Defects and Interfaces in Peridynamics: A Multiscale Approach

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Outline

• Peridynamics background and examples
• Concurrent hierarchical multiscale method
• Calibrating a bond damage model using MD
• Coarse graining
Purpose of peridynamics*

- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.

- Why do this?
  - Avoid coupling dissimilar mathematical systems (A to C).
  - Model complex fracture patterns.
  - Communicate across length scales.

* Peri (near) + dyn (force)
Some ways to treat cracks in an FE mesh

- Tend to get different results when you change the mesh.
- Methods do not reflect realistic crack-tip processes.
- Difficult to apply to complex crack trajectories.
- Methods destroy the accuracy and convergence properties of FEM.

Why do we have to do this sort of thing?
Because the equations that FEM approximate fail to apply.
Peridynamics basics: Horizon and family

- Any point $x$ interacts directly with other points within a distance $\delta$ called the “horizon.”
- The material within a distance $\delta$ of $x$ is called the “family” of $x$, $\mathcal{H}_x$.

General references
- Madenci & Oterkus, Peridynamic Theory & Its Applications (2014)
Point of departure: Strain energy at a point

- **Continuum**
  - Family of \( x \)

- **Discrete particles**
  - Deformation
  - \( x \)

- **Discrete structures**

**Key assumption:** the strain energy density at \( x \) is determined by the deformation of its family.
Potential energy minimization yields the peridynamic equilibrium equation

- Potential energy:
  \[ \Phi = \int_B (W - b \cdot y) \, dV_x \]

  where \( W \) is the strain energy density, \( y \) is the deformation map, \( b \) is the applied external force density, and \( B \) is the body.

- Euler-Lagrange equation is the equilibrium equation:
  \[ \int_{\mathcal{H}_x} f(q, x) \, dV_q + b(x) = 0 \]

  for all \( x \). \( f \) is the pairwise bond force density.
Peridynamics basics: Material model determines bond forces

- Each pairwise bond force vector $f(q, x, t)$ is determined jointly by:
  
  - the collective deformation of $\mathcal{H}_x$, and
  
  - the collective deformation of $\mathcal{H}_q$.

- Bond forces are antisymmetric: $f(x, q, t) = -f(q, x, t)$.
Peridynamics basics: The nature of internal forces

**Standard theory**

Stress tensor field (assumes continuity of forces)

\[ \rho \ddot{u}(x, t) = \nabla \cdot \sigma(x, t) + b(x, t) \]

Differentiation of surface forces

**Peridynamics**

Bond forces between neighboring points (allowing discontinuity)

\[ \rho \ddot{u}(x, t) = \int_{H_x} f(q, x) dV_q + b(x, t) \]

Summation over bond forces

Stress tensor maps surface normal vectors onto surface forces

Force state maps bonds onto bond forces
Peridynamic vs. local equations

- The structures of the theories are similar, but peridynamics uses nonlocal operators.

<table>
<thead>
<tr>
<th>Relation</th>
<th>Peridynamic theory</th>
<th>Standard theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kinematics</td>
<td>$\mathbf{Y}(q - x) = y(q) - y(x)$</td>
<td>$F(x) = \frac{\partial y}{\partial x}(x)$</td>
</tr>
<tr>
<td>Linear momentum balance</td>
<td>$\rho \ddot{y}(x) = \int_{\mathcal{H}} \left( t(q, x) - t(x, q) \right) dV_q + b(x)$</td>
<td>$\rho \ddot{y}(x) = \nabla \cdot \sigma(x) + b(x)$</td>
</tr>
<tr>
<td>Constitutive model</td>
<td>$t(q, x) = T(q - x)$, $T = \hat{T}(\mathbf{Y})$</td>
<td>$\sigma = \hat{\sigma}(F)$</td>
</tr>
<tr>
<td>Angular momentum balance</td>
<td>$\int_{\mathcal{H}} \mathbf{Y}(q - x) \times T(q - x) dV_q = 0$</td>
<td>$\sigma = \sigma^T$</td>
</tr>
<tr>
<td>Elasticity</td>
<td>$T = W_{\mathbf{Y}}$ (Fréchet derivative)</td>
<td>$\sigma = W_F$ (tensor gradient)</td>
</tr>
<tr>
<td>First law</td>
<td>$\dot{\mathbf{e}} = T \cdot \dot{\mathbf{Y}} + q + r$</td>
<td>$\dot{\mathbf{e}} = \sigma \cdot \dot{\mathbf{F}} + q + r$</td>
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</table>

$$T \cdot \dot{\mathbf{Y}} := \int_{\mathcal{H}} T(\xi) \cdot \dot{\mathbf{Y}}(\xi) dV_\xi$$
Bond based material models

- If each bond response is independent of the others, the resulting material model is called bond-based.
- The material model is then simply a graph of bond force density vs. bond strain.
- Damage can be modeled through bond breakage.
- Bond response is calibrated to:
  - Bulk elastic properties.
  - Critical energy release rate.
Linearized theory

- For small displacements (possibly superposed on a large deformation):

\[ \rho \ddot{u}(x, t) = \int_{\mathcal{H}} C(x, q)(u(q, t) - u(x, t)) \, dV_q + b(x, t) \]

where \( C \) is the tensor-valued \textit{micromodulus} field.

- Equation is formally the same as in Kunin’s nonlocal theory.

- Can still have bond breakage.

- Most of the following discussion uses the linearized theory.

- Will see how to get \( C \) by multiscale methods.
Autonomous crack growth

- When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.
EMU numerical method

- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

\[ \rho \ddot{y}(x, t) = \int_{\mathcal{H}} f(x', x, t) \, dV_{x'} + b(x, t) \quad \rightarrow \quad \rho \ddot{y}_i^n = \sum_{k \in \mathcal{H}} f(x_k, x_i, t) \, \Delta V_k + b_i^n \]

- Linearized model:

\[ \rho \ddot{u}_i = \sum_{k \in \mathcal{H}_i} C_{ik} (u_k - u_i) \Delta V_k + b_i \]
Peridynamics fun facts

• Molecular dynamics is a special case of peridynamics
  • Any multibody potential can be made into a peridynamic material model (Seleson & Parks, 2014).
• Classical (local) PDEs are a limiting case of peridynamics as $\delta \to 0$ (SS & Lehoucq, 2008).
• Any material model from the classical theory can be included.
  • e.g., Strain-hardening viscoplastic (Foster & Chen, 2010.)
  • Classical material models with the Emu discretization are similar to
    • RKPM (Bessa, Foster, Belytschko, & Liu, 2014).
    • SPH (Ganzenmüller, Hiermaier, & May, 2014).
• Waves are dispersive
  • Material properties can be deduced from dispersion curves (Weckner & SS, 2011).
• It’s possible to model crack nucleation and growth without damage (!).
  • Use nonconvex bond energy (Lipton, 2014).
Examples: Membranes and thin structures (videos)

Oscillatory crack path

Crack interaction in a sheet

Self-assembly
Dynamic crack branching

• Similar to previous example but with higher strain rate applied at the boundaries.
• Red indicates bonds currently undergoing damage.
  • These appear ahead of the visible discontinuities.
• Blue/green indicate damage (broken bonds).
• More and more energy is being built up ahead of the crack – it can’t keep up.
  • Leads to fragmentation.

More on dynamic fracture: see Ha & Bobaru (2010, 2011)
Dynamic crack branching (video)

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Some peridynamic multiscale methods and results

- Derivation of peridynamic equations from statistical mechanics (Lehoucq & Sears, 2011).
- Higher order gradients to connect MD to peridynamic (Seleson, Parks, Gunzburger, & Lehoucq, 2005).
- Adaptive mesh refinement (Bobaru & Hu, 2011).
- Coarse-graining (SS, 2011).
- Two-scale evolution equation for composites (Alali & Lipton, 2012).
- PFHMM method for atomistic-to-continuum coupling (Rahman, Foster, & Haque, 2014).
Concurrent multiscale method for defects

- Apply the best practical physics at the smallest length scale (near a crack tip).
- Scale up hierarchically to larger length scales.
- Each level is related to the one below it by the same equations.
  - Any number of levels can be used.
- Adaptively follow the crack tip.

The details of damage evolution are always modeled at level 0.
Concurrent solution strategy

- The equation of motion is applied only within each level.
- Higher levels provide boundary conditions on lower levels.
- Lower levels provide coarsened material properties (including damage) to higher levels.

Schematic of communication between levels in a 2D body
Concurrent multiscale example: shear loading of a crack

Bond strain

Damage process zone
Multiscale crack growth in a heterogeneous medium (video)
Branching in a heterogeneous medium

- Crack grows between randomly placed hard inclusions.
Multiscale modeling reveals the structure of brittle cracks

- Material design requires understanding of how morphology at multiple length scales affects strength.
- This is a key to material reliability.

Multiscale model of crack growth through a brittle material with distributed defects

Metallic glass fracture (Hofmann et al, Nature 2008)
Upscaling of material properties

• Suppose we have an accurate model in level 0.
  • How can we obtain material properties in level 1?
  • This is sometimes called “coarse-graining”.
  • Will next describe a method for doing this based on constrained optimization.
Level 1 DOFs

- Divide the region into \( K \) \textit{“cells”} \( C_k \).
- The mean level 0 displacement within each cell is the level 1 DOF:

\[
u_k^1 = \int_{C_k} \varphi(x) u^0(x) \, dx\]

where

\[
\int_{C_k} \varphi(x) = 1.
\]
Level 1 DOF as a constraint

- Pretend all the $u^1_k$ values are given.
- In effect, this places a constraint on the $u^0$ function.
- Constrained potential energy functional:

$$
\Phi = \int_B \left( W^0 (x) - u^0 (x) b(x) \right) \, dx - \sum_{k=1}^{K} \lambda_k \left( \int_{C_k} \varphi (x) u^0 (x) \, dx - u^1_k \right)
$$

where $\lambda_1, \lambda_2, \ldots, \lambda_K$ are Lagrange multipliers.
Force balance on cell \( k \)

- Resulting constrained equilibrium equation:

\[
L^0(x) + b(x) + \lambda_k \varphi(x) = 0
\]

where \( k \) is whichever cell contains \( x \) and \( L^0 \) is the level 0 internal force operator:

\[
L^0(x) = \int_{\mathcal{H}_x} \left( T[x](q - x) - T[q](x - q) \right) dq.
\]

- Observe that the constraint acts like a body force distributed over cell \( k \).
- Integrate the equilibrium equation over cell \( k \), recall \( \int \varphi = 1 \), set \( b \equiv 0 \):

\[
\int_{C_k} L^0(x) \, dx + \lambda_k = 0.
\]

Interaction forces from other cells + constraint force = 0
Level 1 micromodulus

- Set all $u_k^1 = 0$ except for cell $n$: $u_n^1 = \epsilon \ll 1$.
- Solve the constrained equilibrium equation for $u^0(x)$ and the $\lambda_1, \lambda_2, \ldots, \lambda_K$.
- The upscaled micromodulus is

$$c_{kn}^1 = \frac{\lambda_k}{\epsilon}.$$
Example: Rod with a defect

- Upscaling method preserves the effect of a defect embedded within a cell.
Coarser level 1

- If the defect is not exactly at a cell boundary, the method still produces the mean of the level 0 displacements within each cell.
Time-dependent response

- Time-dependent bond force model for level 1:

\[ f(x_n, x_k) = \int_0^t \lambda_k(t - \tau)(\dot{u}(x_k, \tau) - \dot{u}(x_n, \tau)) \, d\tau \]

- \( \epsilon(t) = \) cell n displacement
- \( \lambda_k(t) = \) cell k constraint force
Coarse graining verification: crack in a plate

- Example: Solve the same problem in four different levels using the successively upscaled material properties – results are the same.

Level 0: 16384 nodes
Level 1: 4096 nodes
Level 2: 1024 nodes
Level 3: 256 nodes
Defining damage from coarse-grained material properties

• Define bonds to be damaged if their coarse-grained micromodulus is less than a tolerance.
• This allows damage to be determined without deforming the MD grid.

Level 1 damage contours deduced from coarse-grained properties
Coarse graining MD directly into peridynamics

- The level 0 physics can be anything: PD, standard continuum, MD, MC(?), DFT(?)

Level 0: MD showing thermal oscillations  
Level 1: Coarse grained micromodulus  
MD time-averaged displacements
Summary

- Concurrent multiscale:
  - Adaptively follow crack tips.
  - Apply the best practical physics in level 0.
  - MD time step is impractical. Instead...
- Calibrate a peridynamic damage model from an MD simulation.
  - Derives continuum damage parameters ("parameter passing").
- Coarse-graining:
  - Derives incremental elastic properties at higher levels.
  - Does not rely on a representative volume element (RVE).

- Methods are “scalable:” can be applied any number of times to obtain any desired increase in length scale.
Level 0: calibrating a peridynamic model using molecular dynamics

- The concurrent multiscale method, in spite of subcycling the lower levels, is still not efficient enough to use MD in level 0 for growing cracks.
- Instead: Use MD to calibrate a continuum model.
- Video show smoothed atomic positions in a LAMMPS model of Al polycrystal (courtesy David Newsome, CFD Research Corp.)
- Yellow-red: bond strains > 1.0.
Peridynamic mesoscale simulations using properties determined from MD

- Continuum model of a polycrystal shows the effect of embrittlement due to oxide.

Time-averaged atomic positions (LAMMPS). Colors = peridynamic bond strain.

Calibrated peridynamic bond interactions

Grains

Colors indicate damage (broken bonds)