------------|----------------|
| 0.1 $\mu s$ | 3.51 J         |
| 0.2 $\mu s$ | 3.51 J         |
| 0.3 $\mu s$ | 3.51 J         |
| 0.4 $\mu s$ | NaN            |
| 0.5 $\mu s$ | NaN            |
| 0.6 $\mu s$ | NaN            |
| 0.7 $\mu s$ | NaN            |
| 0.8 $\mu s$ | NaN            |
| 0.9 $\mu s$ | NaN            |
| 1.0 $\mu s$ | NaN            |

### Nodal Stiffness Matrix

max. time step = 0.314  $\mu s$   
max. kinetic energy = 3.51 J

### CFL Limit (element size)

max. time step = 0.329  $\mu s$   
max. kinetic energy = 3.51 J

### Empirical Observation

max. time step = 0.381  $\mu s$   
max. kinetic energy = 3.51 J

### Global Lanczos

max. time step = 0.381  $\mu s$   
max. kinetic energy = 3.51 J

### CFL Limit (horizon)

max. time step = 1.00  $\mu s$   
max. kinetic energy = **unstable**



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# Computational Peridynamics

## 3. Estimation of the maximum stable time step

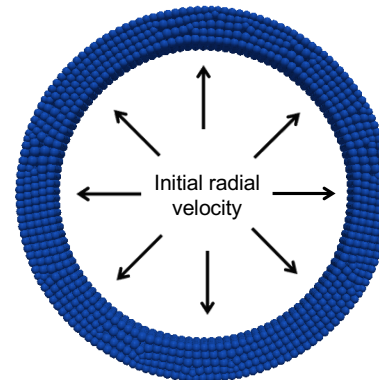
- Investigate material models
  - Microelastic bond-based
  - Linear peridynamic solid state-based
  - Wrapped classical elastic model (nosb)
- Investigate critical time step estimates
  - Empirical
  - 1D approach of Silling and Askari
  - Generalized Silling and Askari
  - Element time step (3x3 stiffness probe)
  - Lanczos global estimate

Simulation

|                         |           |
|-------------------------|-----------|
| Ring Diameter           | 4.5 cm    |
| Ring Width              | 1 cm      |
| Initial Radial Velocity | 200.0 m/s |

Material Parameters

|                  |                       |
|------------------|-----------------------|
| Density          | 7.8 g/cm <sup>3</sup> |
| Young's Modulus  | 300.0 GPa             |
| Poisson's Ratio  | 0.25                  |
| Critical Stretch | 0.01 cm/cm            |
| Horizon          | 0.603 cm              |



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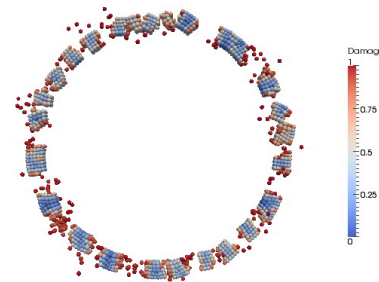


# Computational Peridynamics

## 3. Estimation of the maximum stable time step

Simulation results for  
microelastic material

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



Time step = 5.0  $\mu s$   
46.7% of bonds broken



Time step = 7.5  $\mu s$   
62.7 % of bonds broken



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# 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 $\mu s$ | 40.3 %                     | 3.43 kJ                                   |
| 0.1 $\mu s$  | 40.2 %                     | 3.43 kJ                                   |
| 0.2 $\mu s$  | 40.4 %                     | 3.43 kJ                                   |
| 0.3 $\mu s$  | 41.6 %                     | 3.42 kJ                                   |
| 0.4 $\mu s$  | 42.0 %                     | 3.44 kJ                                   |
| 0.5 $\mu s$  | 44.7 %                     | 3.45 kJ                                   |
| 0.6 $\mu s$  | 95.6 %                     | 4.33 kJ                                   |
| 0.7 $\mu s$  | 97.3 %                     | 5.54 kJ                                   |
| 0.8 $\mu s$  | 98.6 %                     | 7.14 kJ                                   |
| 0.9 $\mu s$  | 99.4 %                     | 19.8 kJ                                   |
| 1.0 $\mu s$  | 99.8 %                     | 62.8 kJ                                   |

### CFL Limit (element size)

max. time step = 0.395  $\mu s$   
percentage of broken bonds = 45.3 %  
max. kinetic energy = 3.51 J

### Global Lanczos

max. time step = 0.494  $\mu s$   
percentage of broken bonds = 42.8 %  
max. kinetic energy = 3.43 kJ

### Nodal Stiffness Matrix

max. time step = 0.505  $\mu s$   
percentage of broken bonds = 44.8 %  
max. kinetic energy = 3.82 kJ

### Empirical Observation

max. time step = 0.509  $\mu s$   
percentage of broken bonds = 50.0 %  
max. kinetic energy = 3.46 kJ

### CFL Limit (horizon)

max. time step = 1.19  $\mu s$   
percentage of broken bonds = 99.1 %  
max. kinetic energy = **unstable**



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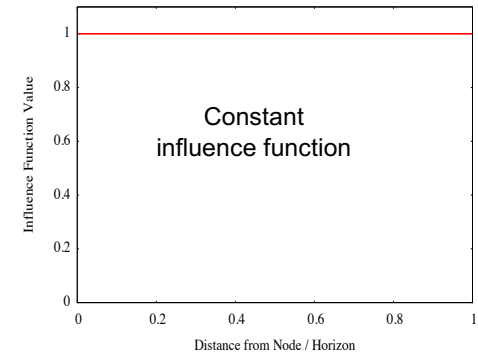
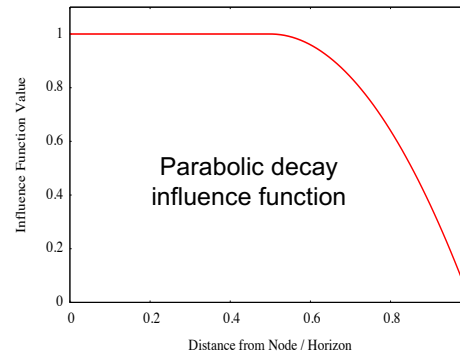
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# Computational Peridynamics

## 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 $\mu$ s                      | 0.434 $\mu$ s               |
| Empirical result       | 0.381 $\mu$ s                      | 0.434 $\mu$ s               |

14% Increase

Correspondence Material Model

|                        | Parabolic decay influence function | Constant influence function |
|------------------------|------------------------------------|-----------------------------|
| Max. Lanczos time step | 0.490 $\mu$ s                      | 0.549 $\mu$ s               |
| Empirical result       | 0.490 $\mu$ s                      | 0.549 $\mu$ s               |

12% Increase



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# Computational Peridynamics

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## 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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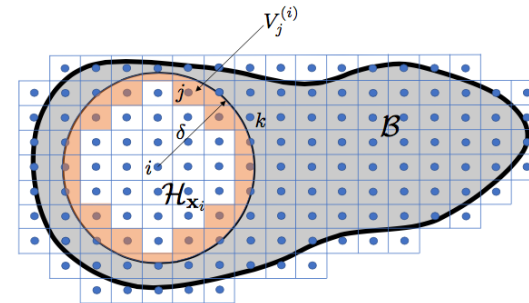
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# Computational Peridynamics

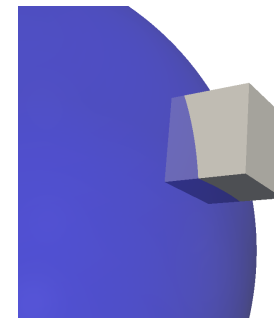
## 5. Convergence of meshfree models

### 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
  - Poor treatment of neighbor-horizon intersections
  - 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. In preparation.



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# Computational Peridynamics

## 5. Convergence of meshfree models

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### *Approaches for improving behavior at neighbor-horizon intersections*

---

**Algorithm 1 : FV**

---

```
1: {Compute bond length}
2:  $|\xi| = |\mathbf{x}_j - \mathbf{x}_i|$ 
3: {Check if node  $j$  is in the family of node  $i$ }
4: if  $|\xi| \leq \delta$  then
5:    $V_j^{(i)} = V_j$ 
6: else
7:    $V_j^{(i)} = 0$ 
8: end if
9: Return  $V_j^{(i)}$ 
```

---

---

**Algorithm 2 : PV-PDLAMMPS**

---

```
1: {Compute bond length}
2:  $|\xi| = |\mathbf{x}_j - \mathbf{x}_i|$ 
3: {Check if cell  $j$  is contained within the neighborhood of node  $i$  (perfect in 1D only)}
4: if  $|\xi| + \frac{h}{2} \leq \delta$  then
5:    $V_j^{(i)} = V_j$ 
6:   {Check if node  $j$  is in the family of node  $i$ }
7: else if  $|\xi| \leq \delta$  then
8:    $V_j^{(i)} = \frac{1}{h} \left[ \delta - \left( |\xi| - \frac{h}{2} \right) \right] V_j$ 
9: else
10:   $V_j^{(i)} = 0$ 
11: end if
12: Return  $V_j^{(i)}$ 
```

---

---

**Algorithm 3 : PV-HHB**

---

```
1: {Compute bond length}
2:  $|\xi| = |\mathbf{x}_j - \mathbf{x}_i|$ 
3: {Check if cell  $j$  is contained within the neighborhood of node  $i$  (perfect in 1D only)}
4: if  $|\xi| + \frac{h}{2} \leq \delta$  then
5:    $V_j^{(i)} = V_j$ 
6:   {Check if node  $j$  is in the family of node  $i$ }
7: else if  $|\xi| - \frac{h}{2} \leq \delta$  then
8:    $V_j^{(i)} = \frac{1}{h} \left[ \delta - \left( |\xi| - \frac{h}{2} \right) \right] V_j$ 
9: else
10:   $V_j^{(i)} = 0$ 
11: end if
12: Return  $V_j^{(i)}$ 
```

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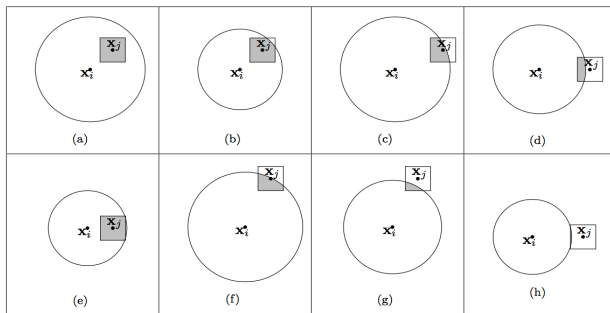
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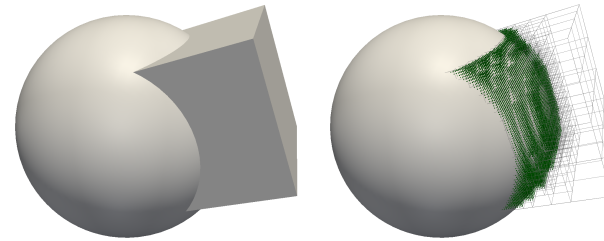
# Computational Peridynamics

## 5. Convergence of meshfree models

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



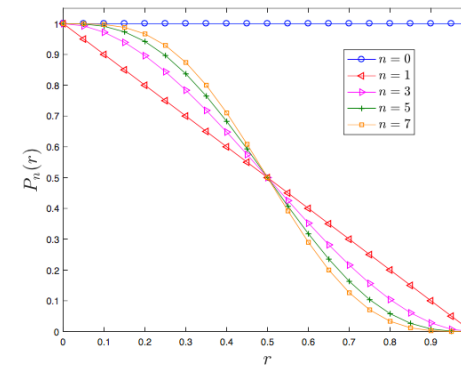
Analytic calculation of partial areas (2D)



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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# Computational Peridynamics

## 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

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

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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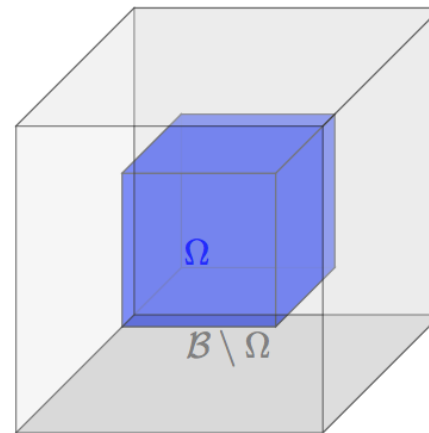
# Computational Peridynamics

## 5. Convergence of meshfree models

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### *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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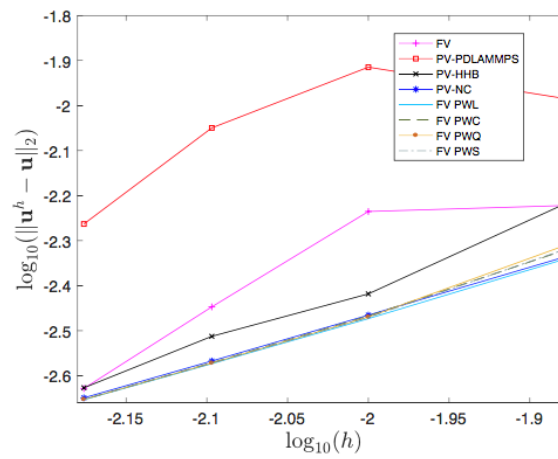
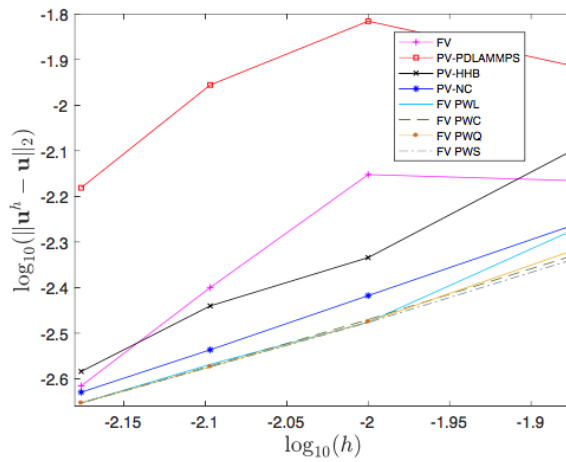
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# Computational Peridynamics

## 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

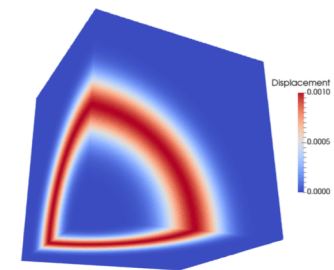
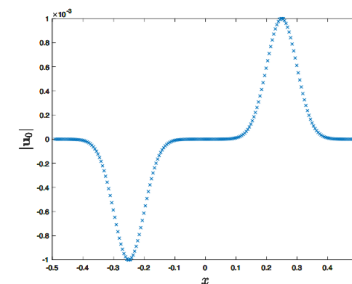
### Numerical experiments: Solution of dynamics problem

- 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

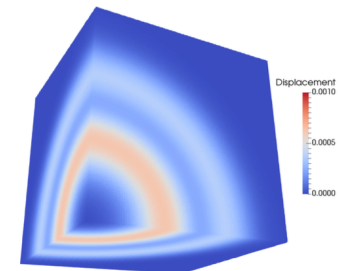
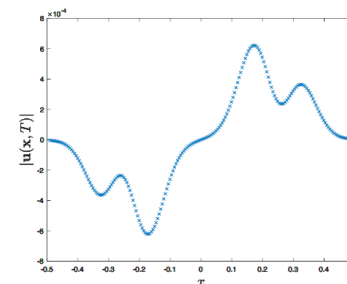
#### Initial conditions

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

Initial displacement



Final displacement



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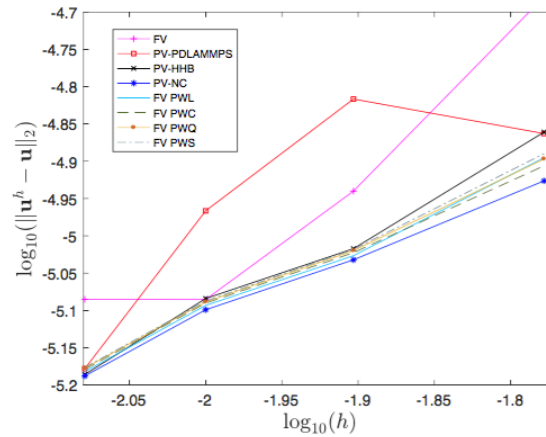
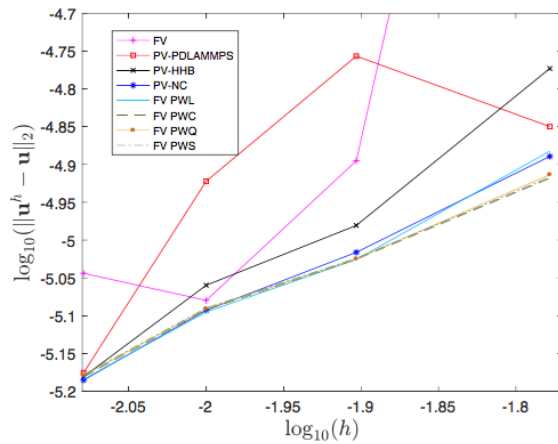
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# Computational Peridynamics

## 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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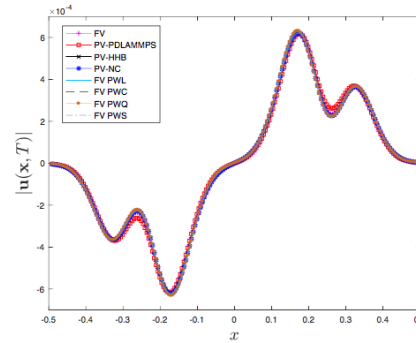
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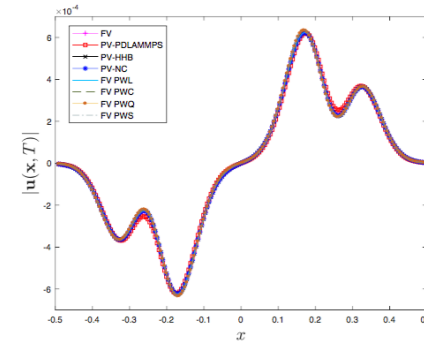
# Computational Peridynamics

## 5. Convergence of meshfree models

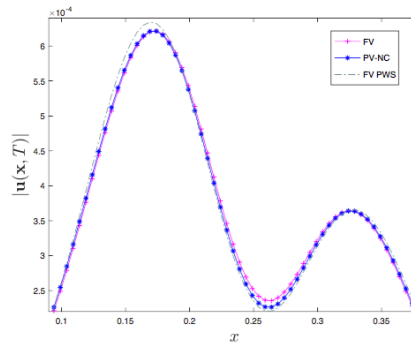
*Changing the influence function changes the underlying model (physics)*



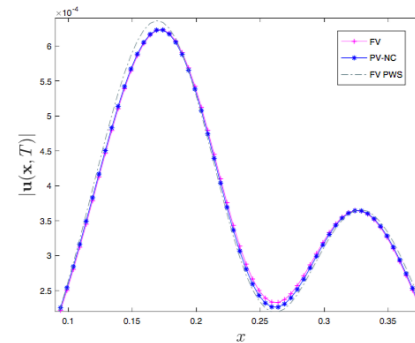
(a)  $\alpha = 0$



(b)  $\alpha = 1$



(c)  $\alpha = 0$  (zoom in)



(d)  $\alpha = 1$  (zoom in)



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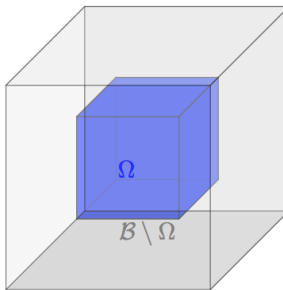
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# Computational Peridynamics

## 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



| $\delta/L$                      | 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 |

| $N_{\text{neig}}$<br>( $\delta/h$ ) | 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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# Computational Peridynamics

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## 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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# 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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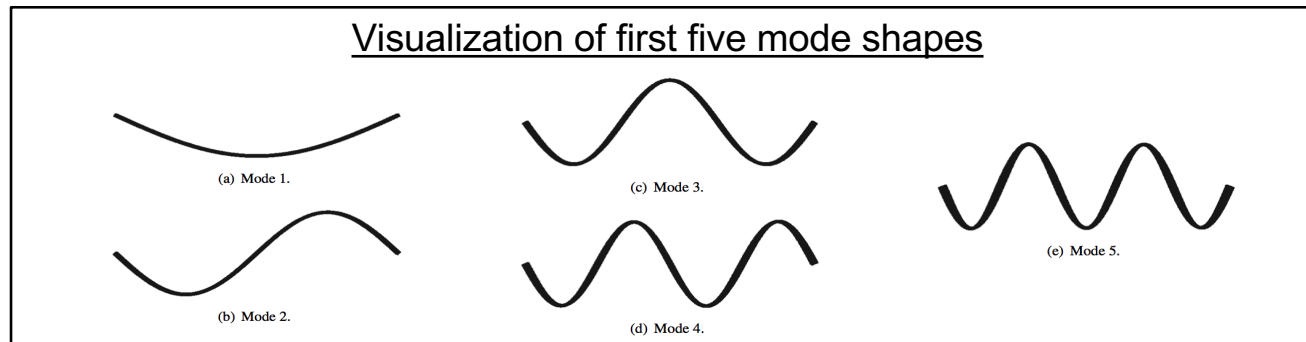
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## 7. Modal analysis of peridynamic models

### 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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# Computational Peridynamics

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- Demonstration of meshfree peridynamics for model analysis
- **Modeling damage and failure**



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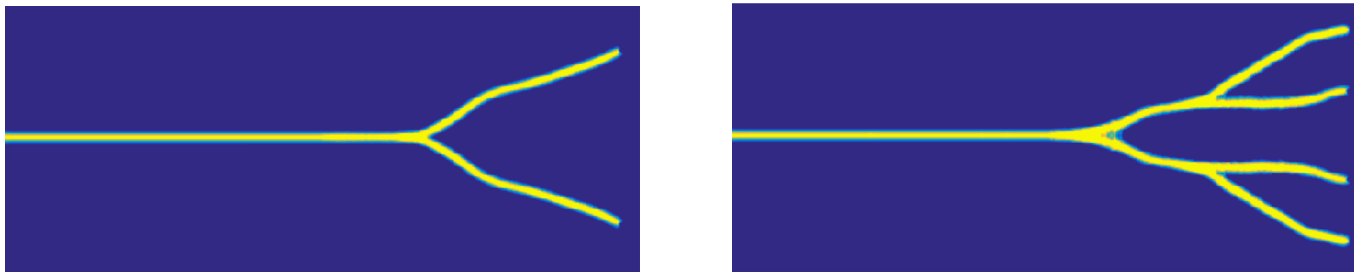
# Computational Peridynamics

## 7. Modeling failure and damage

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### *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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# Computational Peridynamics

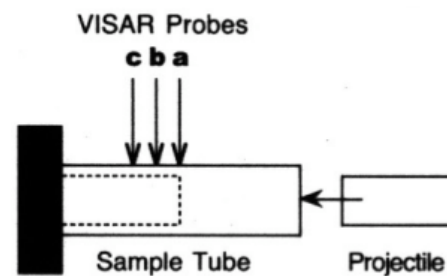
## 7. Modeling failure and damage

### 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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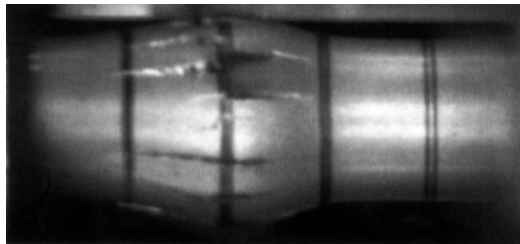
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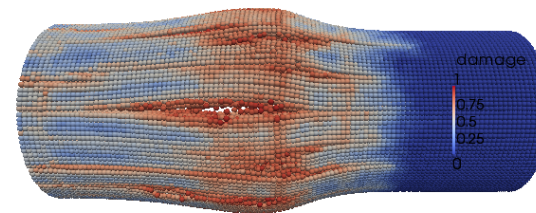
# Computational Peridynamics

## 7. Modeling failure and damage

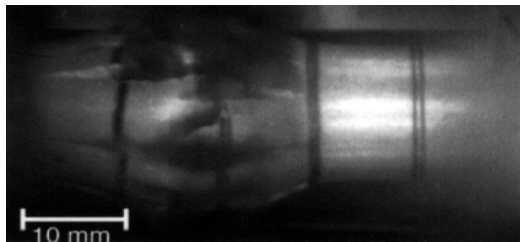
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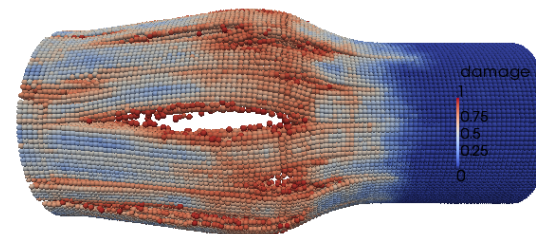
Experimental image at 15.4 microseconds [Vogler et. al]



Simulation at 15.4 microseconds



Experimental image at 23.4 microseconds [Vogler et. al]



Simulation at 23.4 microseconds



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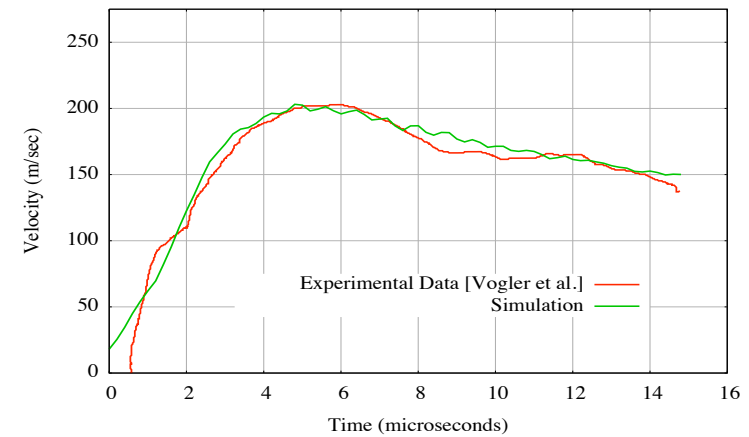
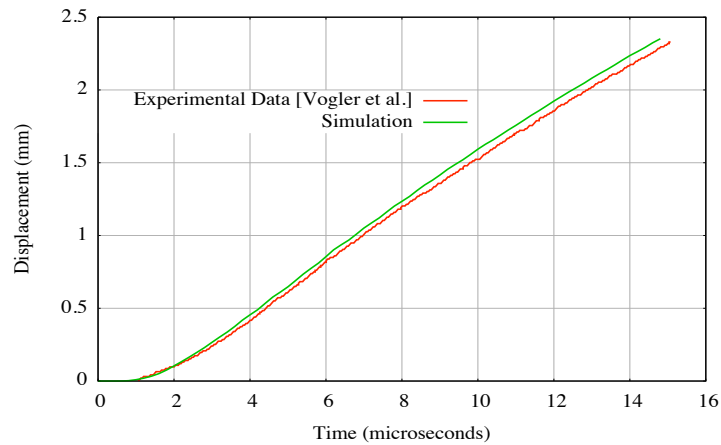
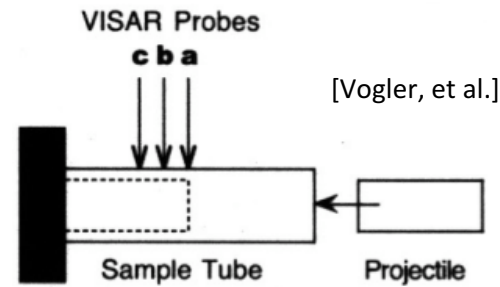
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# Computational Peridynamics

## 7. Modeling failure and damage

Displacement and velocity  
on tube surface  
at probe position A



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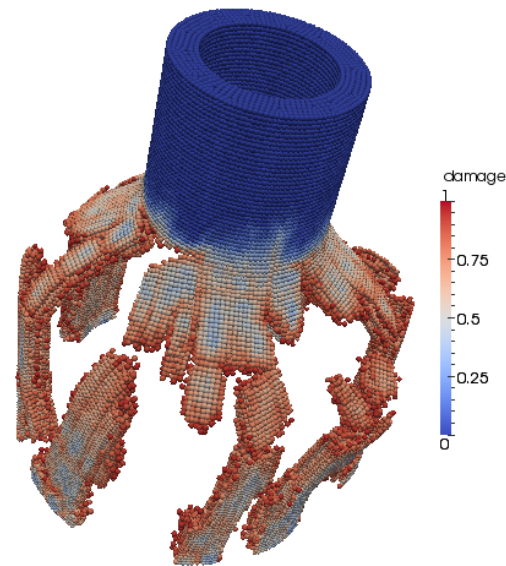
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## 7. Modeling failure and damage

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### 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

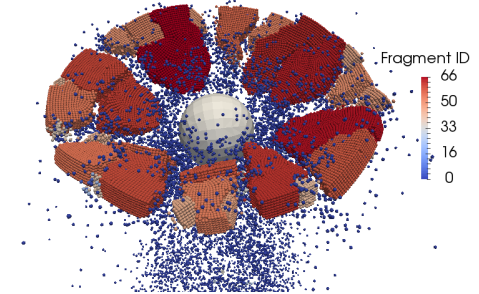
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### *Identification of fragments in a meshfree peridynamic simulation*

- 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



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## Computational Peridynamics

### 7. Modeling failure and damage

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#### *Algorithm for fragment identification*

```
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  $j$ 
```



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# Computational Peridynamics

## 7. Modeling failure and damage

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### *Parallel algorithm for fragment identification*

```
DO initialize fragment numbers to node ids
REPEAT until fragment numbers stop changing across all processors
  REPEAT until on-processor 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  $j$ 
    FOR every node  $i$ 
      DO assign  $\text{global\_max}(F_i)$  to node  $i$  on all processors
```

Additional loop for  
global convergence

Synchronization of fragment  
numbers across processors



# Computational Peridynamics

## 7. Modeling failure and damage

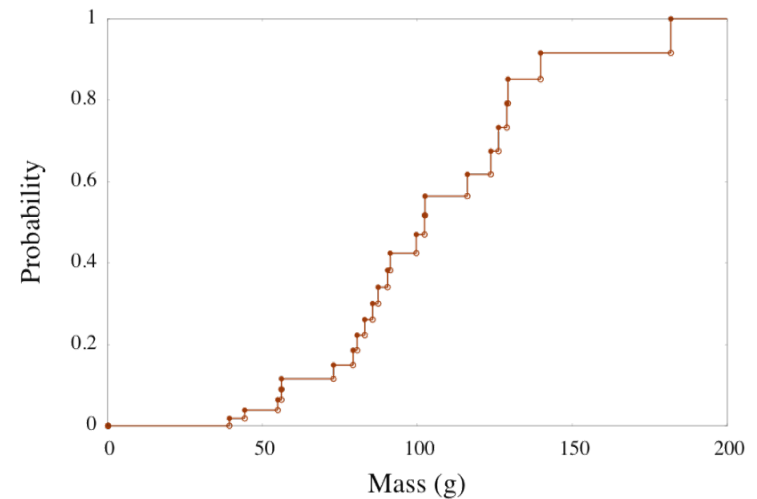
### *Parallel algorithm for fragment identification*

- 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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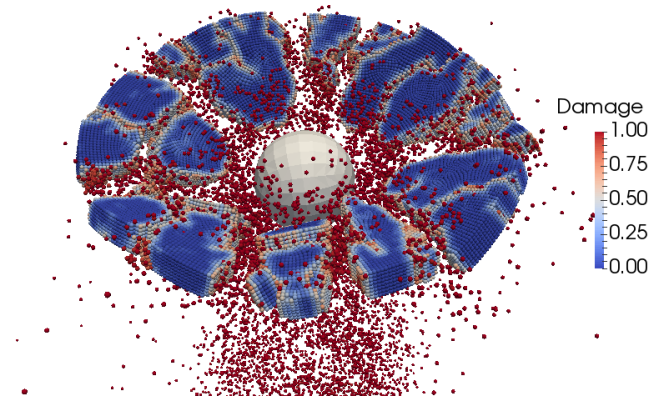
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# Computational Peridynamics

## 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 $\rho$        | 993.1 kg/m <sup>3</sup> |
| Bulk modulus $k$      | 1.0 GPa                 |
| Poisson's ratio $\nu$ | 0.3                     |

Material parameters  
for target

| Parameter                   | Value                    |
|-----------------------------|--------------------------|
| Density $\rho$              | 2200.0 kg/m <sup>3</sup> |
| Bulk modulus $k$            | 14.9 GPa                 |
| Horizon $\delta$            | 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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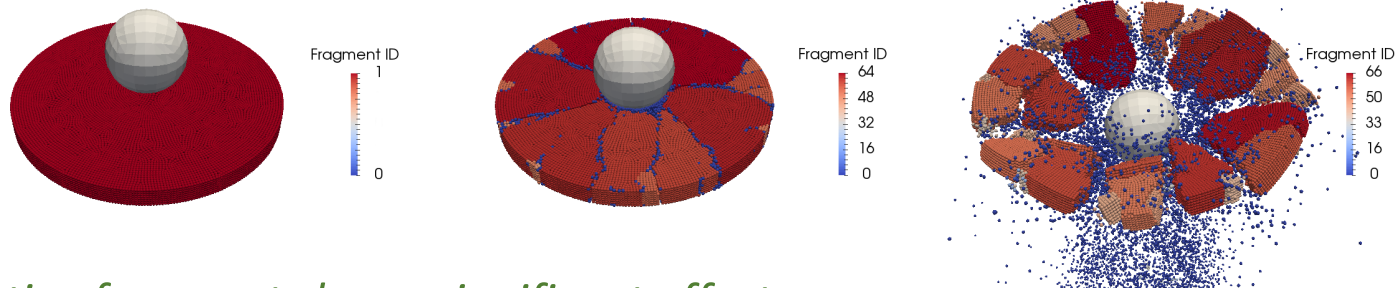
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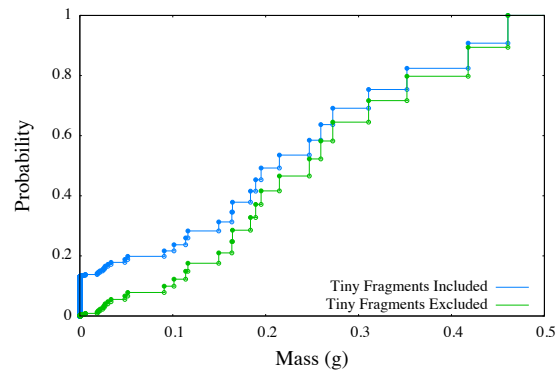
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## 7. Modeling failure and damage

*Algorithm captures evolution of fragmentation process*



*Exclusion of tiny fragments has a significant effect*



| Threshold<br>Fragment Size | Total Mass of<br>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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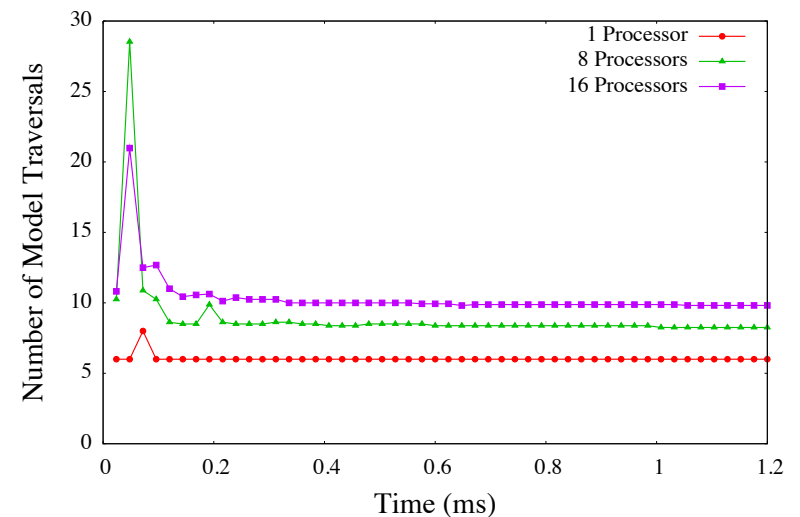
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## Computational Peridynamics

### 7. Modeling failure and damage

#### *Computational expense of fragment identification algorithm*

- Overall computational expense of algorithm was low
  - Fragment identification algorithm called 50 times
  - Computational expense between 0.2% and 0.3% of overall simulation time
- Additional processors resulted in modest increase in number of required iterations
- Number of iterations is highest when fragmentation is occurring
  - Possible result of fragments that are connected by a small number of bonds



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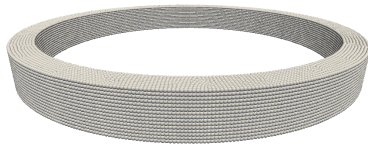
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## 7. Modeling failure and damage

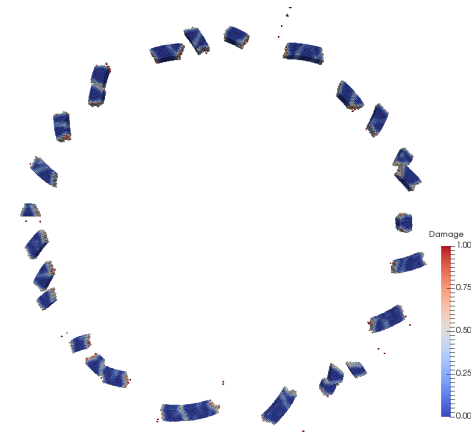
- Fragmentation of an expanding ductile ring
- Bond-based microplastic material model
- Critical stretch bond failure rule
- Inner radius 110.0 mm, outer radius 125.0 mm, height 25.0 mm
- Initial outward radial velocity 100.0 m/s
- ~60,000 nodal volumes

Discretization of ring



Material parameters

| Parameter                   | Value                    |
|-----------------------------|--------------------------|
| Density $\rho$              | 7850.0 kg/m <sup>3</sup> |
| Bulk modulus $k$            | 140.0 GPa                |
| Horizon $\delta$            | 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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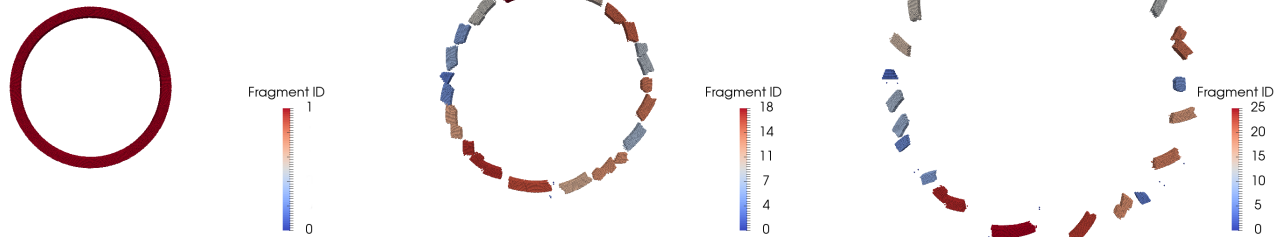
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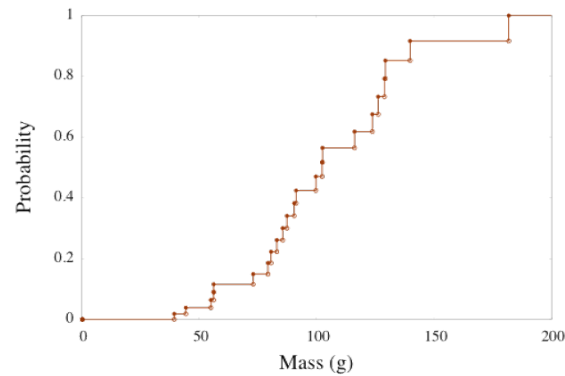
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## 7. Modeling failure and damage

*Algorithm captures evolution of fragmentation process*



*Exclusion of tiny fragments does not affect results*



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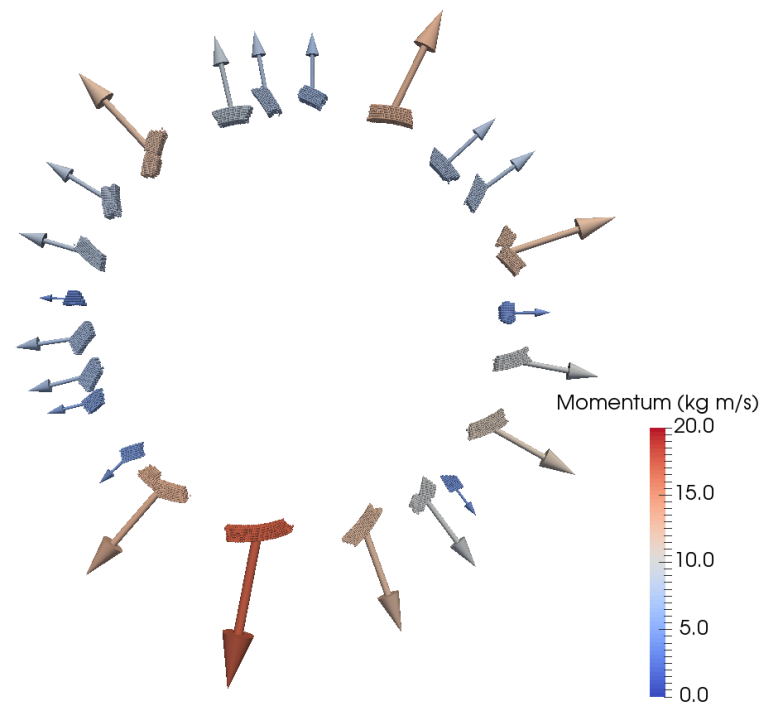
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# Computational Peridynamics

## 7. Modeling failure and damage

Visualization of  
fragment momentum



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