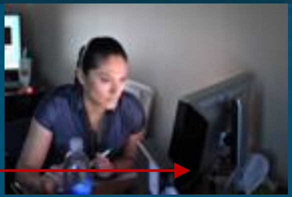
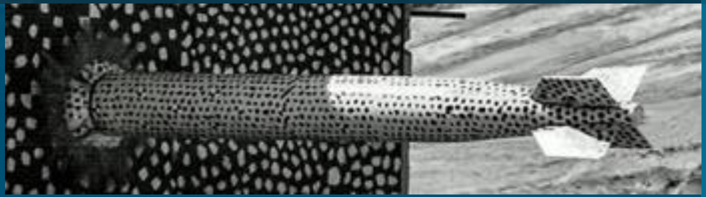
Peridynamics and linear elastic fracture mechanics





Stewart Silling

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Workshop on Experimental and Computational Fracture Mechanics
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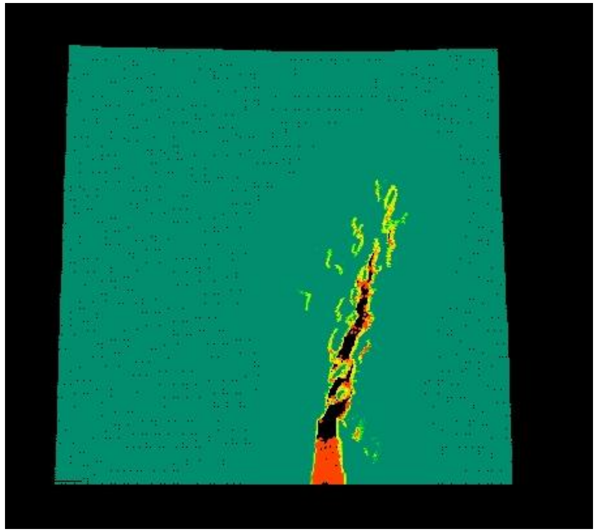
Outline

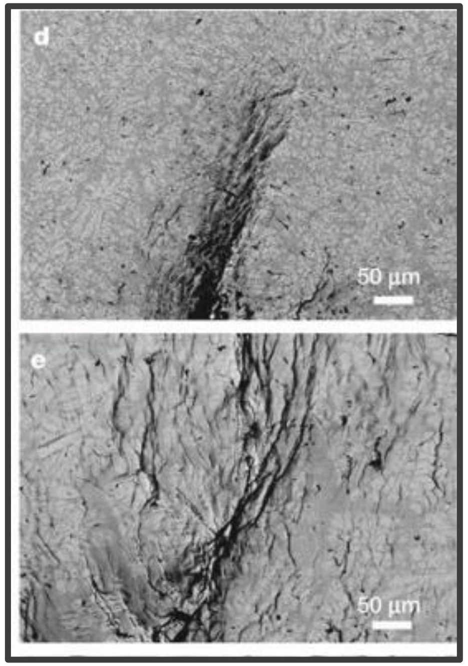
- Peridynamics background
- Autonomous crack growth
- Similarities and differences with linear elastic fracture mechanics (LEFM)
  - Fields near a crack tip
  - Energy dissipation by a growing crack
  - Mixed mode loading
  - Fatigue

Peridynamics: What it is

- It is a theory of solid mechanics that allows for discontinuities within the basic equations.
- It also allows for long-range forces.
- Why?
  - Avoid need to insert discontinuities at the numerical level
  - Seamlessly transition from crack nucleation to growth



Peridynamic simulation



Metallic glass crack tip
Images: Hofmann et al, 2008

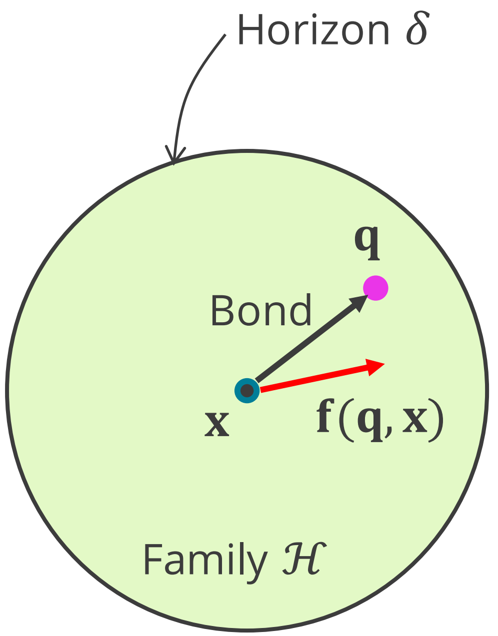
Peridynamic equation of motion

- Peridynamic equation of motion:

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\,\mathrm{d}\mathbf{x} + \mathbf{b}(\mathbf{x},t)$$

  where $\mathbf{y}$ is the deformation map and $\mathbf{b}$ is the external body force density.

- $\mathcal{H}$ is a neighborhood of $\mathbf{x}$ called the *family* of $\mathbf{x}$.
- The radius of $\mathcal{H}$ is called the *horizon* δ.
- $\mathbf{f}(\mathbf{q},\mathbf{x},t)$ is the *pairwise bond force density* that $\mathbf{q}$ exerts on $\mathbf{x}$ (units N/m^3 in 3D).
- There doesn't need to be an actual long-range physical force (like gravity) between $\mathbf{q}$ and $\mathbf{x}$.

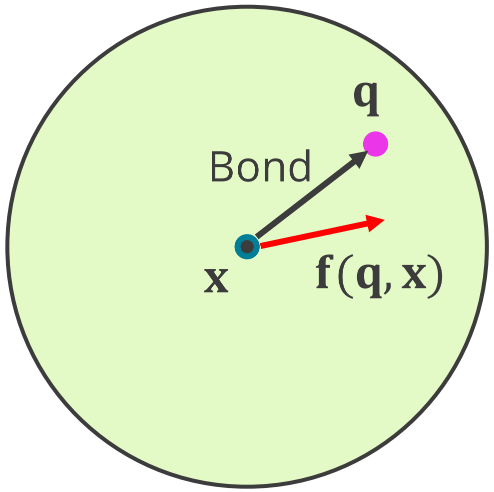


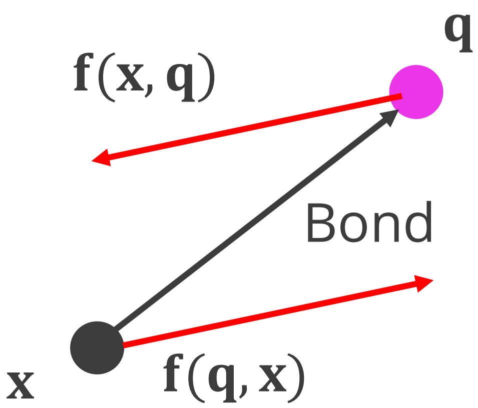
Material model provides values of the bond force

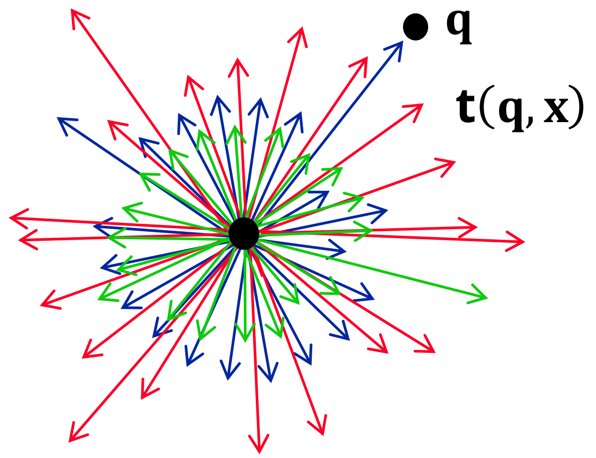
- $\mathbf{f}$ contains contributions from the material response at both $\mathbf{x}$ and $\mathbf{q}$.

$$\mathbf{f}(\mathbf{q},\mathbf{x}) = \mathbf{t}(\mathbf{q},\mathbf{x}) - \mathbf{t}(\mathbf{x},\mathbf{q}).$$

- The *material model* at $\mathbf{x}$ determines $\mathbf{t}(\mathbf{q},\mathbf{x})$ for every deformation of $\mathcal{H}$.







Bond forces

Material modeling: States

- Material modeling uses nonlocal operators called *states*.
- A state maps any bond $\boldsymbol{\xi}$ onto some other quantity.

$$\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle = \mathbf{v}.$$

- The *deformation state* maps any bond onto its deformed image.

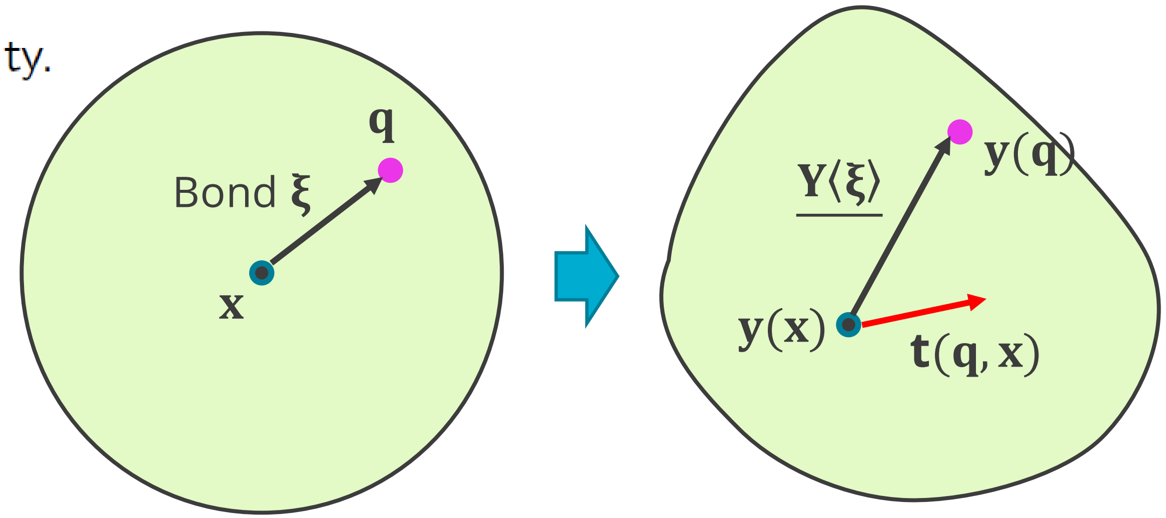
$$\underline{\mathbf{Y}}\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q}) - \mathbf{y}(\mathbf{x}).$$

- The *force state* maps any bond onto its bond force density.

$$\underline{\mathbf{T}}\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{t}(\mathbf{q}-\mathbf{x}).$$

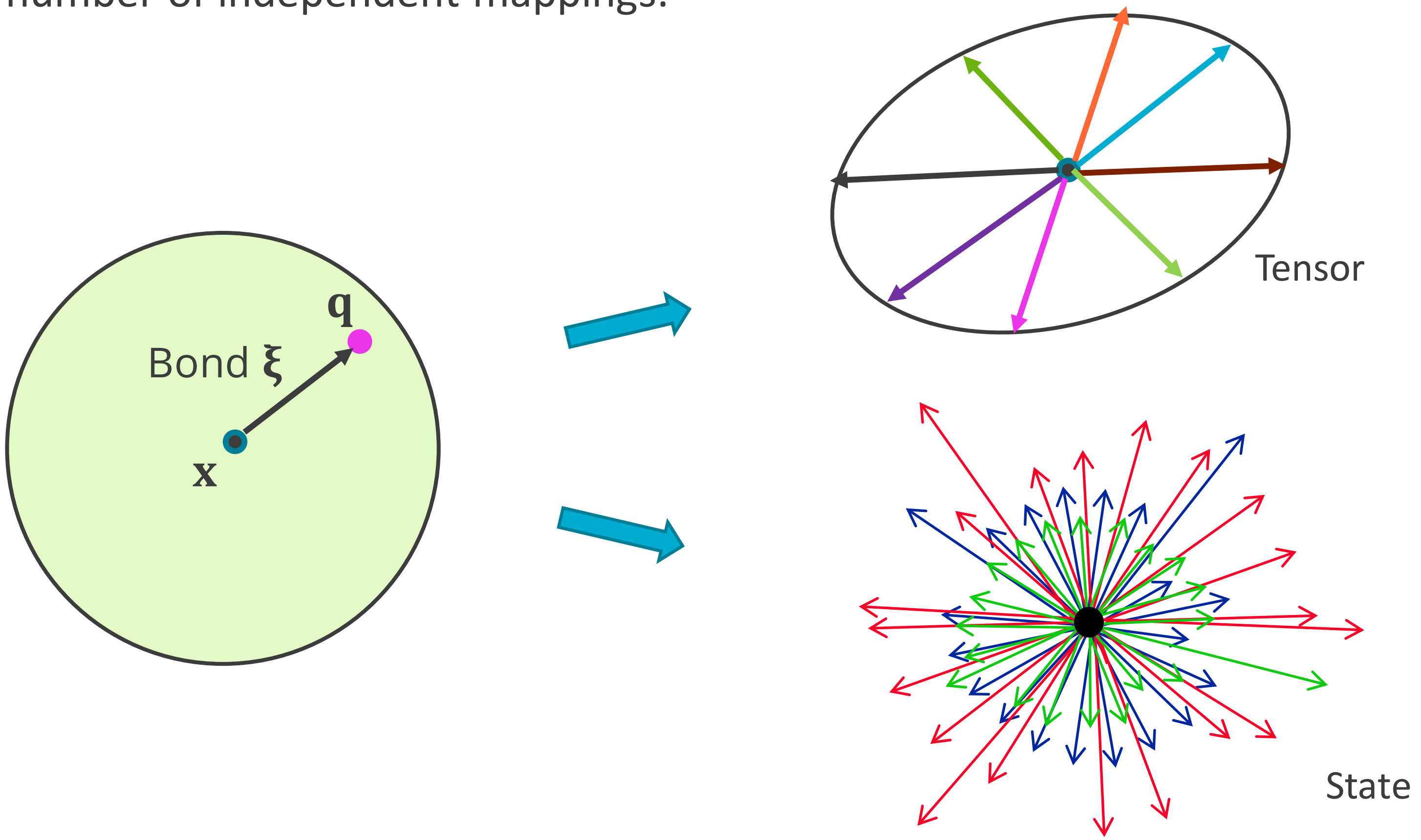
- A material model is a state-valued function of a state.

$$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}).$$



States are like tensors but with more "bandwidth"

- States and 2nd order tensors both map vectors into vectors.
- Tensors: mapping is linear.
  - 9 independent components.
- States: mapping can be nonlinear and even discontinuous.
  - Infinite number of independent mappings.



Finding a stress tensor from a peridynamic model

- The stress tensor does not play a fundamental role in peridynamics.
- But sometimes we want to know it.
- Approximate expression (***partial stress tensor***):

$$\boldsymbol{\sigma} = \frac{1}{2}\int_{\mathcal{H}} \mathbf{f}(\mathbf{q},\mathbf{x}) \otimes (\mathbf{q}-\mathbf{x})\, d\mathbf{q}$$

where $\otimes$ is the dyadic (tensor) product of two vectors.

- Units are force/area. ☺

- SS, D. Littlewood, and P. Seleson, 2015. Variable horizon in a peridynamic medium. *Journal of Mechanics of Materials and Structures*, 10(5), pp.591-612.
- S. Li, 2021. Peridynamic stress is a weighted static virial stress. arXiv:2103.00489.

Discrete form of the peridynamic model

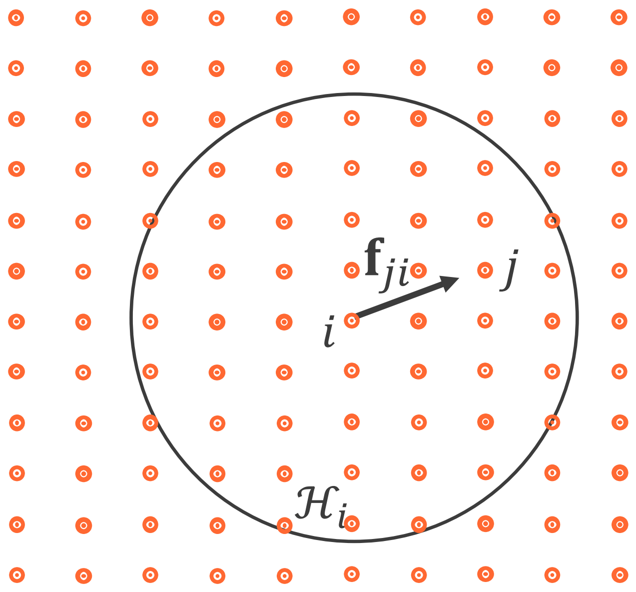
- We will mostly be using the discrete form:

$$m_i \ddot{\mathbf{u}}_i = \sum_{j \in \mathcal{H}_\mathrm{i}} \mathbf{f}_{ji} + \mathbf{b}_i$$

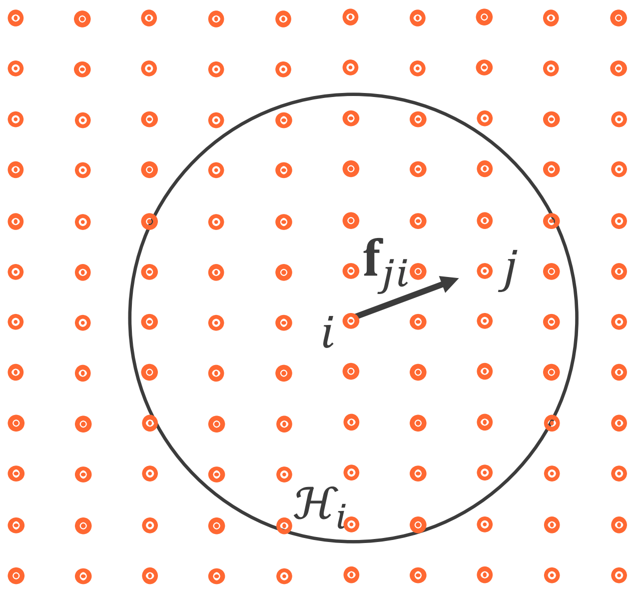
  where i is the node (discrete DOF) number.

- $\mathcal{H}_\mathrm{i}$ is the *family* of i, consisti $m_i \ddot{\mathbf{u}}_i = \sum_{j \in \mathcal{H}_\mathrm{i}} \mathbf{f}_{ji} + \mathbf{b}_i$ that interact with it.

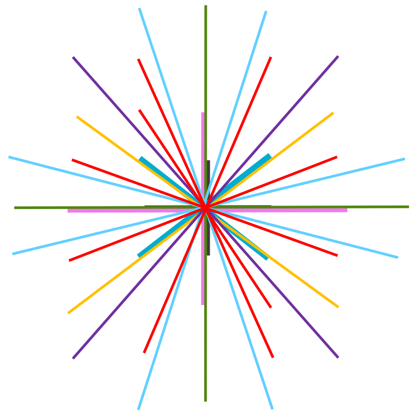
- Usually $\mathcal{H}_\mathrm{i}$ is assumed to have a finite horizon δ.



Bonds in a family (stencil)



Family of node i

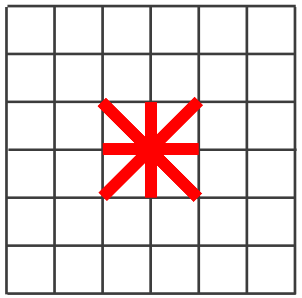


Bond interactions for node i

$$m_i \ddot{\mathbf{u}}_i = \sum_{j \in \mathcal{H}_i} \mathbf{f}_{ji} + \mathbf{b}_i$$

How general is peridynamics?

- Start with what everybody is familiar with: **Finite element** discretization of a PDE $Lu + b = 0$



- Red lines show direct interactions of the node at the center with its neighbors.
- Interactions in terms of the FE stiffness matrix K:

$$\sum_j K_{ij}(u_j - u_i) + b_i = 0$$ for each FE node (row) i.

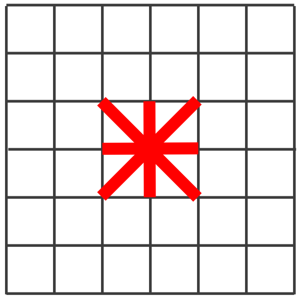
- Compare with peridynamics:

$$\sum_j f_{ji} + b_i = 0$$

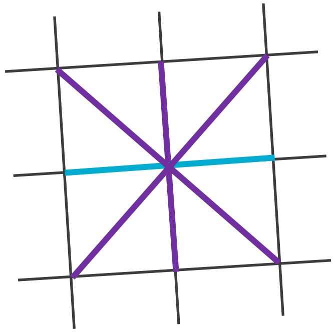
- Set $f_{ji} = K_{ij}(u_j - u_i)$.
- Conclusion is that FEM is (technically) a special case of PD.
- Same is true of MD, SPH, other methods.

How reasonable is nonlocality?

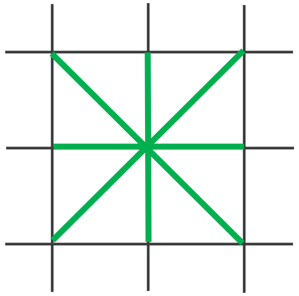
- Already showed that this "stencil" for PD bond interactions provides a reasonable representation of a continuum since FEM does.
- What about the following? They do too for the same reason.



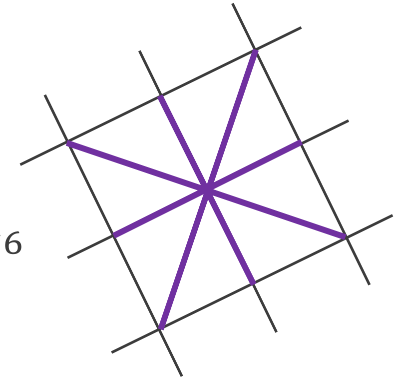
L_1



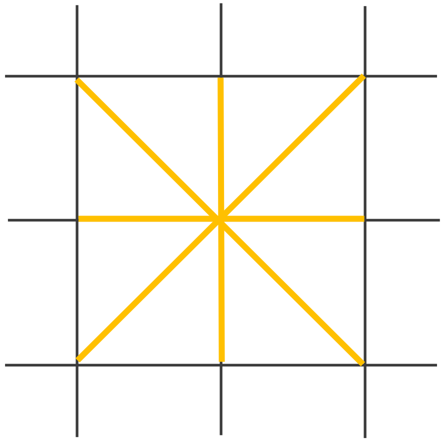
L_5



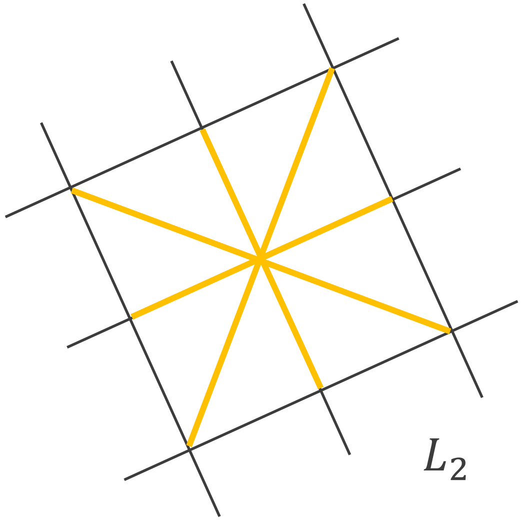
L_4



L_6



L_3

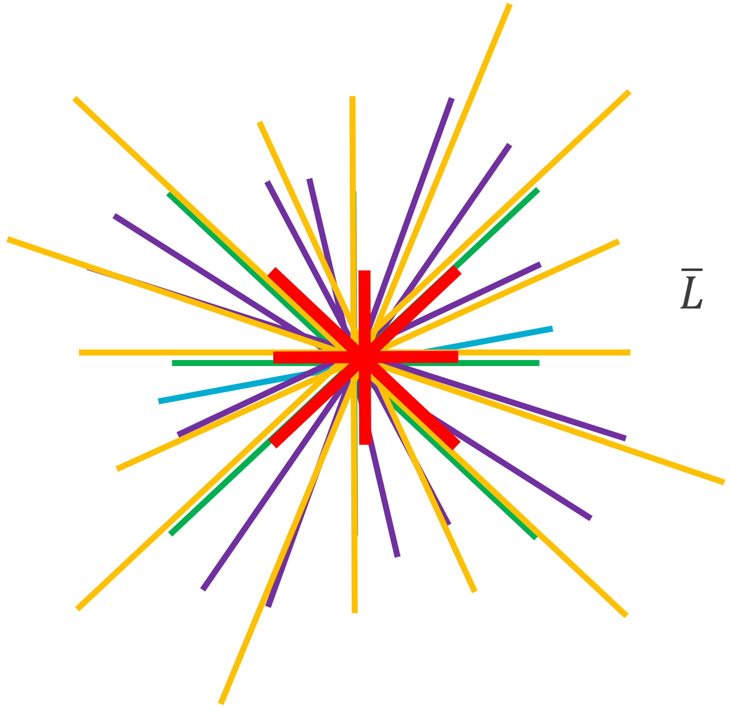


L_2

How reasonable is nonlocality? (ctd.)

- Now take the average of all 6 FEM interactions, each of which provides a reasonable representation of a real continuum:

$$\bar{L} = (L_1 + L_2 + L_3 + L_4 + L_5 + L_6)/6$$



- This is nonlocality in the sense of peridynamics.
- Does not assume that bonds respond independently of each other.
- It does not assume a gravitational of electrostatic type of action-at-a-distance.

Elastic materials and bond damage

- Strain energy density has the same meaning as in the local theory.
- Elastic material model:

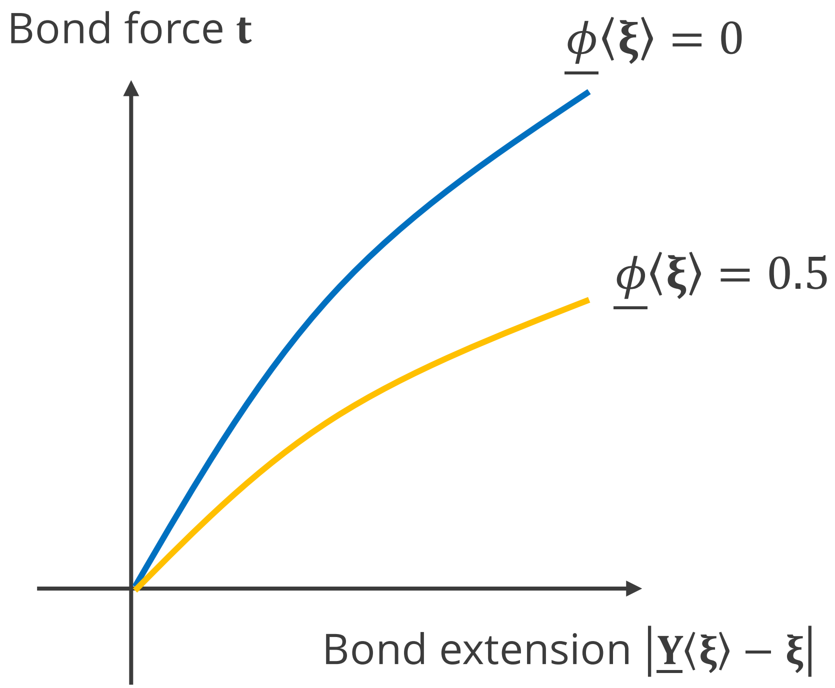
$$W = \hat{W}(\underline{\mathbf{Y}}).$$

- Elastic material with damage:

$$W = \hat{W}(\underline{\mathbf{Y}}, \underline{\phi})$$

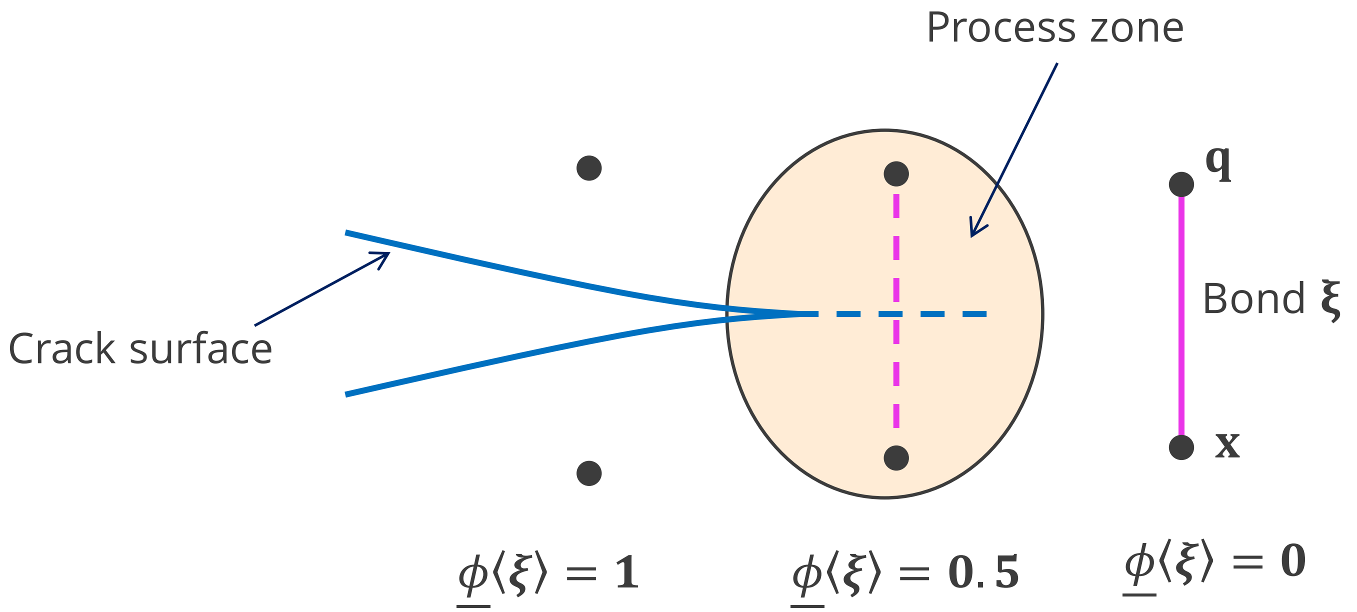
  where $\underline{\phi}$ is the *damage state*.

- Each $\underline{\phi}\langle\boldsymbol{\xi}\rangle$ grows monotonically from 0 to 1 over time according to some evolution law.



Peridynamic process zone

- Bonds are being damaged in a small region (size = $O(\delta)$) near the crack tip.



Autonomous fracture

- The bonds degrade and fail according to conditions within their family.
  - This allows cracks to “do what they want to.”
- As much as possible, we’d like to avoid using
  - Global failure criteria (that involve larger length scales).
  - Supplemental equations that determine crack growth.

Linear peridynamic solid (LPS)

- This is the closest analogue to a classical linear elastic isotropic solid.

$$W = \frac{1}{2}k\theta^2 + \frac{1}{2}\alpha \underline{d} \bullet \underline{d}$$

where θ is the (nonlocal) dilatation

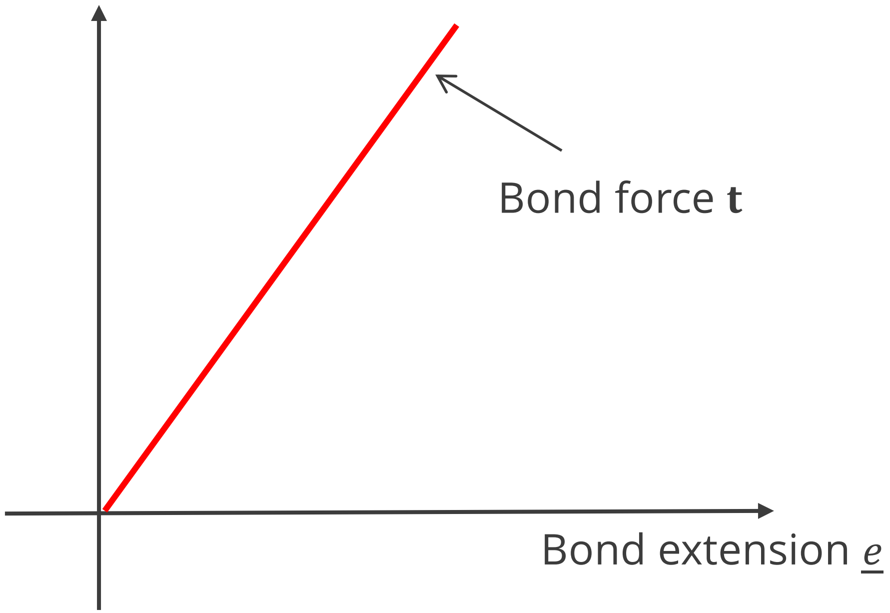
$$\theta = \frac{3\underline{\omega}\,\underline{x} \bullet \underline{e}}{\underline{\omega x} \bullet \underline{x}}$$

and $\underline{d}$ is the deviatoric part of the extension state:

$$\underline{e} = |\underline{\mathbf{Y}} - \underline{\mathbf{X}}|, \qquad \underline{d} = \underline{e} - \frac{\theta \underline{x}}{3}.$$

- k is the usual bulk modulus.
- α is a constant that characterizes the shear response:

$$\alpha = \frac{15\mu}{\underline{\omega}\,\underline{x} \bullet \underline{x}}.$$



LPS with continuous bond damage

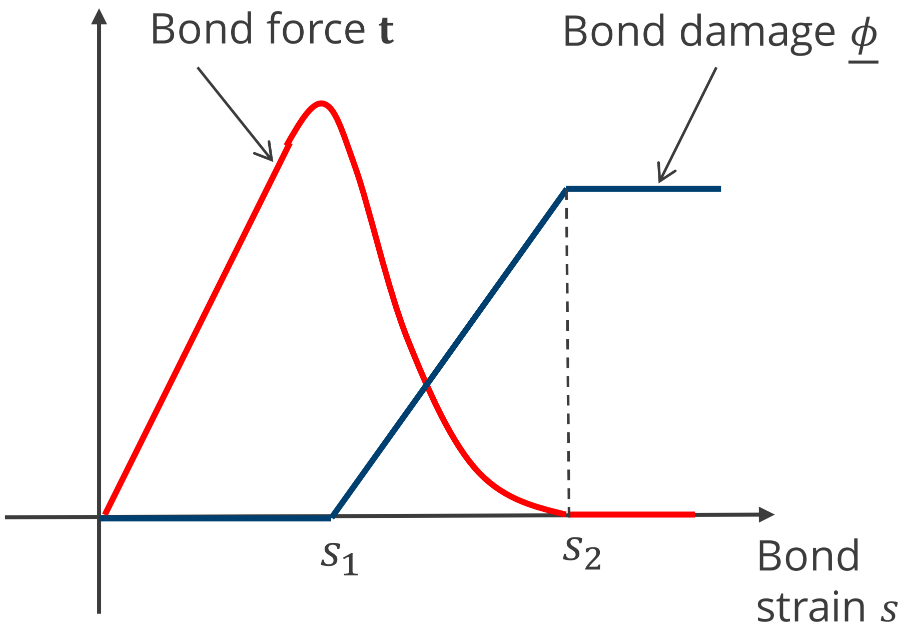
- To include damage, use the same LPS equations but with a modified form of the bond extension:

$$W = \frac{1}{2}k\theta^2 + \frac{1}{2}\alpha \underline{d} \bullet \underline{d}$$

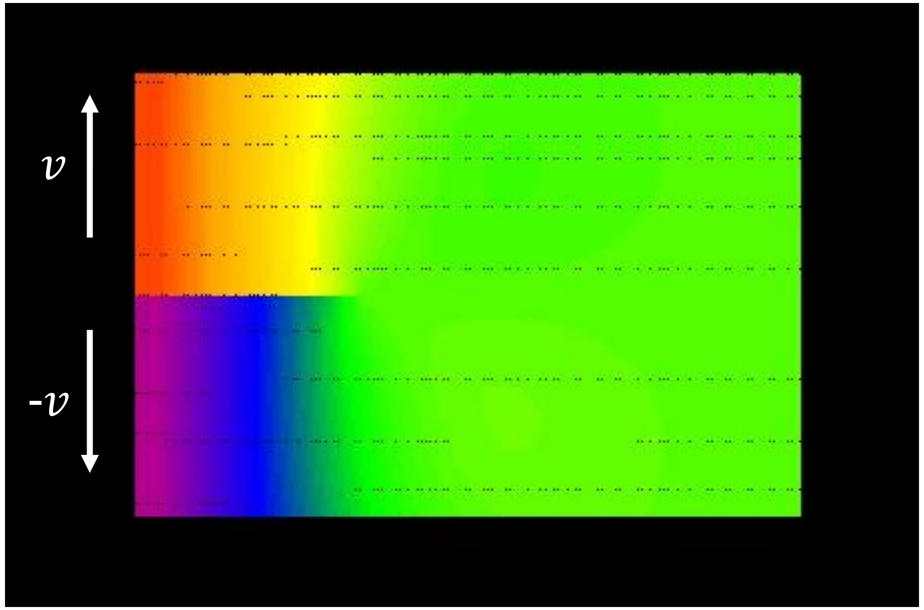
$$\underline{e} = (1 - \underline{\phi})|\underline{\mathbf{Y}} - \underline{\mathbf{X}}|, \qquad \underline{d} = \underline{e} - \frac{\theta \underline{x}}{3}.$$

- The bond damage follows grows linearly with bond strain s, where

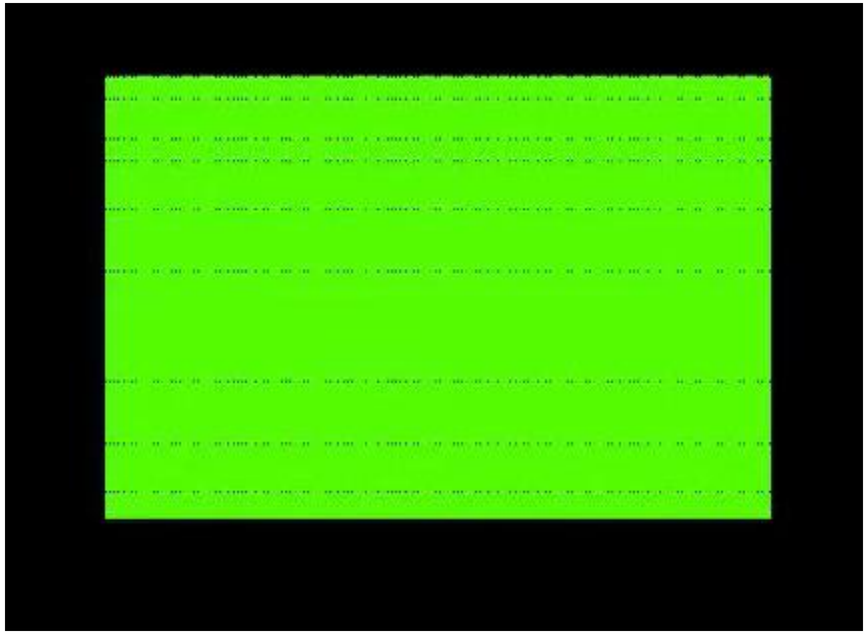
$$s = \frac{\underline{e}}{|\underline{\mathbf{X}}|} - 1.$$



Crack growth in a plate: Mode I



VIDEO



Colors show vertical displacement

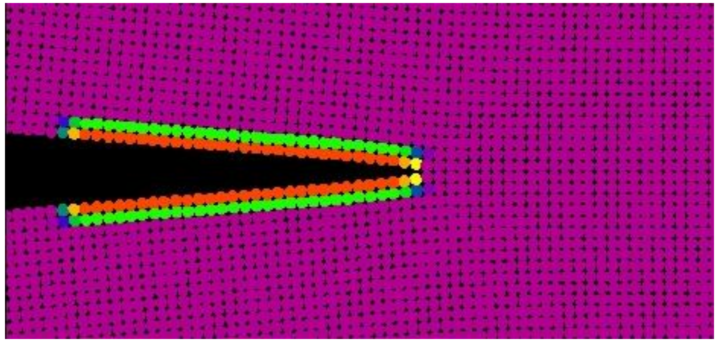
Energy dissipation at a point: the family Joules

- Recall that the free energy depends on both the deformation of the family and the bond damages.

$$W(\underline{\mathbf{Y}}, \underline{\phi}).$$

- The rate of energy dissipation at $\mathbf{x}$ due to damage growth is (basically)

$$\dot{\psi} = -\int_{\mathcal{H}} \frac{\partial W}{\partial \underline{\phi}} \langle \boldsymbol{\xi} \rangle \; \dot{\underline{\phi}} \langle \boldsymbol{\xi} \rangle \; \mathrm{d}\boldsymbol{\xi}$$

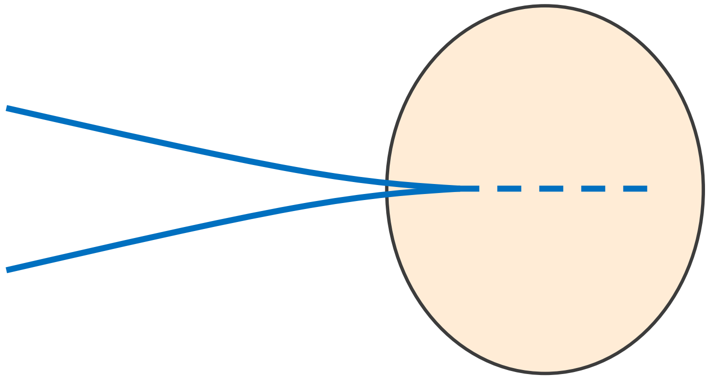


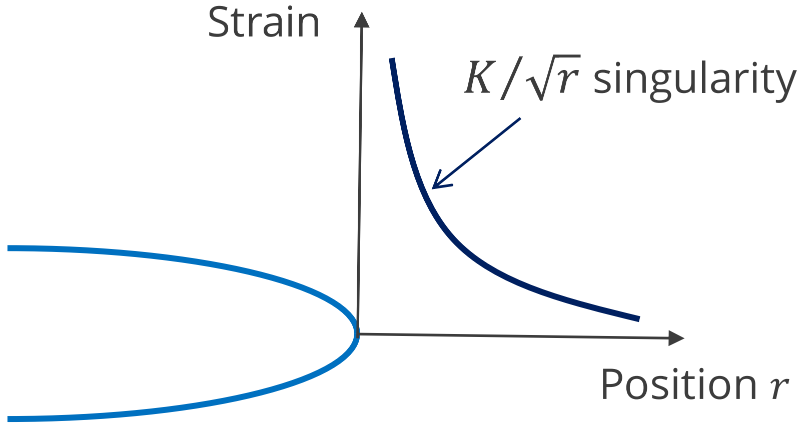
Colors show energy dissipated ψ at each node

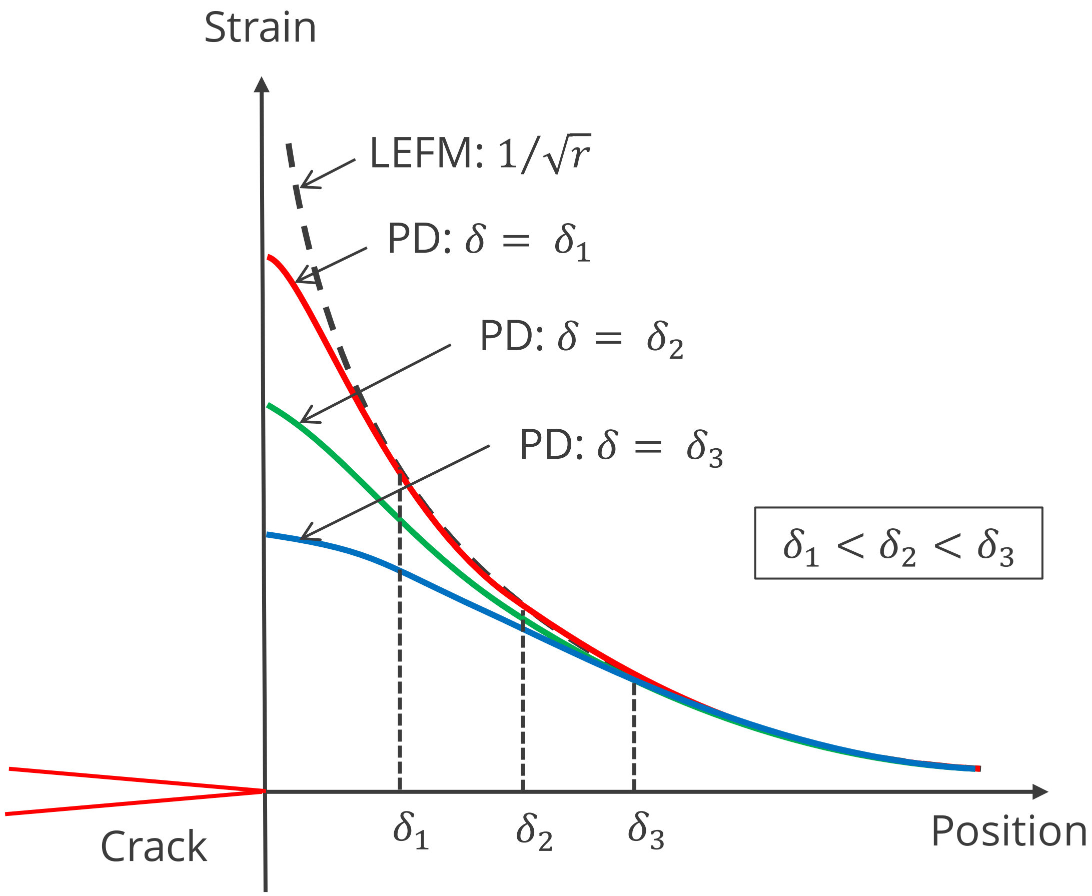
- S.S. & R. Lehoucq, Adv. Appl. Mech (2010)

Peridynamic vs. LEFM crack tip

- Peridynamic crack tip field approaches the LEFM singular field as $\delta \to 0$.



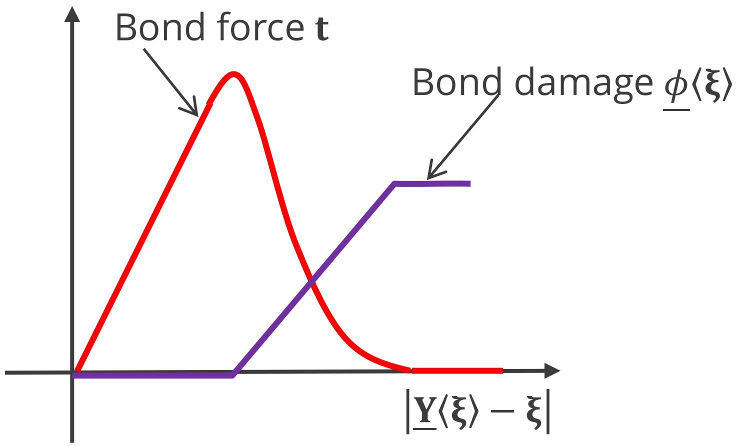


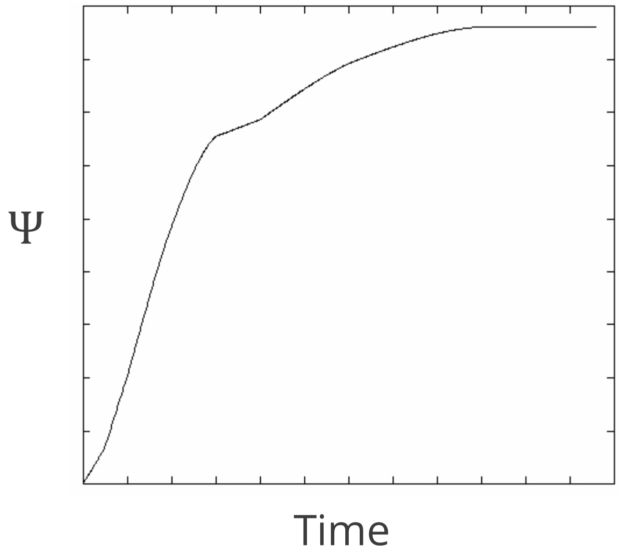


Calibration of the damage law parameters

- Initialize a constant strain everywhere in a square PD model with cross-sectional area A.
- Separate 2 halves using prescribed displacements everywhere.
- Compute the total dissipated energy Ψ.

$$G_{Ic} = \frac{\Psi}{A}$$





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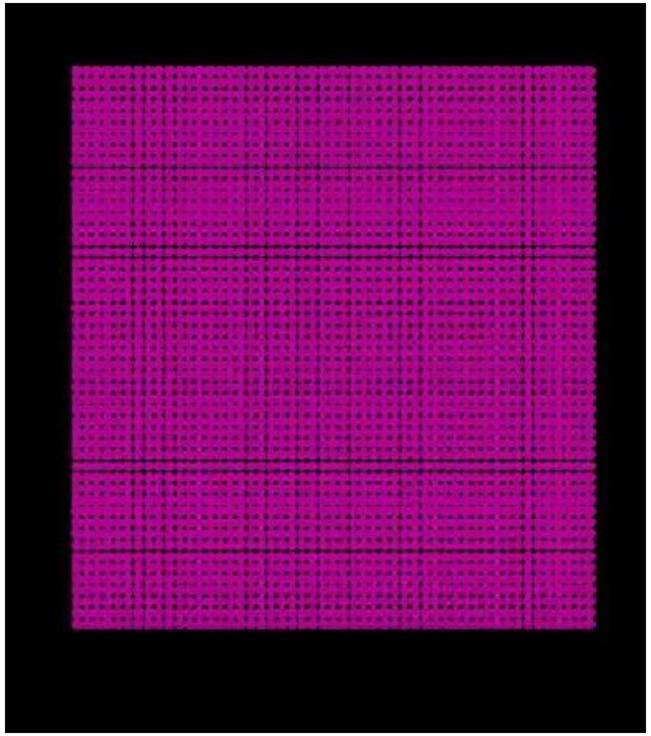


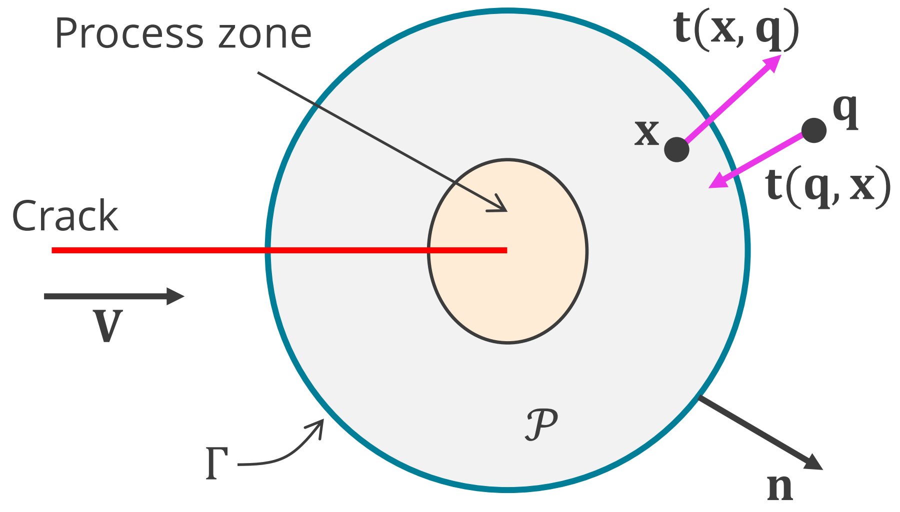
Colors show dissipated energy

Energy release rate in a growing crack

- Let Γ be a contour, $\mathcal{P}$=inside.
- Can show that the rate of energy dissipation in a crack with growth velocity $\mathbf{V}$ (under ideal conditions) is given by $\dot{\Psi} = \int_{\mathcal{B}} \dot{\psi} = \mathbf{V} \cdot \mathbf{J}$ where

$$\mathbf{J} = \int_{\mathcal{P}} \int_{\mathcal{B}-\mathcal{P}} \left[\nabla \mathbf{u}(\mathbf{q}, \mathbf{x}) \cdot \mathbf{t}(\mathbf{x}, \mathbf{q}) - (\nabla \mathbf{u}(\mathbf{x}, \mathbf{q}))^T \cdot \mathbf{t}(\mathbf{q}, \mathbf{x}) \right] \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{x} + \int_{\Gamma} W \mathbf{n} \, \mathrm{d}A.$$

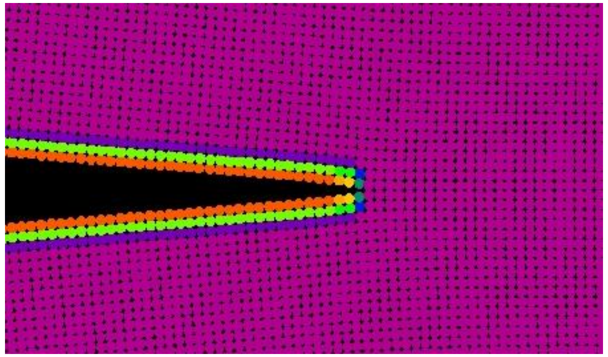
- Can show this nonlocal $\mathbf{J}$ converges to the local (Rice) version as $\delta \to 0$.



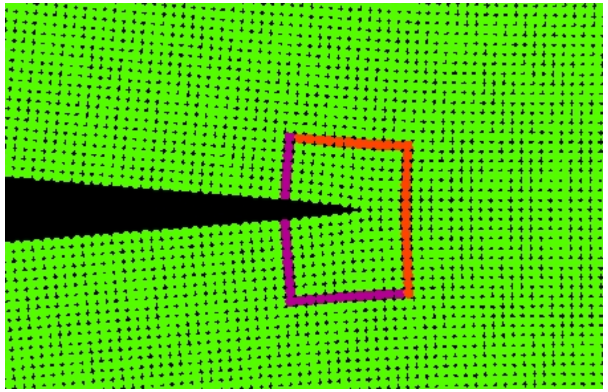
- W. Hu,, et al., Intl. j. Fracture (2012)
- H. Yu and S. Li, JMPS (2020)
- H. Zhang & P. Qiao, CMAME (2020)
- M.-Q. Le,, Intl. J. Fracture
- C. Stenstrom et al. Intl. J. Fracture (2023)

J-integral computed explicitly from PD simulation

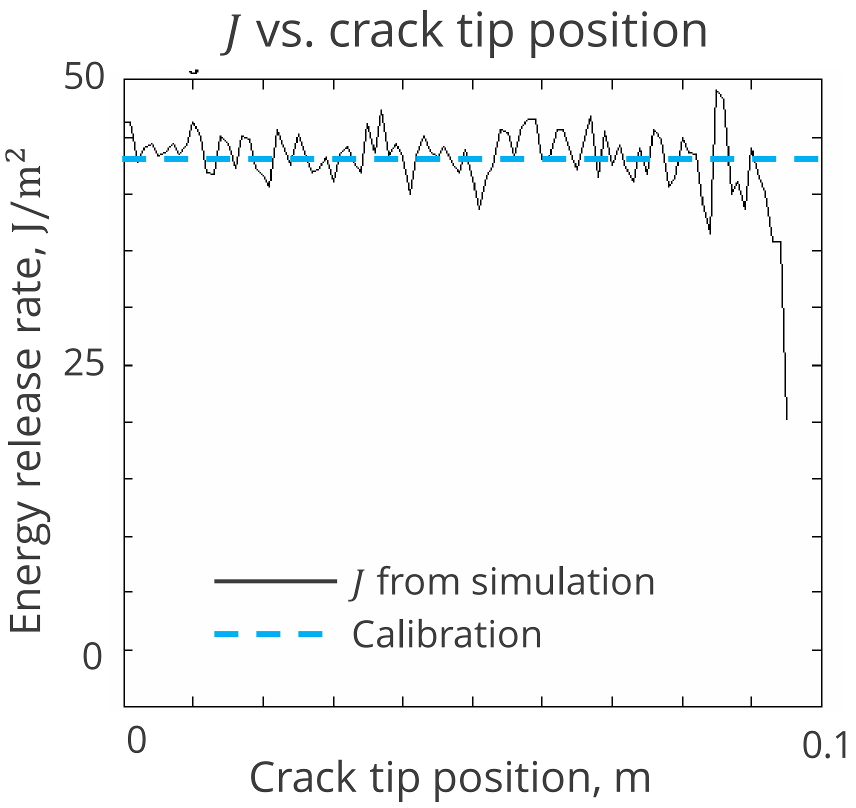
- Confirm that the energy dissipated in the process zone leads to the expected energy release rate.

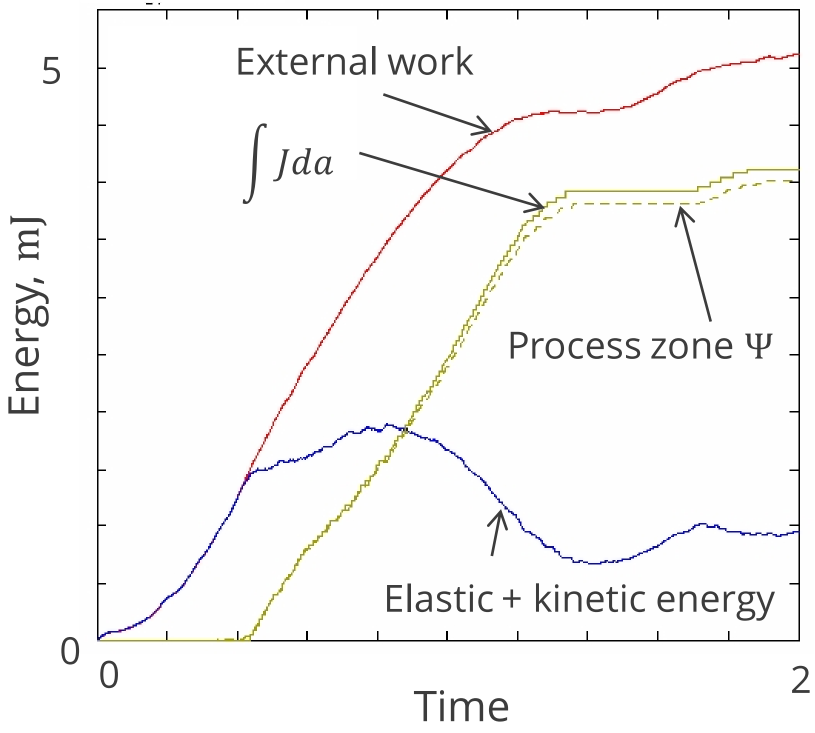


Damage



Contour



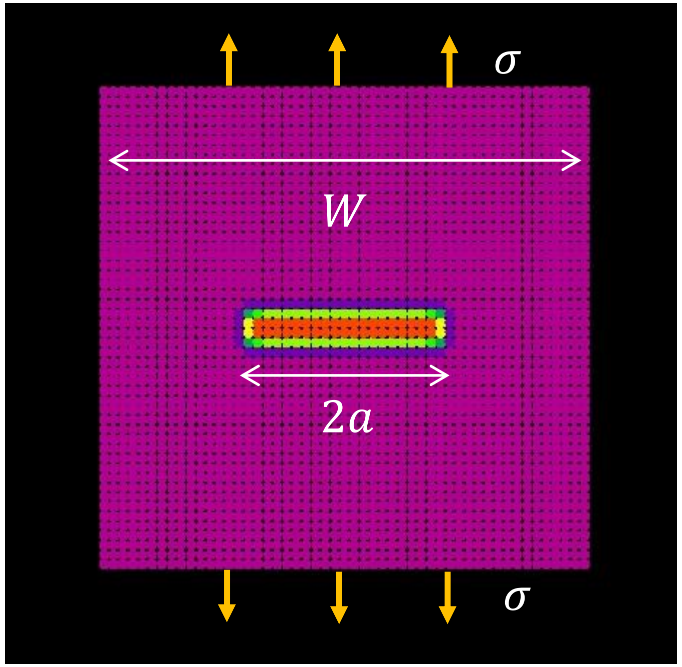


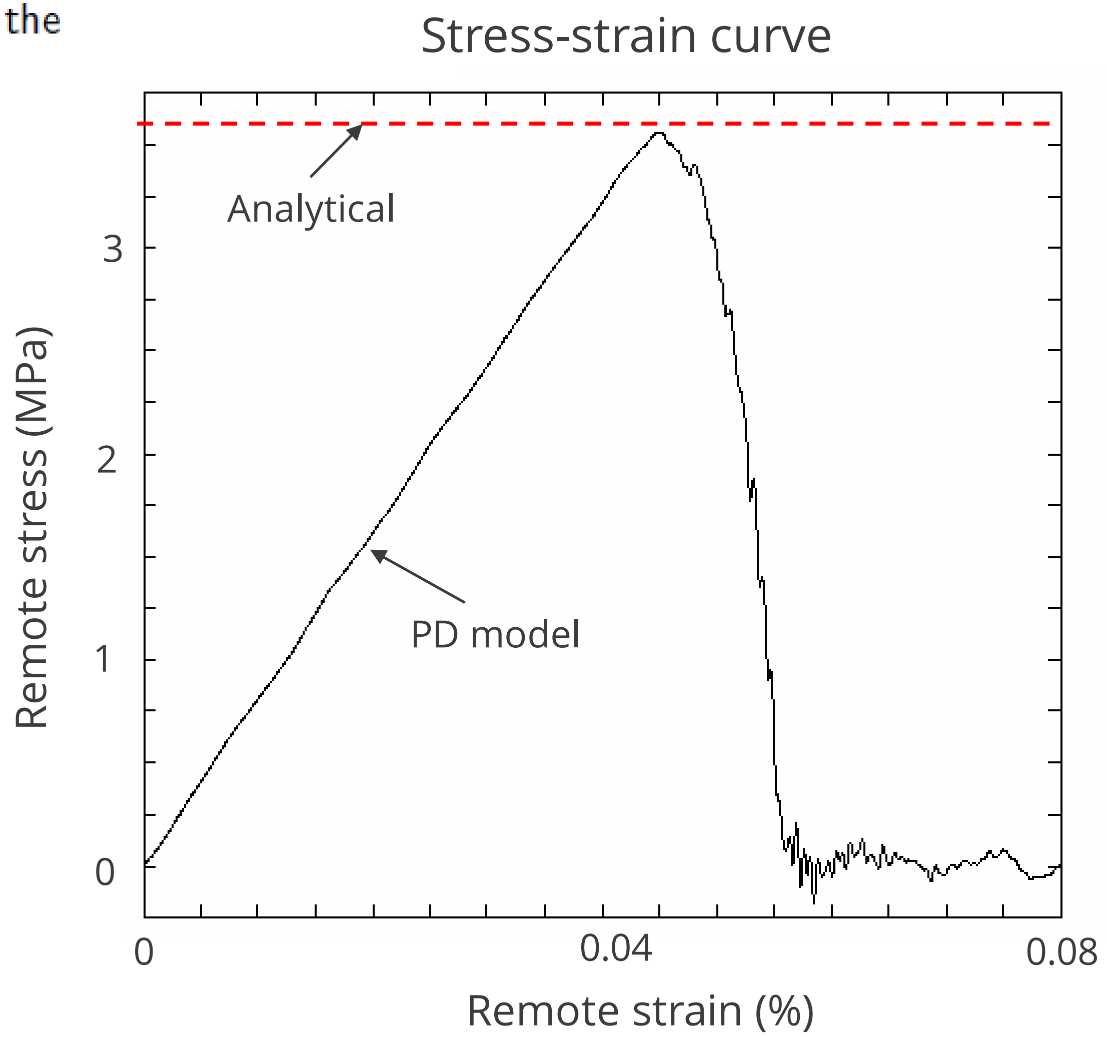
Failure stress in a center-cracked panel

- Using the calibrated value of G from the PD material model, compare the failure load against the analytical value.

$$\sigma = \sqrt{\frac{GE'}{W\tan(\pi a/W)}}$$

where E' is the plane strain Young's modulus.





Accounting for T-stress

- The effect of a normal stress component *parallel* to the crack can be included or excluded by treating it like a Poisson effect.

- Make the damage law parameters s_1 and s_2 dependent on the minimum bond strain in a family:

$$s_m = \min_{\xi \in \mathcal{H}} \frac{\underline{e}\langle \xi \rangle}{|\xi|}$$

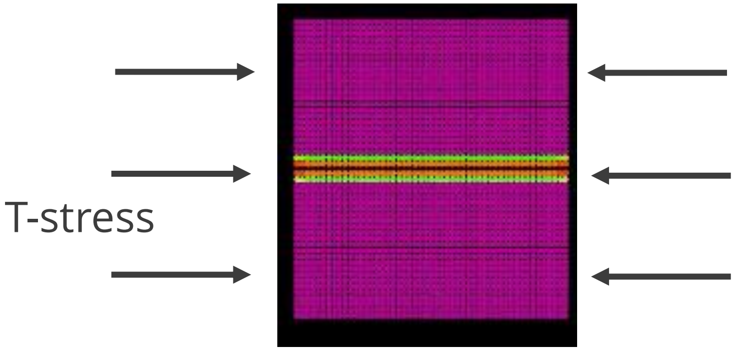
- Then set

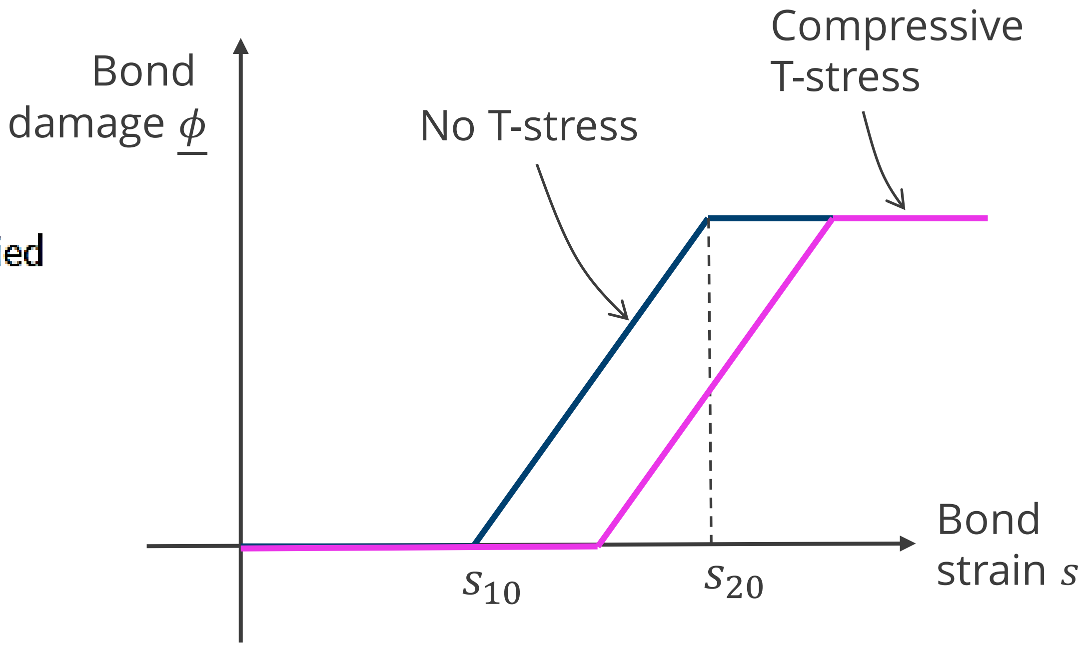
$$s_1 = s_{10} - \beta s_m, \qquad s_2 = s_{20} - \beta s_m$$

  where β, s_{10}, and s_{20} are constants.

- Calibrate β by repeating the half-plane separation runs with an applied T-stress.

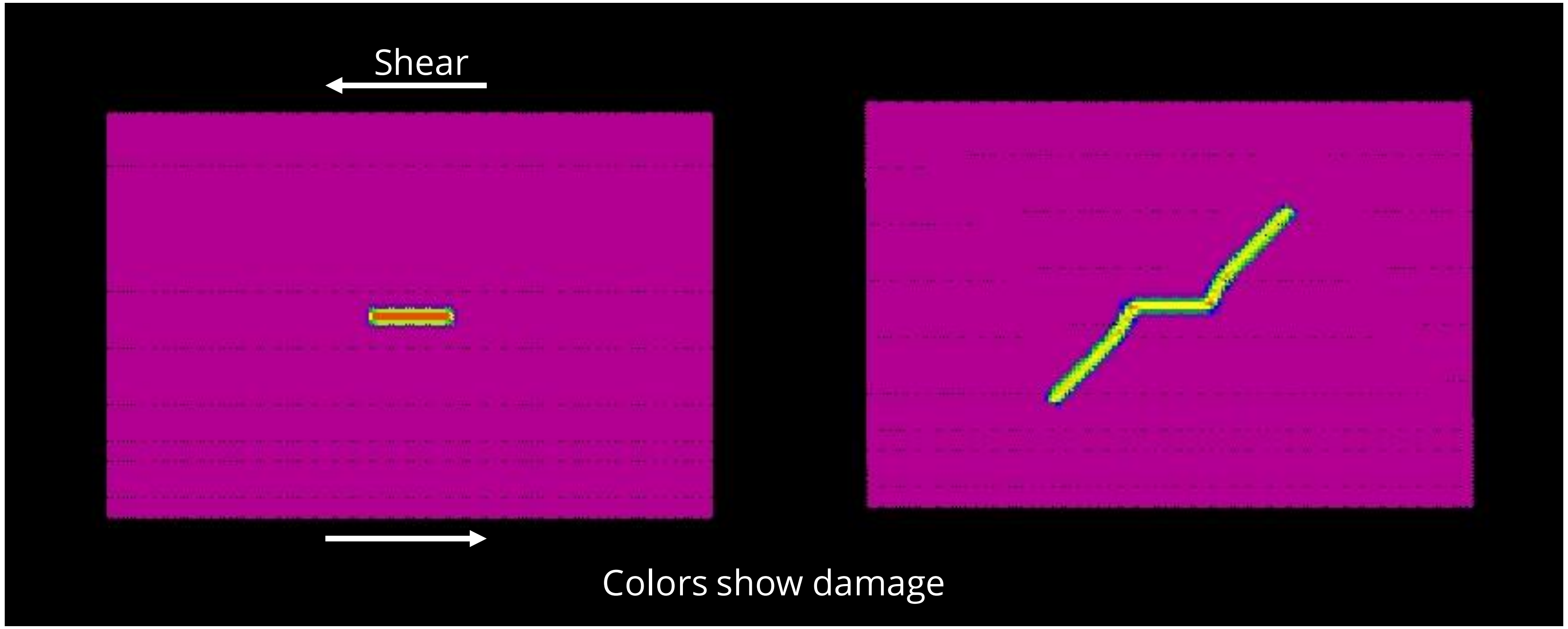
- Typically $\beta \approx \nu/2$ to make G independent of the T-stress.





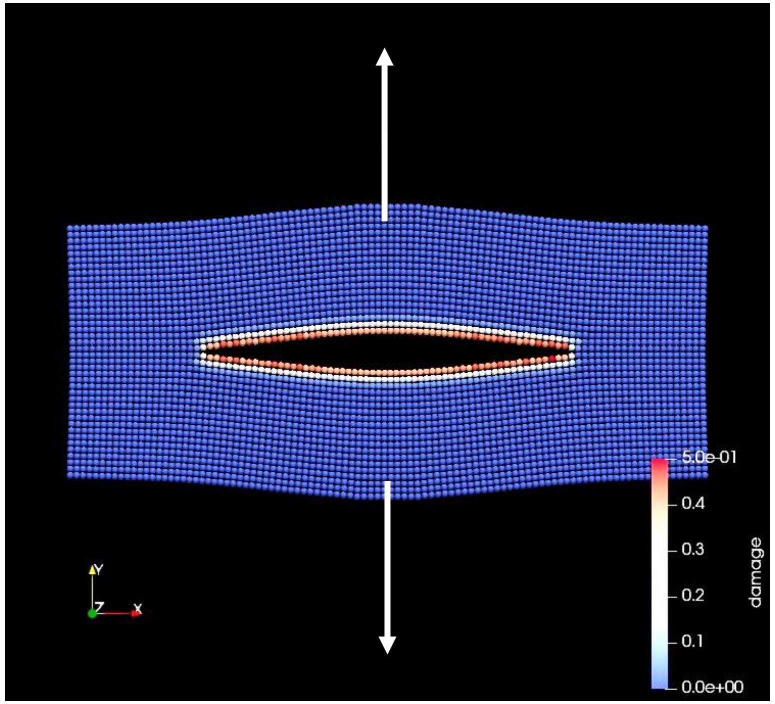
Mode II loading: Crack growth direction

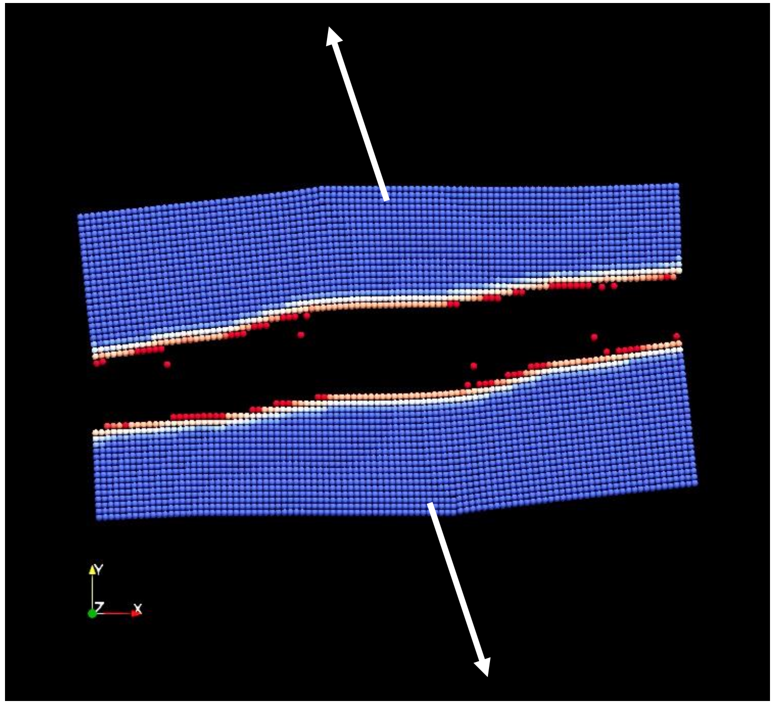
- Initial crack growth direction is typically within a few degrees of what the Maximum Tangential Stress criterion predicts.
- After the crack grows by a few δ further growth is normal to the max principal stress (i.e., mode I).



Mixed mode fracture

- Crack growth direction changes continuously with load direction.



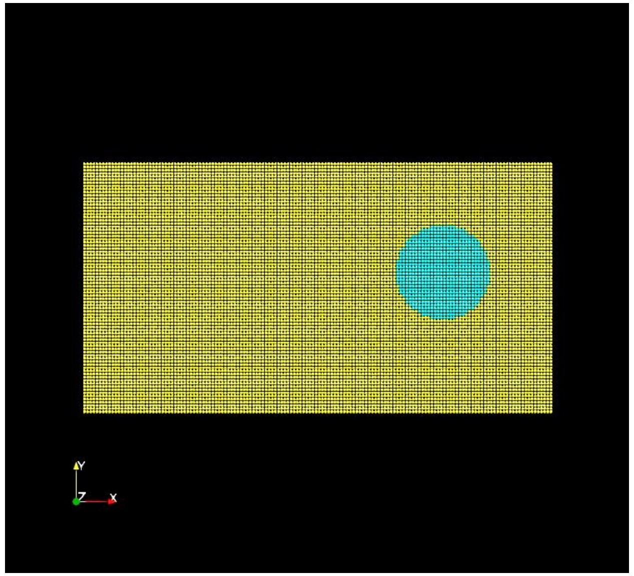


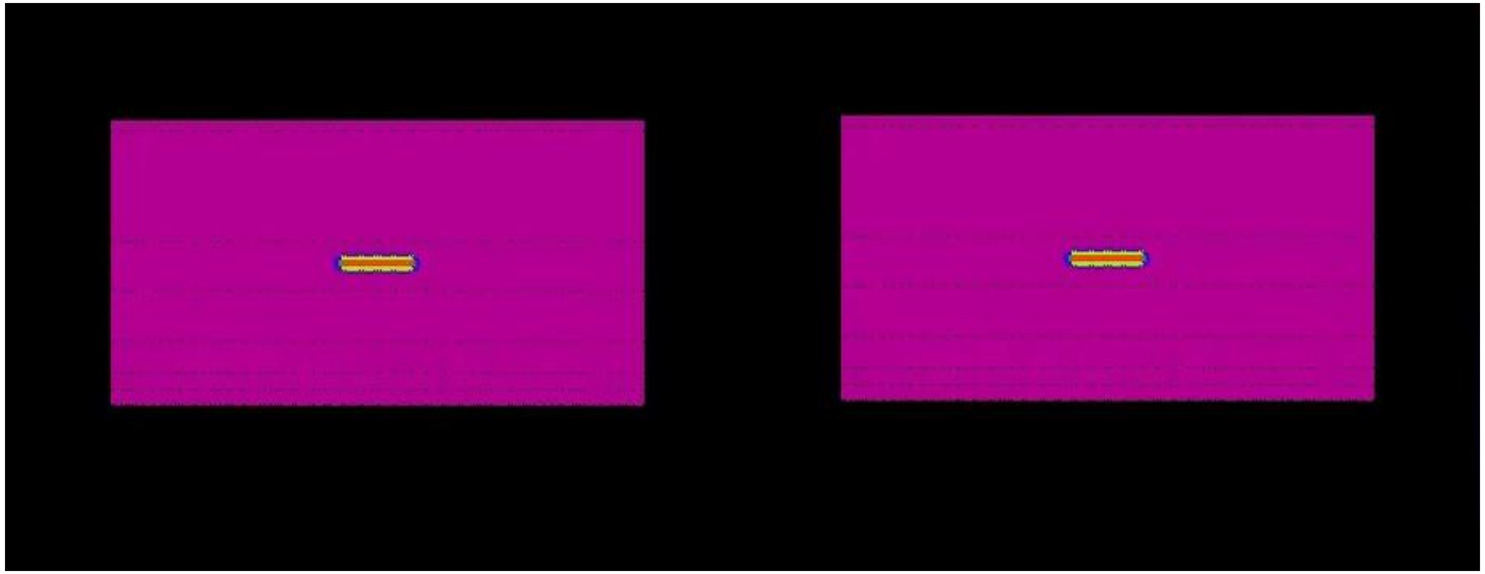
Colors show net damage
Displacements x100

Interfaces can have their own damage law

- Initial crack grows and encounters a hard inclusion.

VIDEOS

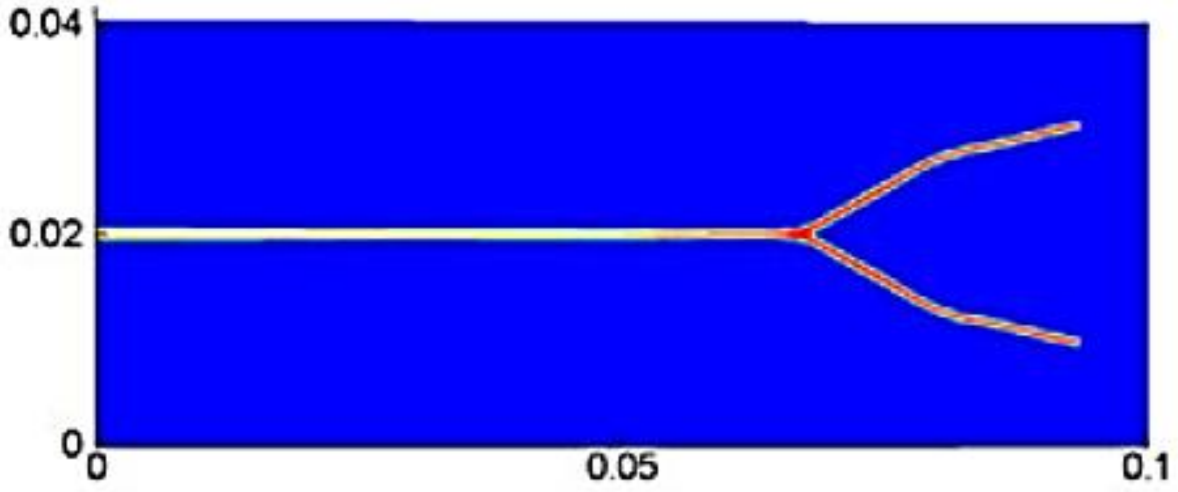


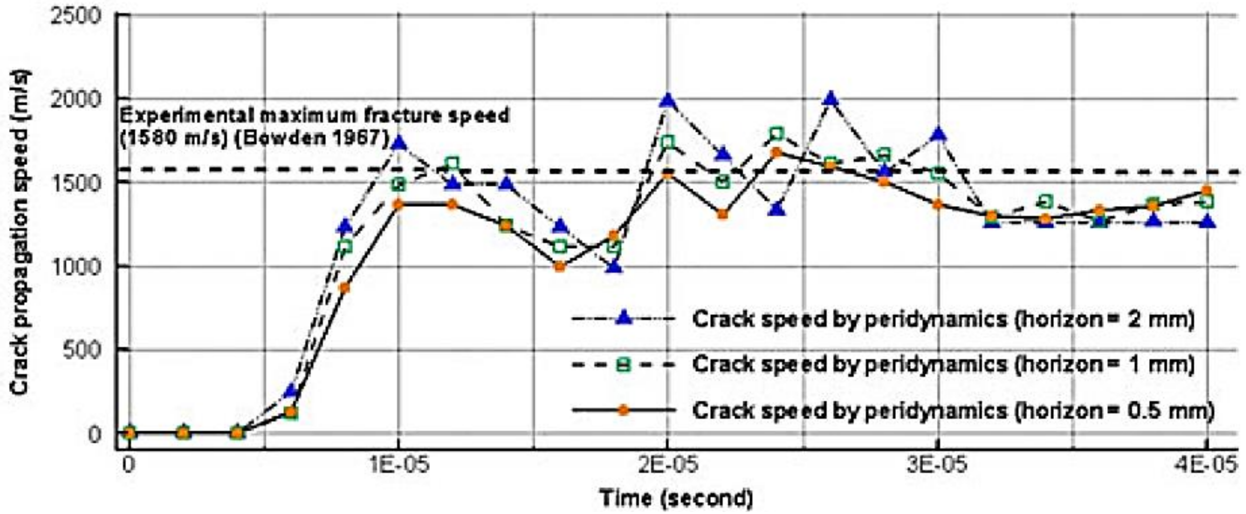


Weak interface Strong interface

Dynamic fracture: crack speed is about right

- Fracture in soda-lime glass



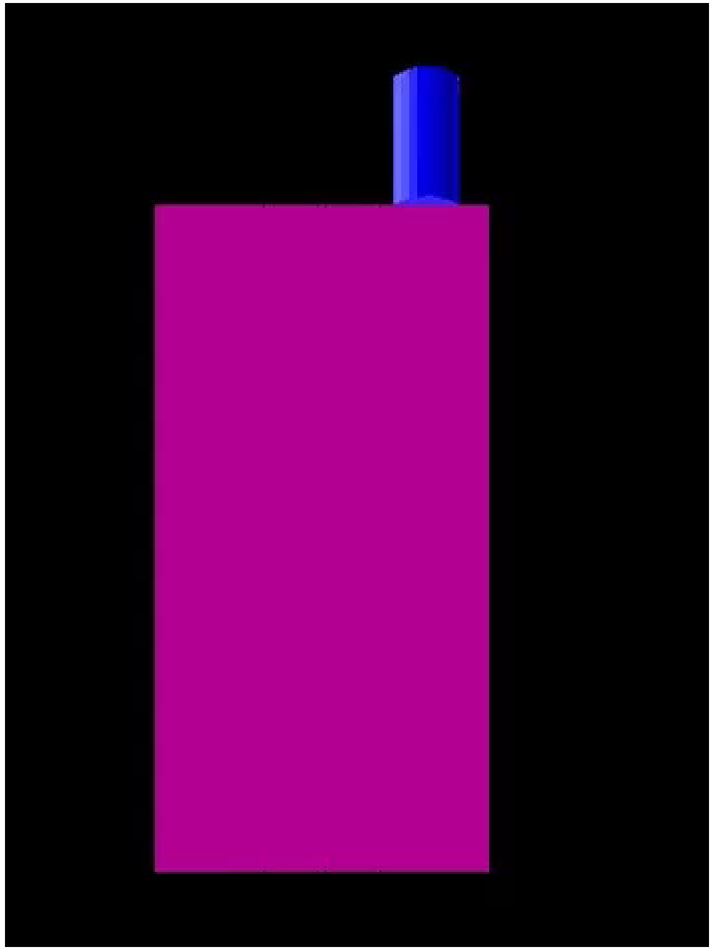


- Ha & Bobaru, *Int J Fracture* (2010)
- *Agwai, Guven, & Madenci, *Int J Fracture* (2011)
- Ha & Bobaru, *Engin Fracture Mech* (2011)
- Dipasquale, Zaccariotto, & Galvanetto, *Int J Fracture* (2014)
- Bobaru & Zhang, *Int. J Fracture* (2015)
- Zhou, Wang, & Qian, *European J Mechanics-A/Solids*. (2016)

Comparison of PD with LEFM

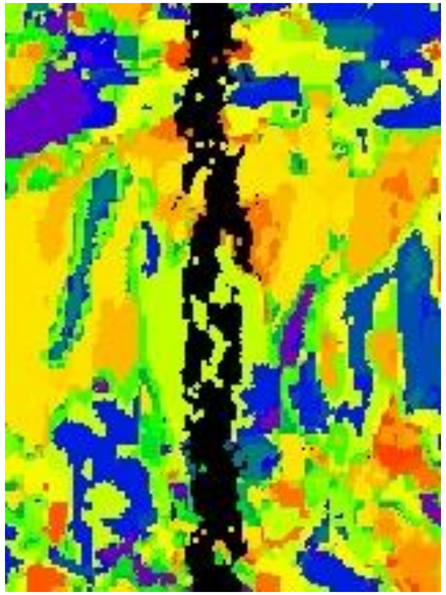
- PD explicitly creates a process zone near a crack tip of size $\approx \delta$.
  - Crack tip field is similar to LEFM outside this process zone.
- PD energy dissipation is consistent with Griffith concept but is explicitly modeled through bond damage.
- Fracture modeling in PD is basically the same in 3D as in 2D.
  - Most LEFM concepts are essentially 2D.
- PD treats crack nucleation as well as growth.
  - Models complex damage progression in structures.
- PD does not need supplemental equation relating SIF to crack advance.

VIDEO

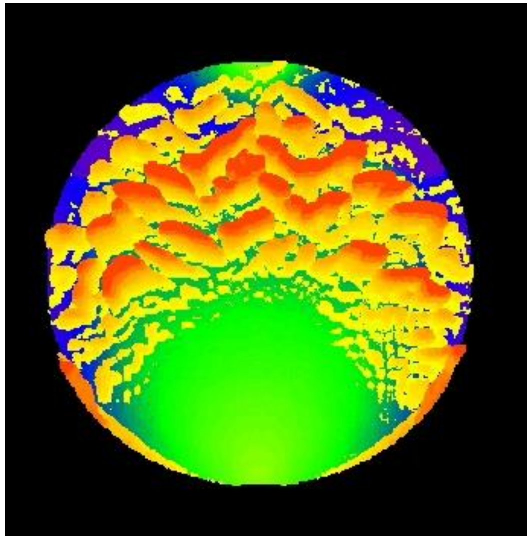


Multiple impacts on a block
Colors show damage

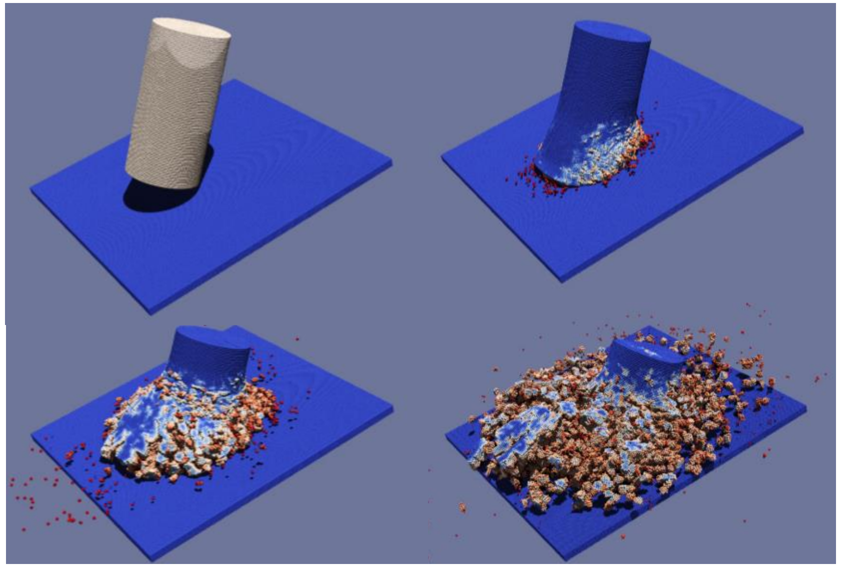
Some applications where PD is a natural choice



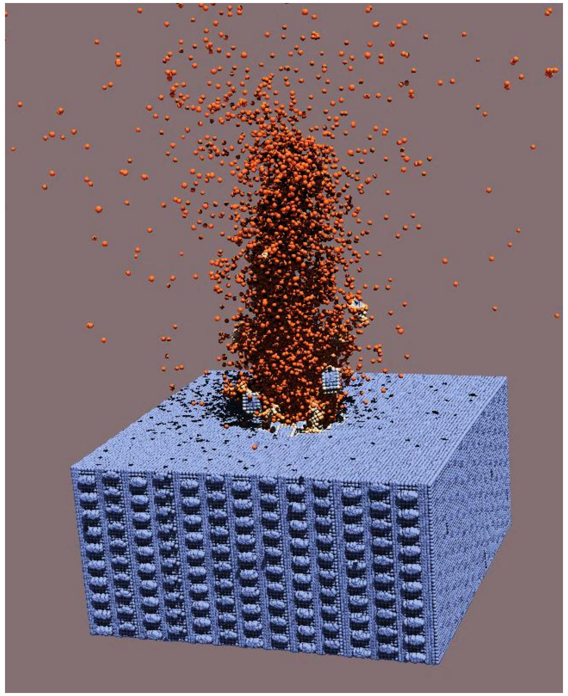
Spall in additively manufactured metals



Mirror-mist-hackle effect in glass



Impact and fragmentation of a brittle projectile

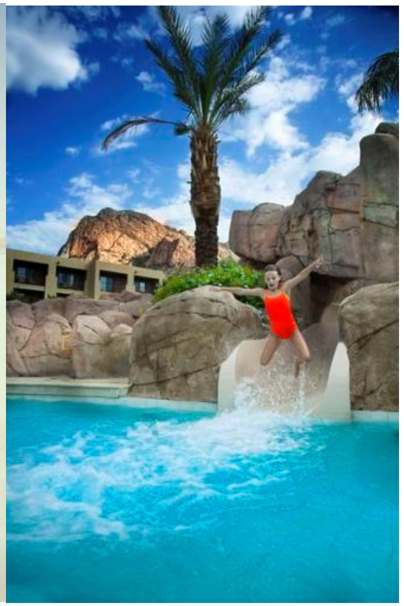


Erosion of a ceramic matrix composite due to impact

Conclusions

- There is a lot of commonality between brittle fracture in peridynamics and LEFM.
- But the real advantages of PD are more easily seen in 3D applications requiring "autonomous crack growth" such as crack nucleation, branching, instability, multiple cracks and fragmentation.

Please join us at…



Questions?

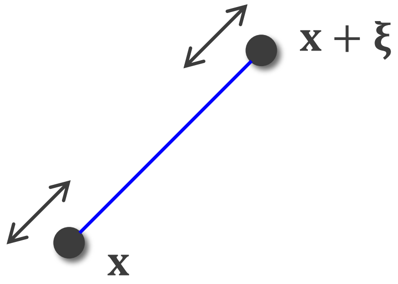
Extra slides

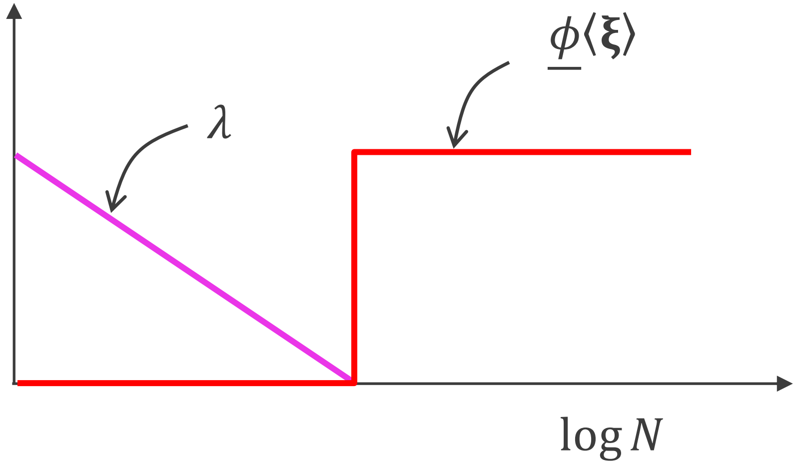
Another damage model: Fatigue

- Let ε be the amplitude of cyclic strain in a bond.
- Let N be the loading cycle in a fatigue test.
- For each bond, define the *remaining life* $\lambda(N)$ such that

$$\lambda(0) = 1, \qquad \frac{\mathrm{d}\lambda}{\mathrm{d}N} = -A\varepsilon^m$$

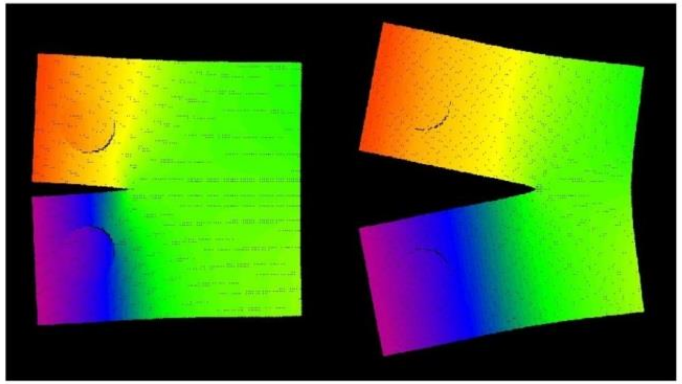
  where A and m are constants.
- Bond damage $\underline{\phi}\langle\xi\rangle$ jumps from 0 to 1 when $\lambda(N) = 0$.
- A and m can be fitted to S-N curves from tests.

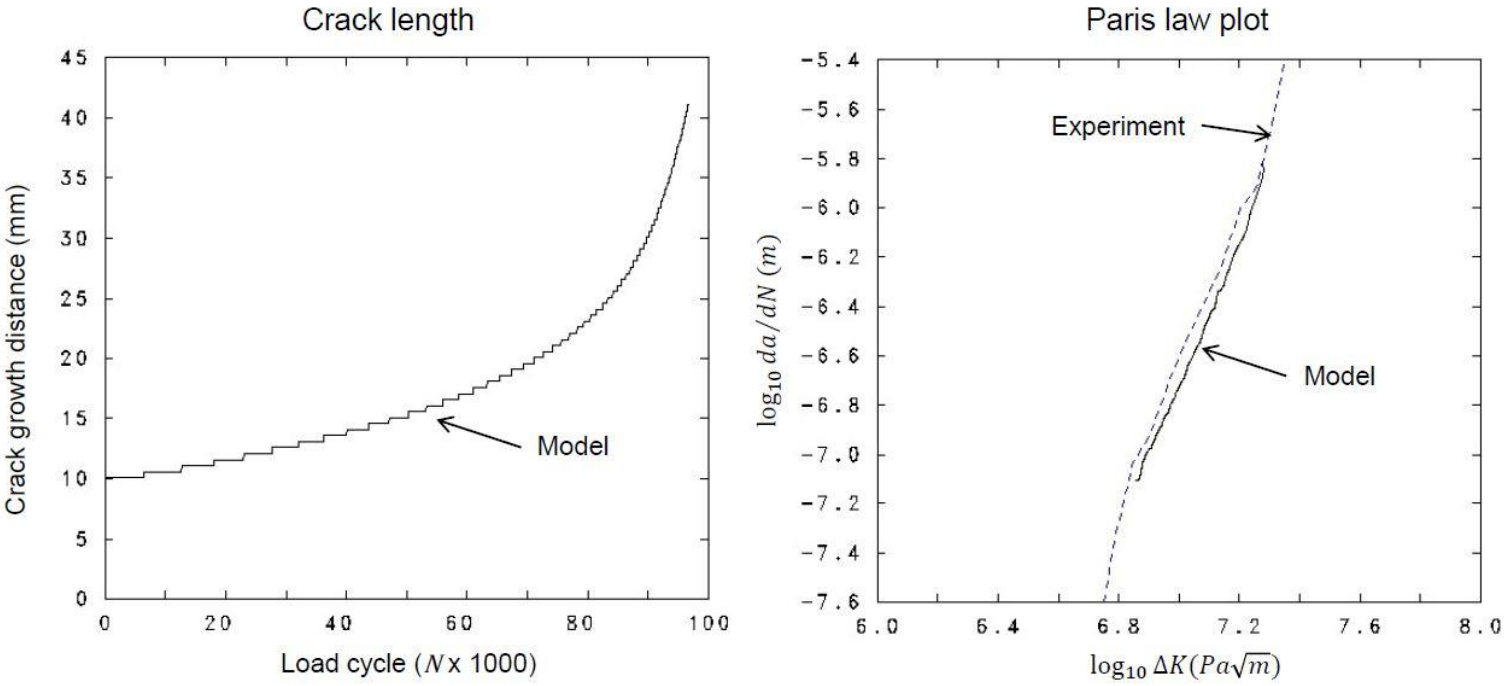




- G. Zhang et al. Engineering Fracture Mechanics (2016)
- D. J. Bang et al. Theoretical and Applied Fracture Mechanics (2021)
- J. Jung & J. Seok, International Journal of Fatigue (2017).
- H. Wang et al., Theoretical and Applied Fracture Mechanics 124 (2023): 103761.

Fatigue crack growth in aluminum alloy





Test data: T. Zhao, J. Zhang, and Y. Jiang. A study of fatigue crack growth of 7075-T651 aluminum alloy. International Journal of Fatigue, 30 (2008) 1169-1180.

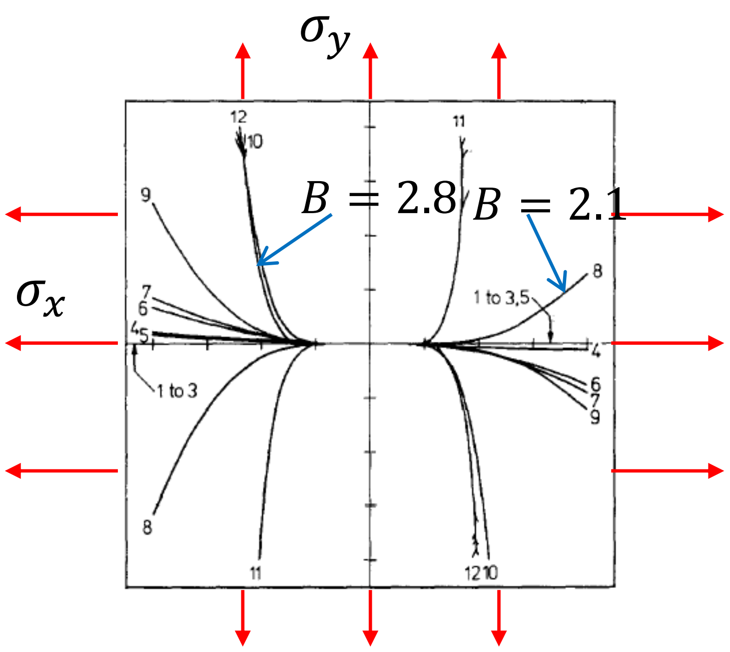
Where does nonlocality come from?

- Long-range physical forces (electrostatic, van der Waals, H bond …)
- Nonlocality is helpful in reproducing many phenomena in nature, such as
  - Anomalous diffusion
  - Wave dispersion
  - Granular flow effects
  - Traffic flow
  - Sea ice transport
  - Adhesion
  - Elastic stability
  - Microstructure evolution
  - Phase boundaries
  - Fracture
- **Can we provide a more <u>intuitive</u> basis for nonlocal modeling?**

Floating ice
Image: NASA

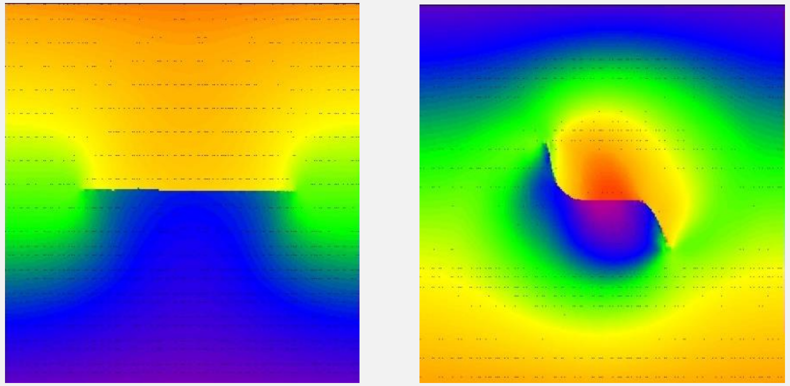
Crack stability and mode transition

- Biaxial loading causes a crack to turn.
- Center defect can grow in an S-shape.
- Biaxiality: $B = \sigma_x/\sigma_y$.

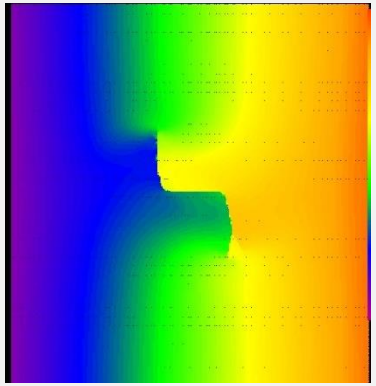


Observed crack paths in PMMA*

Simulated crack paths



$B = 0$ $B = 2.0$

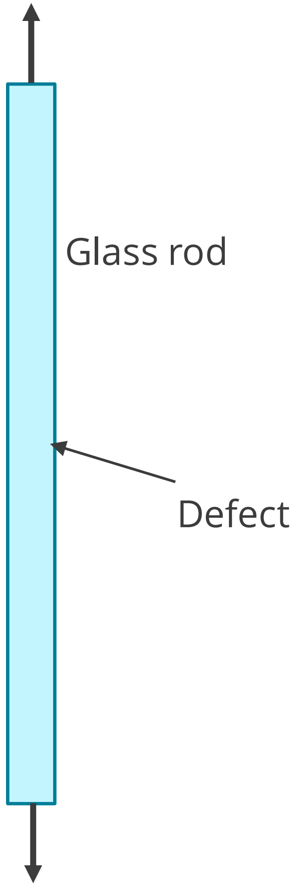


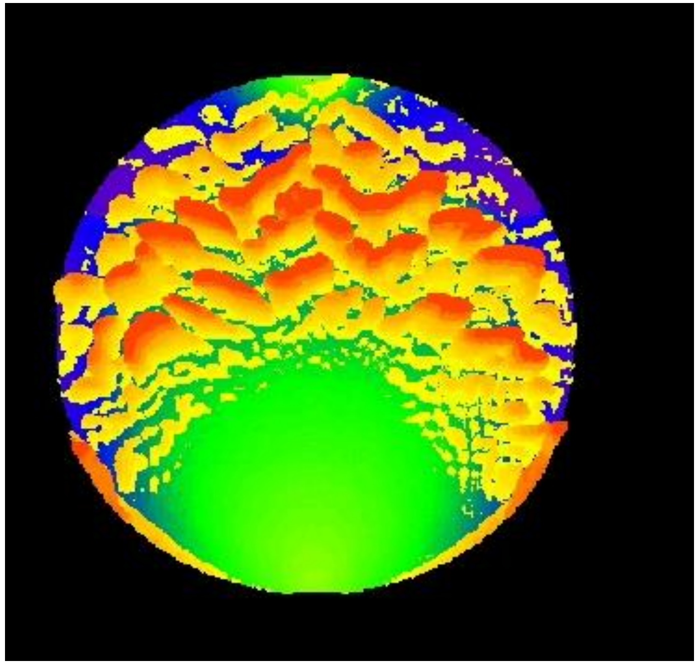
$B = 2.5$

*Leevers, Radon, & Culver JMPS (1976)

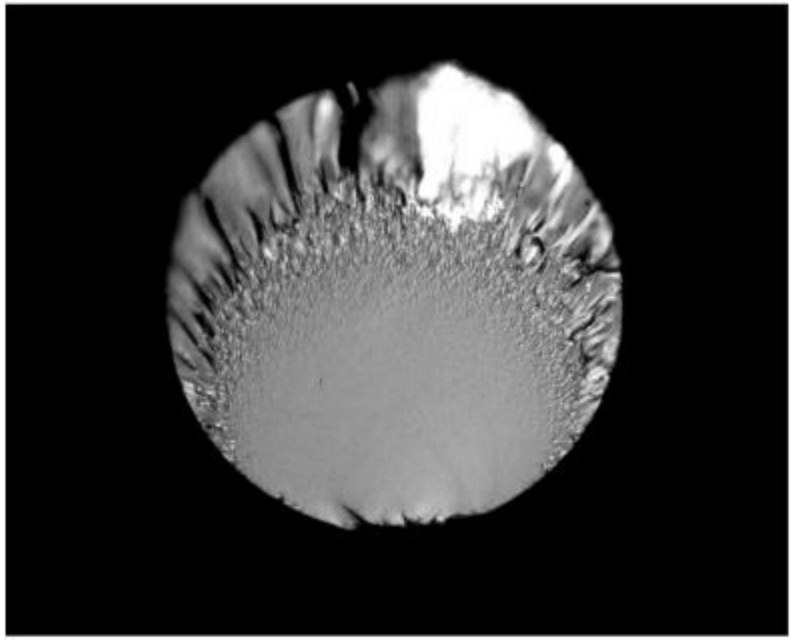
Crack stability: Mirror-mist-hackle transition

- Model predicts microbranches that increase in size as the crack grows.
- Transition radius decreases as initial stress increases – trend agrees with experiments.





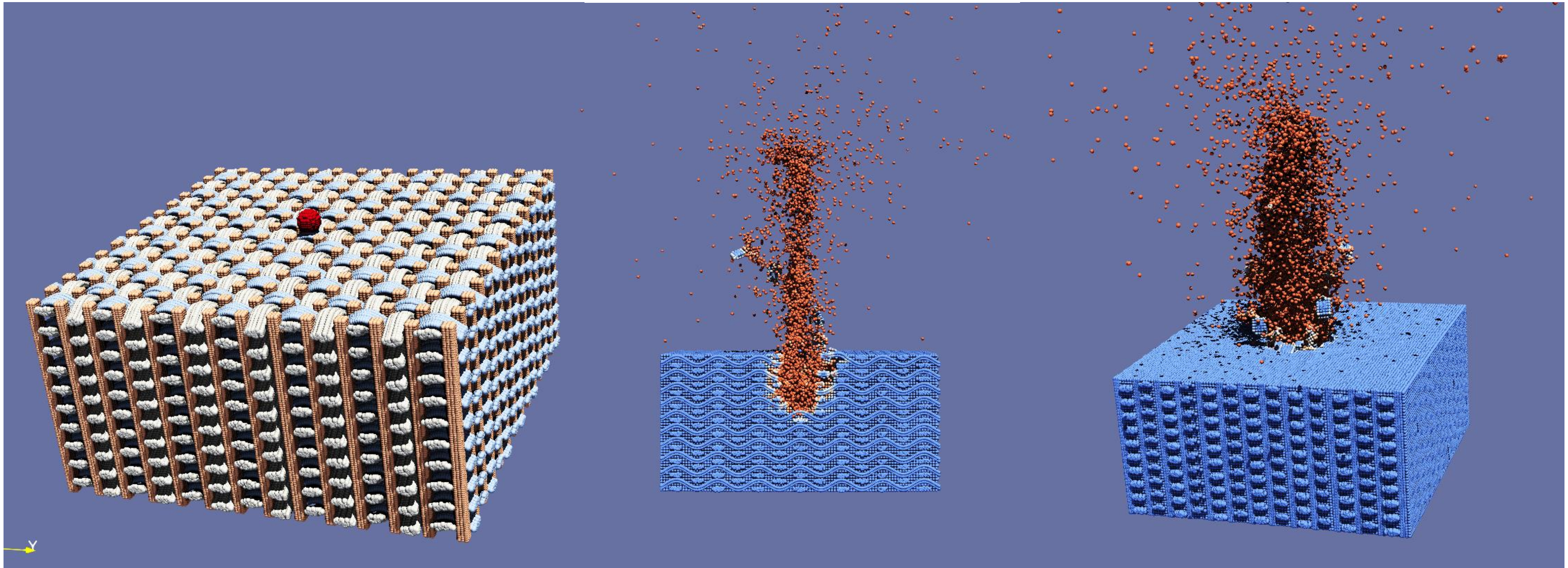
3D peridynamic model
Colors show axial coordinate of damaged nodes.



Fracture surface in a glass optical fiber
Image: Castilone, Glaesemann & Hanson, Proc. SPIE (2002)

Impact and erosion

- 1mm glass sphere into C-C composite, 4000m/s.
- Mie-Gruneisen EOS and critical bond strain damage model.

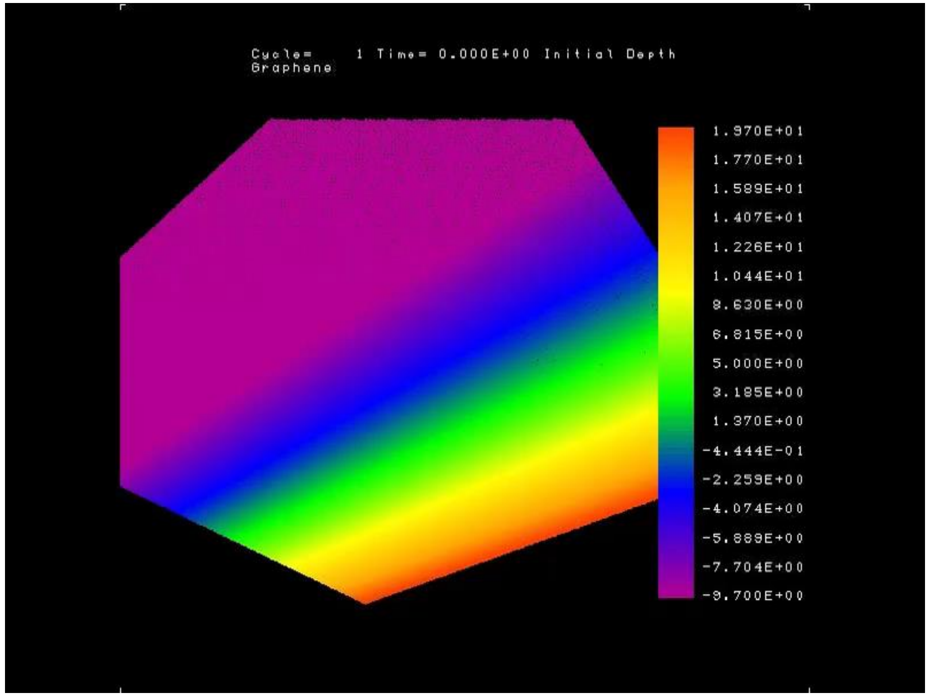


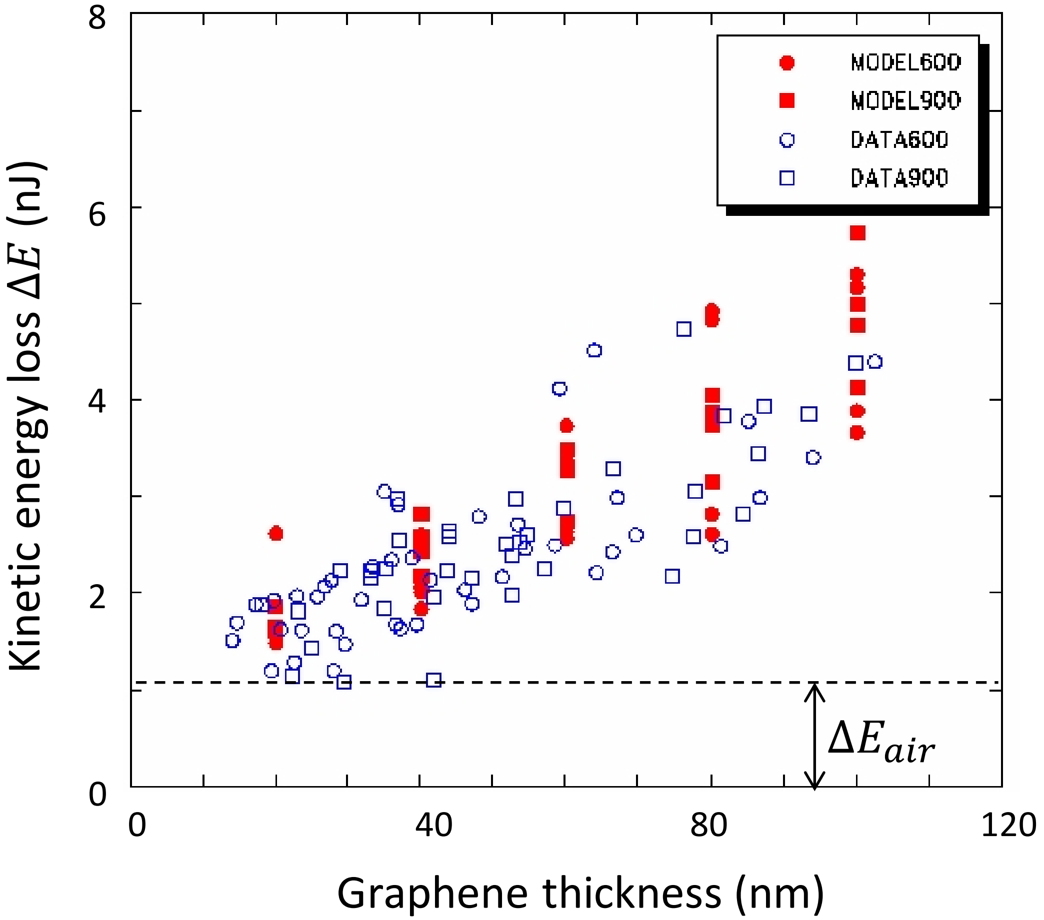
Composite weave

Colors show damage

Microballistic perforation of multilayer graphene

600m/s 3.7μm sphere onto 50nm thick graphene laminate.
VIDEO

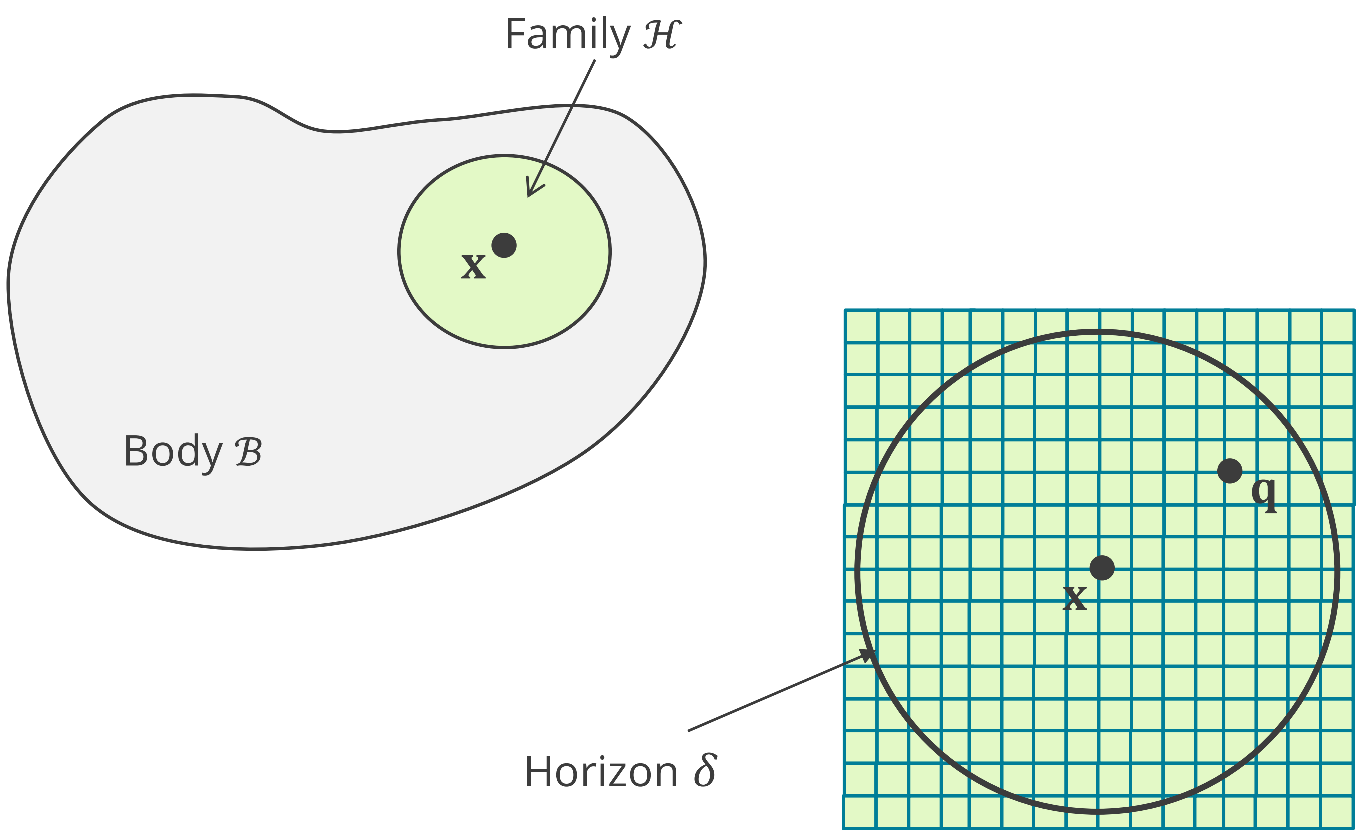


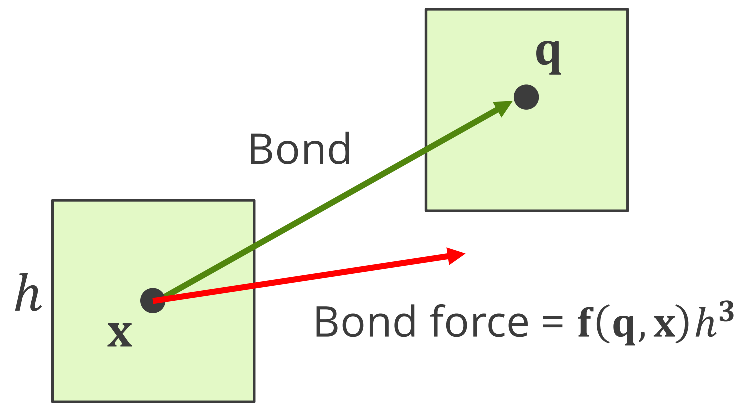


- J-H Lee et al, "Dynamic mechanical behavior of multilayer graphene via supersonic projectile penetration", *Science* (2014)
- SS & M Fermen-Coker, "Peridynamic model for microballistic perforation of multilayer graphene." *Theoretical and Applied Fracture Mechanics*. 2021 Jun 1;113:102947.

Mechanistic picture of peridynamics

- Each material point $\mathbf{x}$ interacts with neighbors $\mathbf{q}$ within a cutoff distance δ (the ***horizon***).





- $\mathbf{f}$ is the bond force density (N/m^6).
- It doesn't necessarily represent a physical force.