Peridynamic Modeling of Localization in Ductile Metals

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Peridynamics

WHAT IS PERIDYNAMICS?

Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles.

HOW DOES IT WORK?

- Peridynamics is a *nonlocal* extension of continuum mechanics.
- Remains valid in presence of discontinuities, including cracks.
- Balance of linear momentum is based on an integral equation:

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

Divergence of stress replaced with integral of nonlocal forces.


Peridynamics

CONSTITUTIVE LAWS IN PERIDYNAMICS

- Peridynamic bonds connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds

\[
\begin{align*}
\mathbf{T}[\mathbf{x}, t] & \quad \left\langle \mathbf{x}' - \mathbf{x} \rightangle \\
\text{Force State} & \quad \text{Bond}
\end{align*}
\]

- Force states are determined by constitutive laws and are functions of the deformations of all points within a neighborhood
- Material failure is modeled through the breaking of peridynamic bonds
  - Example: critical stretch bond breaking law

DISCRETIZATION OF A PERIDYNAMIC BODY

A body may be represented by a finite number of sphere elements

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

**LINEAR PERIDYNAMIC SOLID (ELASTIC MODEL)**

\[ \theta (e) = \frac{3}{m} (\omega x) \bullet e \]

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

**ELASTIC-PLASTIC MODEL**

\[ t = \frac{3k\theta}{m} \omega x + \frac{15\mu}{m} \omega \left( e^d - e^{dp} \right) \]


ADAPTATION: NON-ORDINARY STATE-BASED PERIDYNAMICS

- Apply existing (local) constitutive models within nonlocal peridynamic framework
- Utilize approximate deformation gradient based on positions and deformations of all elements in the neighborhood

1. Compute regularized deformation gradient

\[
\bar{F} = \left( \sum_{i=0}^{N} \omega_i \mathbf{Y}_i \otimes \mathbf{X}_i \Delta V_{x_i} \right) K^{-1}
\]

2. Classical material model computes stress based on regularized deformation gradient

3. Convert stress to peridynamic force densities

\[
\mathbf{T} \langle \mathbf{x}' - \mathbf{x} \rangle = \omega \sigma \mathbf{K}^{-1} \langle \mathbf{x}' - \mathbf{x} \rangle
\]

4. Apply peridynamic hourglass forces as required to stabilize simulation (optional)

Suppression of Zero-Energy Modes

**Approach**: Penalize deformation that deviates from regularized deformation gradient

Predicted location of neighbor

\[ x_{n}^{*} = x_{n} + \bar{F}_{n} \left( x'_{o} - x_{o} \right) \]

Hourglass vector

\[ \Gamma_{hg} = x_{n}^{*} - x'_{n} \]

Hourglass vector projected onto bond

\[ \gamma_{hg} = \Gamma_{hg} \cdot \left( x'_{n} - x_{n} \right) \]

Hourglass force

\[ f_{hg} = -C_{hg} \left( \frac{18k}{\pi \delta^4} \right) \frac{\gamma_{hg}}{\left\| x'_{o} - x_{o} \right\|} \frac{x'_{n} - x_{n}}{\left\| x'_{n} - x_{n} \right\|} \Delta V_{x} \Delta V_{x'} \]

- Micro-modulus
- Hourglass stretch
- Bond unit vector
The peridynamic horizon introduces a length scale that is independent of the mesh size.

Decoupling from the mesh size enables consistent modeling of material response in the vicinity of discontinuities.

Example: Mesh independent plastic zone in the vicinity of a crack.
Can the Peridynamic Horizon Have Physical Meaning?

MANY PHYSICAL PROBLEMS HAVE NATURAL LENGTH SCALE(S)

- **Interatomic forces**
  
  \[ F_{ij} \sim \left( \frac{a}{r_{ij}} \right)^{12} - \left( \frac{a}{r_{ij}} \right)^6 \]

- **Van der Waals forces**
  - Force between a pair of atoms as they are separated:
    
    \[ F_{ij} \sim \frac{1}{r_{ij}^6} \]
  - Net force between half-space and sphere occurs over a much larger length scale*

  \[ F_{\text{sphere}} \sim \frac{1}{D} \]

Physical Interpretation of Peridynamic Horizon

**NONLOCALITY AS A RESULT OF HOMOGENIZATION**

- Homogenization (neglecting natural length scales) often leads to poor results.
- Nonlocality (length scale) can be an essential feature of a realistic homogenized model of a heterogeneous material.
- Example: Concrete indentor

![Diagram showing stress and homogenized local versus real response](Courtesy S. Silling)
Physical Interpretation of Peridynamic Horizon

**PROPOSED EXPERIMENTAL METHOD FOR MEASURING THE PERIDYNAMIC HORIZON**

- Measure how much a step wave spreads as it goes through a heterogeneous sample
- Fit the horizon in a peridynamic model to match observed spread

![Diagram showing experimental setup and data analysis](image)

- Local model would predict zero spread

[Courtesy S. Silling]
Peridynamics and Higher-Order Gradient Methods

- Local models contain no length scale
  \[ \ddot{u}(x) = au''(x) \]

- Higher-order gradients introduce length scale in a weak sense
  \[ \ddot{u}(x) = au''(x) + bu''''(x) \]
  Dimensional analysis shows that \( \sqrt{b/a} \) has units of length

- Peridynamics is a (strongly) nonlocal model

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Necking Experiment

CAN A PERIDYNAMIC MODEL PREDICT LOCALIZATION?

- **Test setup:**
  - 304L stainless steel (very ductile)
  - Quasi-static loading conditions
  - Standard tensile test results provided for calibration

- **Challenge:**
  - Predict force and engineering strain at peak load
  - Predict engineering strain when force has dropped to 95% of peak load
  - Predict chord lengths when force has dropped to 95% of peak load
Necking Experiment: Calibration of Peridynamic Model

**TENSILE TEST CALIBRATION DATA**

- Force versus engineering strain
- Cross-sectional area at the point where the force dropped to 75% of peak load

Cross-sectional Area

Initial value: 0.0310 in\(^2\)
At 75% peak load: 0.0107 in\(^2\)
Necking Experiment: Calibration of Peridynamic Model

ELASTIC-PLASTIC MODEL WITH PIECEWISE LINEAR HARDENING CURVE

- Quasi-static simulations carried out with *Sierra/SolidMechanics*
- Initial calibration taken from classical finite-element model of tensile test (automated calibration tool)
- Hardening curve manually adjusted past ultimate tensile strength

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus</td>
<td>199.95e3 MPa</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.285</td>
</tr>
<tr>
<td>Yield Stress</td>
<td>220.0 MPa</td>
</tr>
</tbody>
</table>
Necking Experiment: Calibration of Peridynamic Model

**LOCALIZATION IN TENSILE TEST**

Cross-sectional Area
- Initial value: 0.031 in\(^2\)
- Simulation at 75% peak load: 0.0129 in\(^2\)

![Image showing cross-sectional area changes](image)

**Graph:**
- X-axis: Engineering Strain (in/in)
- Y-axis: Cross Sectional Area (in\(^2\))
- Red line: Peridynamic Simulation
- Blue circle: Experimental Result
Necking Experiment: Test Geometry

DIRECT TRANSFER OF CALIBRATION PARAMETERS

- Peridynamic horizon and mesh refinement were sufficient for calibration geometry but insufficient for test geometry
- Failed to predict response of test geometry

![Experimental DIC image [Boyce] and Simulation result](image)
Necking Experiment: Test Geometry

**REDUCTION OF PERIDYNAMIC HORIZON**

- Peridynamic horizon reduced from 1.055 mm to 0.353 mm
- Mesh density increased from 189K elements to 1,507K elements
- Dramatically improved agreement between peridynamic model and experimental data

Experimental DIC image [Boyce]  
Simulation result
Questions?

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RESOURCES

Advanced Simulation and Computing (ASC)
http://www.sandia.gov/asc/

Peridigm: A publicly-available peridynamics code
https://software.sandia.gov/trac/peridigm/