Numerical fracture experiments using nonlinear nonlocal models

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Joint work with
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Overview of the talk

- Why Peridynamics?
- Peridynamics as an alternative framework
- Introduction to bond-based peridynamics
- Numerical results
- Discussion and future works
Why peridynamics?

- Strain/stress can’t be defined near crack
- Phase field introduces another field which is to be solved along with displacement field
- Handle situations where crack is not apriori known but is found by solving the evolution equation subjected to boundary conditions and initial conditions.

Key researchers in this area:
Stewart Silling & co., Florin Bobaru & co., Kaushik Dayal, Erdogan Madenci & co., John Foster, Olaf Weckner, Pablo Seleson, Erkan Oterkus

Peridynamics: Advantages

- Formulation completely bypasses the computation of derivatives of displacement field.
- A priori location of crack is not required.
- Only unknown field in the theory is displacement field.
- For smooth deformation the Peridynamics theory converges to the elastodynamics theory in the limit of nonlocal length scale going to zero.
- It has been shown numerically, as well as theoretically (for nonlinear model), that one recovers sharp-crack as the nonlocal length scale tends to zero.
- The elastic and fracture properties of the material fully determine the parameters in peridynamic constitutive law.
Peridynamics: Disadvantages

- No physical interpretation of the nonlocal length scale.
- While for smooth deformation, the peridynamics recovers elastodynamics solution, as nonlocal length scale goes to zero, it remains to show how the deformation behaves within the fracture zone in vanishing nonlocality.
- Need more thorough validation of the theory and show that it predicts the material behavior accurately for fairly large class of problems.
- Computationally expensive due to nonlocal nature of force. The computational complexity is of the form $O(Nr^d)$, where $d$ is the dimension, $r$ is the ratio of nonlocal length scale and mesh size, and $N$ is the total number of mesh nodes.
**Bond-based peridynamics**

**Displacement.** Let \( u(x) \) denote the displacement of material point \( x \in D \). Throughout this talk we will make **small-deformation** assumption.

**Nonlocal length scale.** Let \( \epsilon > 0 \) be the nonlocal length scale. We refer to it as “Horizon”. The material point \( x \in D \) interacts with all other points \( y \in B_\epsilon(x) \).

**Bond strain.** For any two material points \( x, y \in D \), we define the bond strain as

\[
S(y, x) = \frac{u(y) - u(x)}{|y - x|} \cdot \frac{y - x}{|y - x|}
\]

Here \( |y - x| \) is the initial length of bond , \( u(y) - u(x) \) is the relative stretch after deformation, and \( \frac{y - x}{|y - x|} \) is the unit vector pointing towards \( y \) from \( x \).
Internal forces. Force at material point $x \in D$ is given by the integration of the pairwise forces between the point $x$ and the neighboring points $y \in B_\epsilon(x)$.

Suppose $\hat{f}^\epsilon(y, x)$ denotes the force applied on $x$ from the neighboring point $y$. Then total force at $x$ is given by

$$f^\epsilon(x) = \int_{B_\epsilon(x)} \hat{f}^\epsilon(y, x) dy$$
Example 1: Linear force

Example 1. Linear peridynamic force

\[ \hat{f}^\epsilon(y, x) = \frac{c}{\epsilon |B_\epsilon(0)|} S(y, x) \frac{y - x}{|y - x|} \]

If displacement field is sufficiently smooth, we can show that

In 2-d/3-d

\[ \mathbf{f}^\epsilon(x) = \nabla \cdot \mathbf{C} \nabla \mathbf{u} + O(\epsilon^2), \]

\[ \mathcal{E} \mathbf{u} = \frac{\nabla \mathbf{u} + \nabla \mathbf{u}^T}{2} \]

\[ \mathbf{C}_{ijkl} = 2\mu \left( \frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2} \right) + \lambda \delta_{ij}\delta_{kl} \]

\[ \lambda = \mu = \frac{c}{12} \text{ in 2-d}, \quad \lambda = \mu = \frac{c}{20} \text{ in 3-d} \]

In 1-d

\[ \mathbf{f}^\epsilon(x) = \frac{\partial}{\partial x} \left( \frac{c}{2} \frac{\partial \mathbf{u}(x)}{\partial x} \right) + O(\epsilon^2) \]
Example 2. Adding fracture to the model

\[ f^\varepsilon(y, x) = \mu(S(y, x)) \frac{c}{\varepsilon |B_\varepsilon(0)|} S(y, x) \frac{y - x}{|y - x|} \]

where \( \mu(S) = 1 \) if \( |S| < S_c \) and \( \mu(S) = 0 \) if \( |S| \geq S_c \).

While constant \( c \) is determined by elastic properties of the material, the critical strain \( S_c \) will be determined by the fracture properties of the material.

In 3-d, given Young’s modulus \( E \) and the critical energy release rate \( G_c \), we have\(^1\)

\[ c = 8E, \quad S_c = \sqrt{\frac{10G_c}{c\pi\varepsilon^5}} \]

Example 3: Nonlinear force

Example 3. Nonlinear peridynamic model\(^1\)

\[
\hat{f}^\varepsilon(y, x) = \frac{1}{\varepsilon |B_\varepsilon(0)|} \frac{\partial S}{\partial r}(|y - x| S(y, x)^2) \frac{y - x}{|y - x|}
\]

If function \(r \mapsto \psi(r)\) is linear, i.e., \(\psi(r) = cr/2\) then we get linear peridynamic model

\[
\hat{f}^\varepsilon(y, x) = \frac{c}{\varepsilon |B_\varepsilon(0)|} S(y, x) \frac{y - x}{|y - x|}
\]

Equation of motion

Equation of motion.

\[ \rho(x)\ddot{u}(x, t) = f^e(x; u(t)) + b(x, t), \quad \forall x \in D, t \in [0, T] \]

Boundary condition.

\[ u(x, t) = g(x, t) \quad \forall x \in D_u, t \in [0, T] \]
\[ b(x, t) = f_{ext}(x, t) \quad \forall x \in D_f, t \in [0, T] \]

Initial condition. \( u(x, 0) = u_0(x), \dot{u}(x, 0) = v_0(x) \) for all \( x \in D \)

Weak form. Multiplying peridynamic equation by smooth test function \( \tilde{u} \) such that \( \tilde{u} = 0 \) on \( D_u \), and integrating over \( D \), and using nonlocal integration by parts, gives

\[ (\rho \ddot{u}(t), \tilde{u}) + a^e(u(t), \tilde{u}) = (b(t), \tilde{u}) \]

where

\[ a^e(u, w) = \frac{1}{\epsilon|B_\epsilon(0)|} \int_D \left[ \int_{B_\epsilon(x)} \psi'(|y - x|S(u)^2)|y - x|S(u)S(w)dy \right] dx \]
Well-posedness of nonlinear peridynamic model

Using the fact that nonlinear peridynamic force is bounded and Lipschitz continuous with respect to displacement field $u \in L^2_0(D)$, the existence of solutions over any finite time domain $[0, T]$ is shown [1].

To prove existence of solutions in more regular spaces, we introduce boundary function $\omega$ into Peridynamic force. $\omega(x) = 1$ in the interior and smoothly decays to 0 as $x$ approaches boundary $\partial D$.

To perform apriori error analysis of finite difference approximation, we consider Hölder space $C^{0, \gamma}_0(D)$, $\gamma \in (0, 1]$. In [2] we show existence of solutions in Hölder space $C^{0, \gamma}_0(D)$. In [3] we extend the results to state-based peridynamic models.

For apriori error analysis of finite element approximation using continuous piecewise linear elements, we consider natural space $H^2(D) \cap H^1_0(D)$. In [4] we show existence of solutions in $H^2(D) \cap H^1_0(D)$.

Well-posedness

Let $W$ be either $C^0_0,\gamma(D)$ or $H^2(D) \cap H^1_0(D)$ space. We assume $u \in W$ is extended by zero outside $D$. Domain $D$ is assumed to be sufficiently smooth (precise details in [1,2]). Two key steps to show existence:

- Obtain Lipschitz bound on peridynamic force in $W$.
- Using Lipschitz bound, show local existence of unique solutions. Show that local existence of unique solutions can be repeatedly applied to get global existence of solutions for any time domain $(-T, T)$.

**Theorem 1. Existence and uniqueness of solutions over finite time intervals**

Let $\nu(t) = \dot{u}(t)$, and $X = W \times W$. For any initial condition $x_0 \in X$, time interval $I_0 = (-T, T)$, and right hand side $b(t)$ continuous in time for $t \in I_0$ such that $b(t)$ satisfies $\sup_{t \in I_0} \|b(t)\|_W < \infty$, there is a unique solution $(u(t), \nu(t)) \in C^1(I_0; X)$ of Peridynamic equation of motion with initial condition $x_0$. Moreover, $(u(t), \nu(t))$ and $(\dot{u}(t), \dot{\nu}(t))$ are Lipschitz continuous in time for $t \in I_0$.

Finite difference approximation

We approximate peridynamic equation using **piecewise constant interpolation** and central in time discretization. Let $u_i^k$ denote the discrete displacement at mesh node $x_i$ and time $t^k = k\Delta t$. We consider following piecewise constant function

$$u_h^k(x) = \sum_{i, x_i \in D} u_i^k \chi_{U_i}(x)$$

Discrete problem is

$$\frac{u_h^{k+1} - 2u_h^k + u_h^{k-1}}{\Delta t^2} = f^e_{h}(t^k) + b_h^k,$$

where

$$f^e_{h}(x, t^k) = \sum_{i, x_i \in D} f^e(x_i, t^k) \chi_{U_i}(x),$$

$$b_h(x, t^k) = \sum_{i, x_i \in D} b(x_i, t^k) \chi_{U_i}(x)$$
Convergence of finite difference approximation

Error at time step $k$ is defined as: $E^k = ||u^k_h - u(t^k)||$.

**Theorem 1.** Let $\epsilon > 0$ be fixed. Let $(u, v)$ be the solution of peridynamic equation. We assume $u, v \in C^2([0, T]; C^{0, \gamma}(D; \mathbb{R}^d))$. Then the finite difference scheme is consistent in both time and spatial discretization and converges to the exact solution uniformly in time with respect to the $L^2$ norm. If we assume the error at the initial step is zero then the error $E^k$ at time $t^k$ is bounded and satisfies

$$
\sup_{0 \leq k \leq T/\Delta t} E^k \leq O \left( C_t \Delta t + C_s \frac{h^\gamma}{\epsilon^2} \right),
$$

where constant $C_s$ and $C_t$ are independent of $h$ and $\Delta t$. Constants $C_t, C_s$ depend on the $\epsilon$ and Hölder norm of the exact solution.


Finite element approximation

Let $V_h \subset H^1_0(D)$ be given by linear continuous interpolations over tetrahedral or triangular elements $\mathcal{T}_h$ where $h$ denotes the size of finite element mesh. We assume elements are conforming and the mesh is shape regular.

For a continuous function $u$ on $\bar{D}$, $\mathcal{I}_h(u)$ is the continuous piecewise linear interpolant on $\mathcal{T}_h$ and is given by

$$\mathcal{I}_h(u)(x) = \sum_{T \in \mathcal{T}_h} \left[ \sum_{i \in N_T} u(x_i) \phi_i(x) \right].$$

Assuming that the size of each element in triangulation $\mathcal{T}_h$ is bounded by $h$, we have

$$||u - \mathcal{I}_h(u)|| \leq ch^2||u||_2, \quad \forall u \in H^2_0(D; \mathbb{R}^d).$$

**Projection:** Let $r_h(u) \in V_h$ is the projection of $u \in H^2(D) \cap H_0^1(D)$ such that

$$||u - r_h(u)|| = \inf_{\tilde{u} \in V_h} ||u - \tilde{u}||$$
Central difference time discretization

$(u_h^k, v_h^k)$ and $(u^k, v^k)$ denote the approximate and the exact solution at $k^{th}$ step. Projection is denoted as $(r_h(u^k), r_h(v^k))$. Approximate initial condition $u_0, v_0$ by their projection $r_h(u_0), r_h(v_0)$ and set $u_h^0 = r_h(u_0), v_h^0 = r_h(v_0)$.

For $k \geq 1$, $(u_h^k, v_h^k)$ satisfies, for all $\tilde{u} \in V_h$,

$$
\left( \frac{u_h^{k+1} - u_h^k}{\Delta t}, \tilde{u} \right) = (v_h^{k+1}, \tilde{u}),
$$

$$
\left( \frac{v_h^{k+1} - v_h^k}{\Delta t}, \tilde{u} \right) = (f^e(u_h^k), \tilde{u}) + (b_h^k, \tilde{u}),
$$

where we denote projection of $b(t^k), r_h(b(t^k))$, as $b_h^k$. Combining the two equations delivers central difference equation for $u_h^k$. We have

$$
\left( \frac{u_h^{k+1} - 2u_h^k + u_h^{k-1}}{\Delta t^2}, \tilde{u} \right) = (f^e(u_h^k), \tilde{u}) + (b_h^k, \tilde{u}), \quad \forall \tilde{u} \in V_h.
$$
Convergence of approximation

Error at time step $k$ is defined as: $E^k = ||u^k_h - u(t^k)||$.

Theorem 3. Convergence of Central difference approximation
Let $(u, v)$ be the exact solution of peridynamics equation and let $(u^k_h, v^k_h)$ be the FE approximate solution. If $u, v \in C^2([0, T], H^2(D) \cap H^1_0(D))$, then the scheme is consistent and the error $E^k$ satisfies following bound

$$\sup_{k \leq T/\Delta t} E^k = C_t \Delta t + C_s \frac{h^2}{\epsilon^2}$$

where constant $C_t$ and $C_s$ are independent of $h$ and $\Delta t$ and depends on the horizon and the norm of exact solution. Constant $L/\epsilon^2$ is the Lipschitz constant of peridynamic force in $L^2$.

Setting up peridynamic model

- Pairwise potential: \( \psi(r) = c(1 - \exp[-\beta r^2]) \)

- Influence function: \( J(r) = 1 - r \) for \( 0 \leq r < 1 \) and \( J(r) = 0 \) for \( r \geq 1 \)

- Critical strain: \( S_c(y, x) = \frac{\pm \bar{r}}{\sqrt{|y - x|}} \), where \( \bar{r} \) is the inflection point of function \( \psi \)

- We fix \( \rho = 1200 \text{ kg/m}^3 \), bulk modulus \( K = 3.24 \text{ GPa} \), critical energy release rate \( G_c = 500 \text{ J/m}^{-2} \)

- Using relation between nonlinear peridynamic model and linear elastic fracture mechanics\(^1\), we find
  \[
  c = 4712.4, \quad \beta = 1.7533 \times 10^8, \quad \bar{r} = \frac{1}{\sqrt{2\beta}} = 5.3402 \times 10^{-5}
  \]

Mode-I crack propagation

- Final time $T = 34 \mu s$, time step $\Delta t = 0.004 \mu s$
- Uniform grid on square domain $D = [0, 0.1 \text{ m}]^2$
Convergence wrt mesh size

- Three set of horizons $\epsilon = 8, 4, 2$ mm. For each fixed $\epsilon$, simulations were run with three different meshes of size $h = \epsilon/2, \epsilon/4, \epsilon/8$. 

![Graph showing L^2 rate of convergence over time for different mesh sizes. The graph has three lines, each representing a different mesh size: $\epsilon = 8$ mm, $\epsilon = 4$ mm, and $\epsilon = 2$ mm. The x-axis represents time in microseconds, ranging from 5 to 35, and the y-axis represents the L^2 rate of convergence, ranging from 0.8 to 2.2. Each line shows peaks and troughs at different times, indicating the rate of convergence for each mesh size.]
Localization of softening zone

$\epsilon = 8 \text{ mm}$

$\epsilon = 4 \text{ mm}$

$\epsilon = 2 \text{ mm}$
Mode I crack propagation: Setup

Goal: Localization of crack and convergence to classical fracture mechanics for simple mode-I crack propagation

- Final time $T = 560 \mu s$, time step $\Delta t = 0.02 \mu s$
- Uniform grid on square domain $D = [0, 0.1 \text{ m}] \times [-0.15 \text{ m}, 0.15 \text{ m}]$
- Experiment with three different horizons $\epsilon = 2.5, 1.25, 0.625 \text{ mm}$
- Body force $b^\epsilon(x, t) = (0, f_0 h(t)/\epsilon)$ on top layer and $b^\epsilon(x, t) = (0, -f_0 h(t)/\epsilon)$ on bottom layer
- $h(t)$ is a step function such that $h(t) = t$ for $t \leq 350 \mu s$ and $h(t) = 1$ for $t > 350 \mu s$
- Mesh size is fixed by relation $h = \epsilon/4$

Localization of softening zone

\[ t = 460 \, \mu s \]

(a) \hspace{1cm} (b) \hspace{1cm} (c)

\[ t = 520 \, \mu s \]

(d) \hspace{1cm} (e) \hspace{1cm} (f)
Localization of softening zone

\[ t = 520 \mu s \]
Crack tip location and velocity
Energy into crack

The energy associated to crack is given by\textsuperscript{1}

\[
E(\Gamma_\delta(t)) = \frac{1}{|B_\epsilon(0)|} \int_{P_\delta(t)} \int_{P_\delta(t) \cap B_\epsilon(x)} \partial_S W(S(y, x; u(t))) \frac{y - x}{|y - x|} \cdot (\dot{u}(x, t) + \dot{u}(y, t)) dy dx.
\]

Here $W$ is the peridynamic pairwise energy density. $P_\delta(t)$ is the rectangle domain with crack tip at its center. It is moving with tip. $P_\delta^c(t)$ is the complement of $P_\delta(t)$.

Energy into crack

![Graph showing energy into crack over time]
Mix mode crack propagation

Material properties are same as in the Mode-I problem. We set

- Horizon $\epsilon = 0.5$ mm
- Mesh size $h = 0.125$ mm
- Final time $T = 140 \, \mu s$
- Time step size $\Delta t = 0.004 \, \mu s$

![Setup diagram](image)

$\begin{align*}
  f_x &= f_y = -5.0 \times 10^{13} \, N \\
  \theta &= 72.5^\circ \\
  f_x &= f_y = 5.0 \times 10^{13} \, N
\end{align*}$

![Damage profile](image)

![Experiment result](image)

![$u_x$ plot](image)

![$u_y$ plot](image)

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Crack-void interaction

Material properties are same as in the Mode-I problem. We set

- Horizon $\epsilon = 0.4$ mm
- Mesh size $h = 0.1$ mm
- Final time $T = 800$ $\mu$s
- Time step size $\Delta t = 0.004$ $\mu$s

(a) Setup (units in mm)

(b) Damage profile

(c) Magnitude of symmetric gradient of displacement

(d) Numerical experiment results using FEM, Boundary element method [2]


Wave reflection effect on crack velocity

We consider a softer material with shear modulus $G = 35.2$ kPa, density $\rho = 1011$ kg/m$^3$, and critical energy release rate $G_c = 20$ J/m$^{-2}$. Poisson ratio is fixed to $\mu = 0.25$. Domain is $D = [0, 0.12 \text{ m}] \times [0, 0.03 \text{ m}]$.

- Horizon $\epsilon = 0.6$ mm, mesh size $h = 0.15$ mm
- Time $T = 1.1$ s, $\Delta t = 2.2$ $\mu$s
Wave reflection effect on crack velocity

- Max crack length = 0.12 m
- Rayleigh wave speed $c_R = 5.502 \text{ m/s}$
Ongoing and future works

- In [1] we show that the classical kinetic relation is embedded in peridynamics and we have \( \lim_{\varepsilon \to 0} J(t) = G_c \), where \( J(t) \) is the nonlocal J-integral. In LEFM, the classical kinetic relation for the crack velocity is postulated. In contrast, we obtain the classical kinetic relation from the Peridynamics in the limit of vanishing nonlocality.

- Open source computational library for nonlocal modeling. This is a joint work with Patrick Diehl (LSU) and Robert Lipton (LSU).

- Study of granular material using nonlinear nonlocal model.

Thank you!