Multiphysics-based Damage Modeling and Crack propagation using Meshless Peridynamics Approach

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- Prof. Max Gunzburger (Florida State University)

Outline

- Background
  - Challenges with damage, crack propagation
  - Peridynamics based meshless modeling approach

- ACT’s Development of Peridynamics based meshless tools for damage and crack propagation
  - Multi-physics based modeling of corrosion damage in metals
  - Crack propagation in composites
  - Other examples

- Summary

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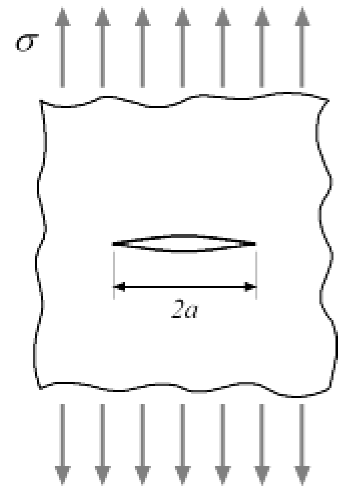
- Conventional Failure Analysis (strength of materials approach)
  - Most straight forward design consideration to avoid structural failure is to keep the stresses, strains, or strains in a material within the *material strength* limits and use a *factory of safety*.

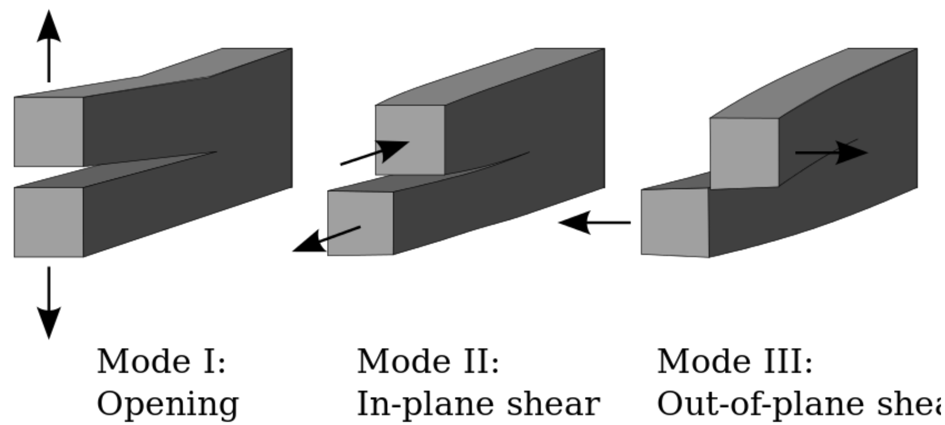
Maximum Stress ↔ Strength of Material

Applied Stress ↔ Failure Criterion



$$K_I = \sigma\sqrt{\pi a}$$

- Fracture Mechanics approaches define three basic modes of crack tip deformation



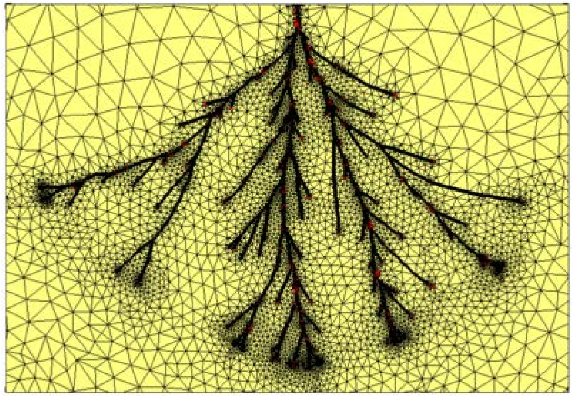
- Common analysis includes finding the stress intensity factor, K.
  - For example, a plate with crack (shown on right)
  - Relations strain energy release f

- Several relations between strain energy release rate and stress intensity factors (for different conditions, geometry) have been developed
  - **Griffith's (energy) criterion, Irwin's formula, CTOD, J-integral**

Challenge of predicting crack propagation

- Despite development in finite element methods, fracture mechanics and several advancements in theory of applying fracture mechanics approaches for failure prediction, challenges exist on how can the crack be modeled

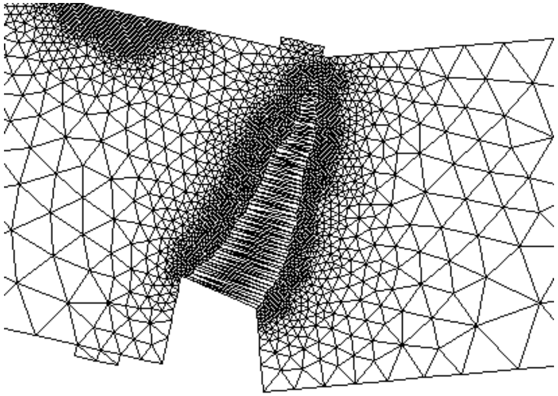
- Things to consider:
  - Crack propagation path
  - Branching of cracks (splitting)
  - Load redistribution due to crack



Crack propagation and branching

The challenge …

- Crack in conventional mechanics is a singularity which needs explicit tracking (i.e., its location need to be specified for the mechanics problem of σ evolution).
- FEM lends itself well for solving the continuum mechanics equation, but needs:
  - prescription of crack path and
  - re-meshing of the domain for every crack propagating step



FE mesh near a crack tip

The purpose of Peridynamics

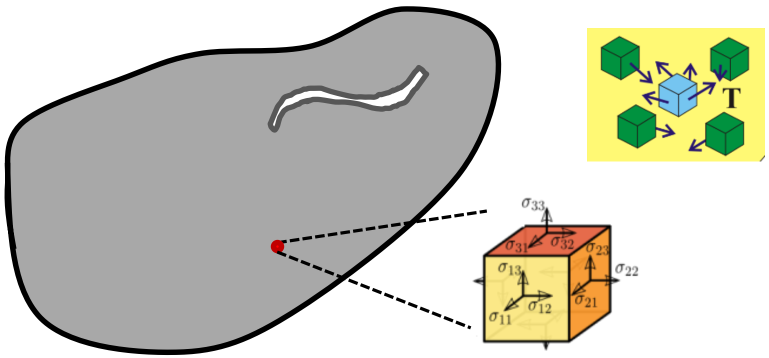
- To unify the mechanics of continuous and discontinuous media within a single set of equations.

- Why do this?
  - Provide a unified mathematical description of the material without the issues of discontinuity (crack)
  - Model complex fracture patterns
  - Avoid coupling of dissimilar mathematical systems
- To accomplish this, the *Peridynamics* approach was proposed as a reformulation of elasticity theory, by Stewart Silling (Sandia) in 2000.

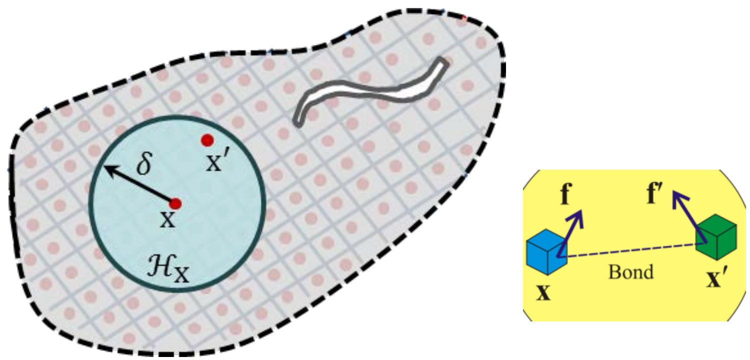
Peridynamics Theory

- Peridynamics (PD) is a nonlocal reformulation of classical elasticity theory that permits modeling materials with discontinuities such as cracks.

peri "near" and *dynamic* "force" (Greek) → *peridynamics*



Classical continuum solid with crack



Peridynamic solid with crack

Classical/Cauchy equation of motion

$$\rho\ddot{u}(\mathbf{x,t}) = \nabla \cdot \sigma(\mathrm{x,t}) + b(\mathbf{x,t})$$

- Assumes differentiable displacement field
- Continuous distribution of mass
- Local interactions through contact forces
- Crack(discontinuity) treated as a pathology

Peridynamic equation of motion

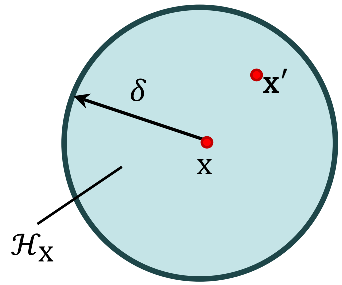
$$\rho\ddot{u}(\mathbf{x,t}) = \int_{\mathcal{H}_{\mathbf{X}}} \mathrm{f}(\mathrm{u}'-\mathrm{u},\mathrm{x}'-\mathrm{x})dV + b(\mathrm{x,t})$$

- Allows discontinuous fields (singularities)
- Material points interaction through bond forces, a force function, f which defines constitutive model
- Non-local integral allows for interaction over a distance

Peridynamics : Basics

- Reformulation of classical elasticity theory, proposed by Stewart Silling, 2000.
- The internal forces within a body is treated as a network of interactions between material points
- The **governing equation** given by local conservation of linear momentum as,

$$\rho(\mathrm{x})\ddot{\mathbf{u}}(\mathrm{x},t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{u}(\mathbf{x}',t) - \mathbf{u}(\mathbf{x},t), \mathbf{x}' - \mathbf{x})\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$



x is material point (reference configuration)

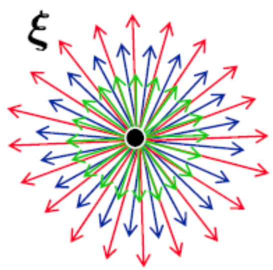
$\mathbf{u}(\mathrm{x},t)$ is displacement of material point x

$\mathbf{f}$ is nonlocal force density (vector function),

force exerted by material point x' on point x

$\mathbf{b}(\mathrm{x},t)$ is external body force density

$\rho(\mathrm{x})$ is mass density



$\mathcal{H}_{\mathrm{x}}$ is neighborhood (family) of x over which interactions occur

$\boldsymbol{\xi} = \mathrm{x}' - \mathrm{x}$ represents a bond in reference configuration

$\boldsymbol{\eta} = \mathbf{u}(\mathrm{x}',t) - \mathbf{u}(\mathrm{x},t)$ relative displacement

$\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ describes material behavior by mapping deformation given by $\boldsymbol{\eta}$ for bond $\boldsymbol{\xi}$

Bond based PD model

- Simple version of Peridynamics model

$$\rho(\mathrm{x})\ddot{\mathbf{u}}(\mathrm{x},t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t),\mathbf{x}'-\mathbf{x})dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

- f (,) is a pairwise force function, value is a force vector (force/volume[2])
- $(\boldsymbol{\xi}+\boldsymbol{\eta})\times\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = 0$ and $\mathbf{f}(-\boldsymbol{\eta},-\boldsymbol{\xi}) = -\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})$

  where, $\boldsymbol{\xi}+\boldsymbol{\eta}$ is current relative position vector between particles

Example, <u>Prototype micro-elastic brittle (PMB)</u>

- Force density described as ,

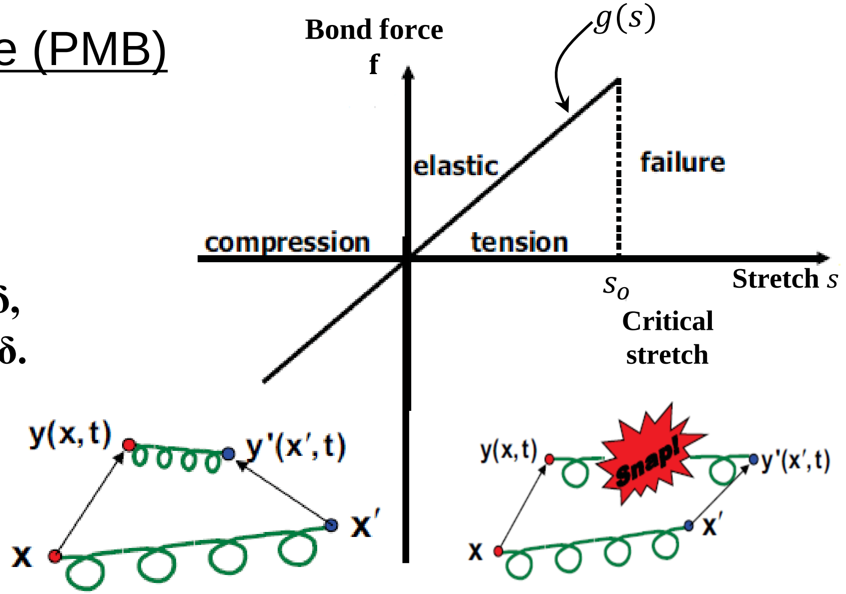
$$\mathbf{f}(\boldsymbol{\eta},\xi) = \mathbf{g}(\boldsymbol{\eta},\xi)\frac{\boldsymbol{\eta}+\xi}{|\boldsymbol{\eta}+\xi|},$$

$$\text{where, } \mathbf{g}(\boldsymbol{\eta},\xi) = \begin{cases} cs(t,\boldsymbol{\eta},\xi)\mu(t,\boldsymbol{\eta},\xi), & |\xi|\le\delta, \\ 0, & |\xi|>\delta. \end{cases}$$

c = stiffness of material

$s = \frac{|\boldsymbol{\eta}+\xi|-|\xi|}{|\xi|}$ is bond stain

$$\mu(t,\boldsymbol{\eta},\xi) = \begin{cases} 1 & \text{unbroken bonds} \\ 0 & \text{broken bonds} \end{cases}.$$



PMB material model

Peridynamic Material Models : State based

- **State based PD model**
  - Generalized PD model, admits materials with any Poisson ratio.
    (PMB materials have Poisson ratio of ¼ only)
  - Each bond force depends on collective deformation of all bonds within the horizon, i.e., Forces within each bond are not independent

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

$\underline{\mathbf{T}}$ is a force state vector material point in reference configuration

$\underline{\mathbf{T}}\,[\mathrm{x},t]\langle\cdot\rangle$ is a mapping of $\mathrm{x}'-\mathrm{x}$ to a force vector field

$\mathrm{x}'-\mathrm{x}$ is the bond between displacement point x and x'

  - PD state are continuum equivalent of multibody potentials (like EAM) of classical particle mechanics

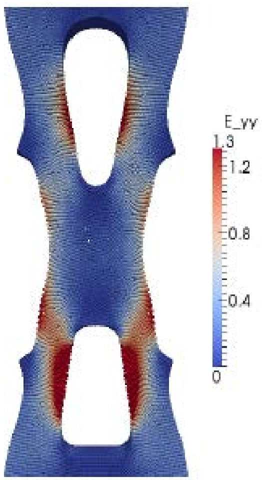
- **Linear Peridynamic solid**

$$\rho(\mathrm{x})\ddot{\mathbf{u}}(\mathrm{x},t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbb{C}(\mathbf{x}'-\mathbf{x})(\eta'-\eta) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

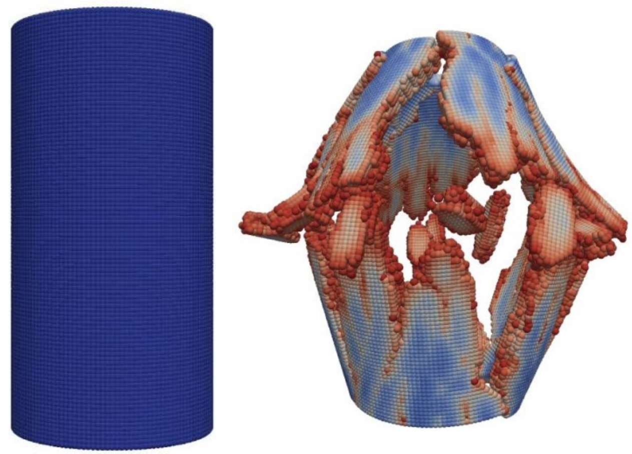
  - $\mathbb{C}(\mathrm{x}'-\mathrm{x})$ is micromodulus function

What can Peridynamics model?

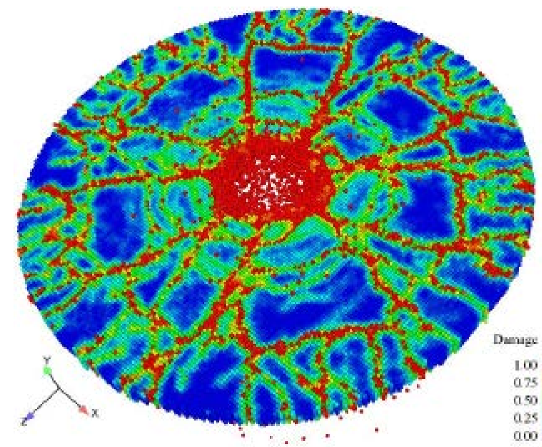
- Crack propagation and fracture failure



Necking under uniaxial tension [Littlewood et al.]



Cylinder before and after fragmentation simulated using PERIDIGM [Parks et al.]



Fracture patterns in a disc after impact with a hard ball, simulated using PD LAMMPS [Seleson et al.]

- Failure of composite laminate
- Fatigue failure
- Transient heat conduction
- Electromigration
- Corrosion, Corrosion Fatigue modeling ← ACT’s work

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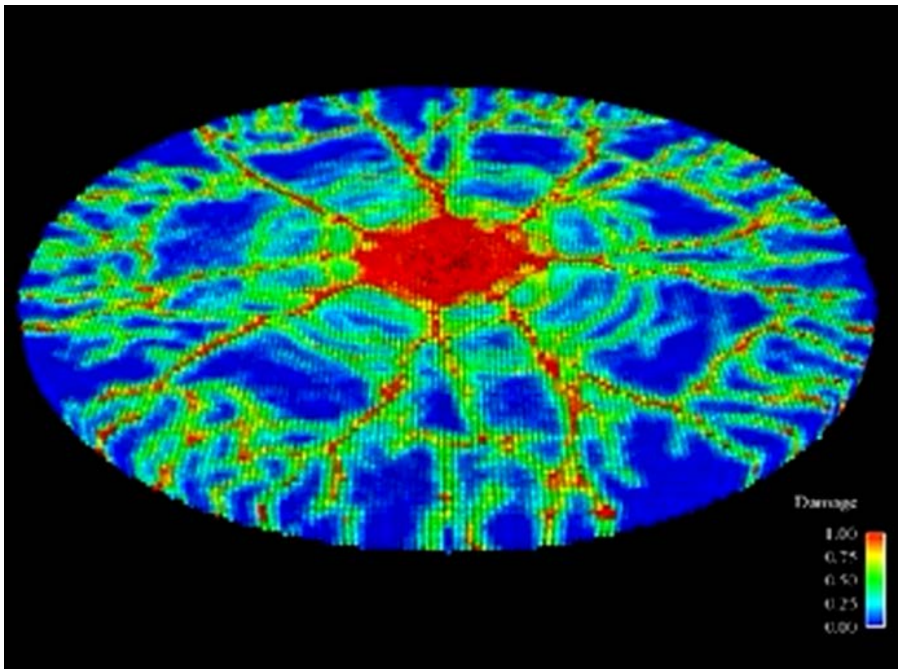
PD Simulation of Fracture Patterns during Impact

- Evolution of fracture patterns in a disc after impact with a hard ball (ball not shown for clarity)



disc.mp4

- Video credit : Pablo Seleson, University of Texas
  (work done during PhD with Prof. Gunzburger, Florida State Univ.)

Summary

- The peridynamics approach automatically enables simulation of cracks propagation and failure, without the need for complicated crack path algorithms like that of XFEM or cohesive element method.

- We developed a peridynamics framework for multiple applications:
  - Modeling corrosion damage phenomena mechanistically, taking into account material weakening due to pitting.
  - Modeling crack propagation in composites, taking into account the degradation of composites
  - Brittle fracture
- Corrosion test cases: illustrate capture of pit nucleation, growth and coalescence phenomena, both with and without manifestation of stress.

- Composite crack propagation cases: illustrates the failure propagation in composites under tensile loads.

- ☞ Peridynamics based damage modeling tools provide a framework for physics-based prediction, prognostics and maintenance in different applications.

Thank you

- Our modeling services include:
  - Modeling of crack propagation and damage using meshless (peridynamics methods)
  - Damage propagation and failure in composites
  - Corrosion damage and fatigue modeling
  - Modeling multiphysics of semiconductors and battery materials Combustion modeling
  - Modeling hypersonic phenomena
  - Computational chemistry and chemical kinetics

- We provide/develop custom modeling capabilities for all the above applications.

- Contact us:

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