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Progress in peridynamics

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COLUMBUS, OHIO

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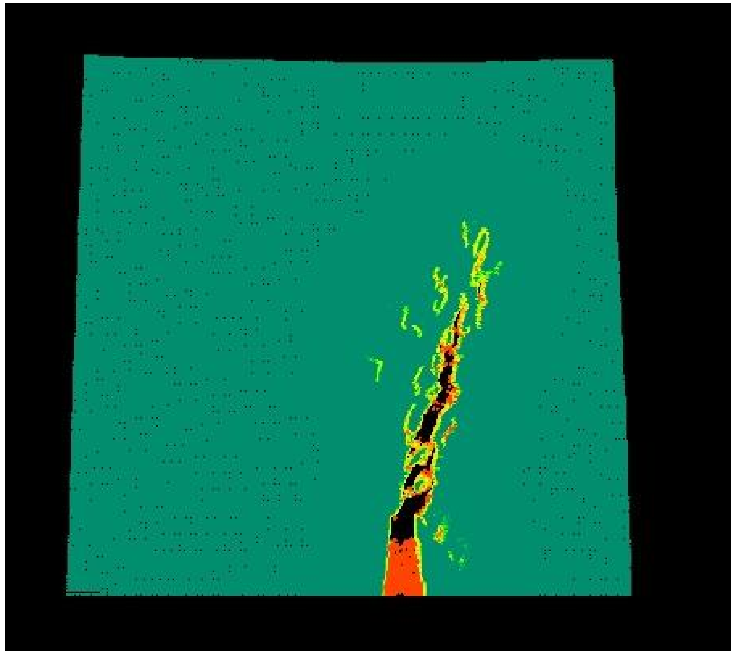
What this talk will cover

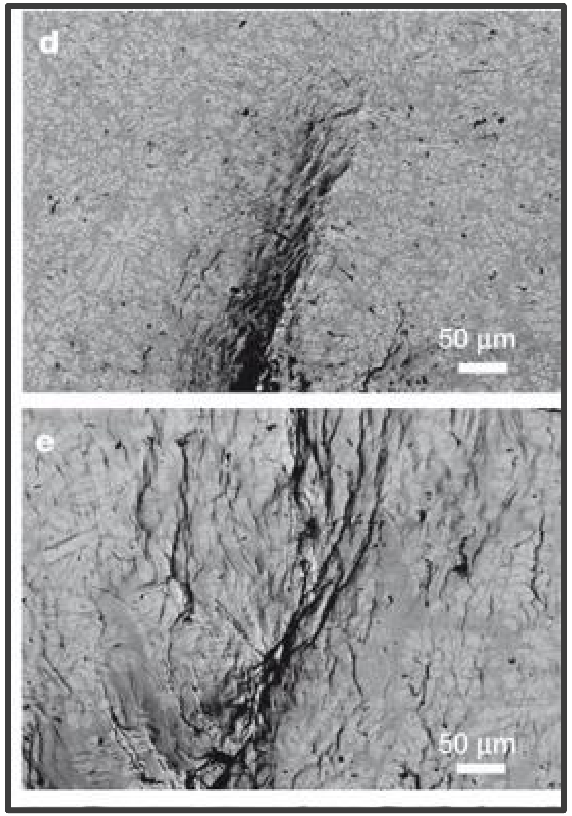
- What is peridynamics?
- What capabilities does it provide?
- Examples of analysis
  - Bird strike
  - Brittle dynamic fracture & fragmentation
  - Composite material failure
  - Pharmaceutical tablet manufacture
- Use with commercial codes
- Relation to machine learning & AI
- Some current research topics

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.



Peridynamic simulation



Metallic glass crack tip
Images: Hofmann et al, 2008

Motivation: Fracture modeling

- The standard PDEs of solid mechanics are incompatible with fracture.
- So, people have created ingenious fixes implemented within a discretized model to model fracture…

Remesh

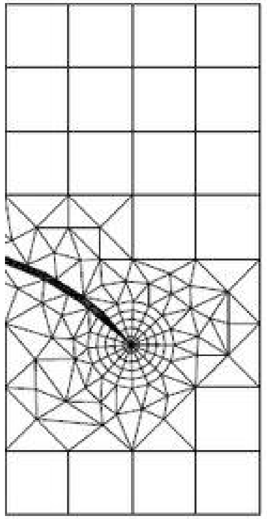


Image: Rege & Lemu, 2017

Element deletion

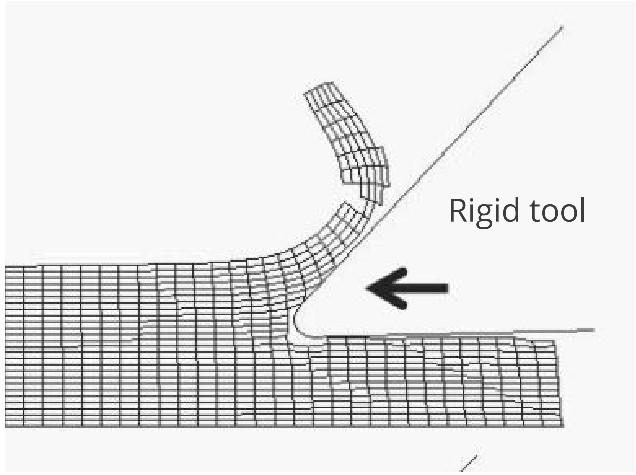


Image: Lee, Choi, Jung, & Im, 2009

Cohesive elements

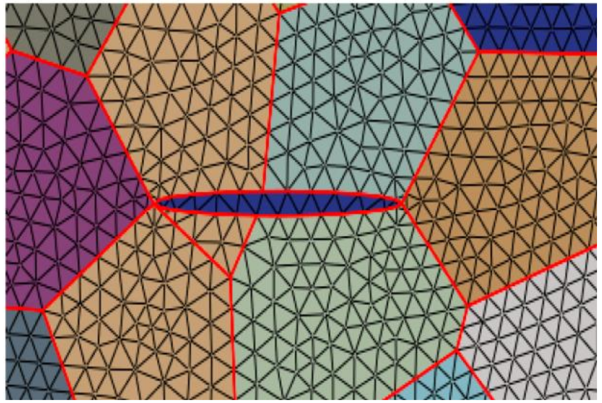


Image: Zhang et al, 2019

XFEM

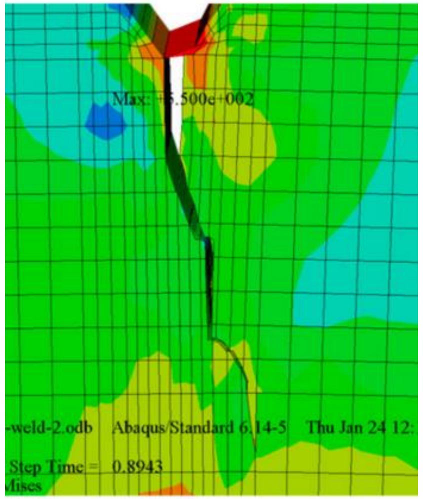
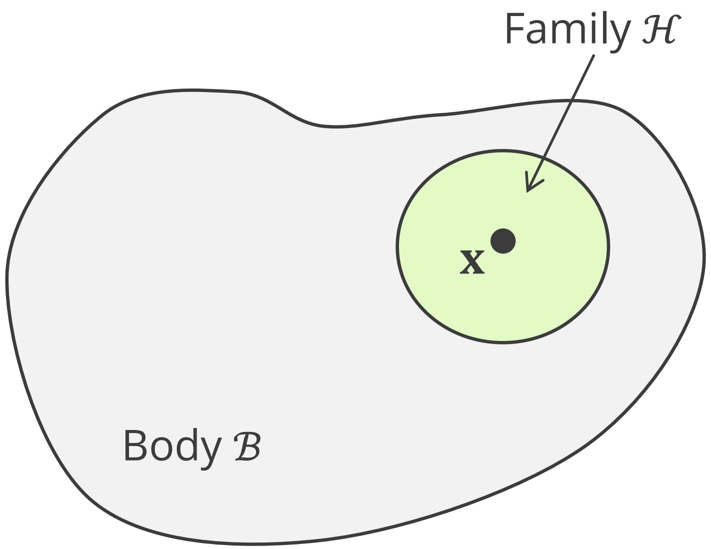


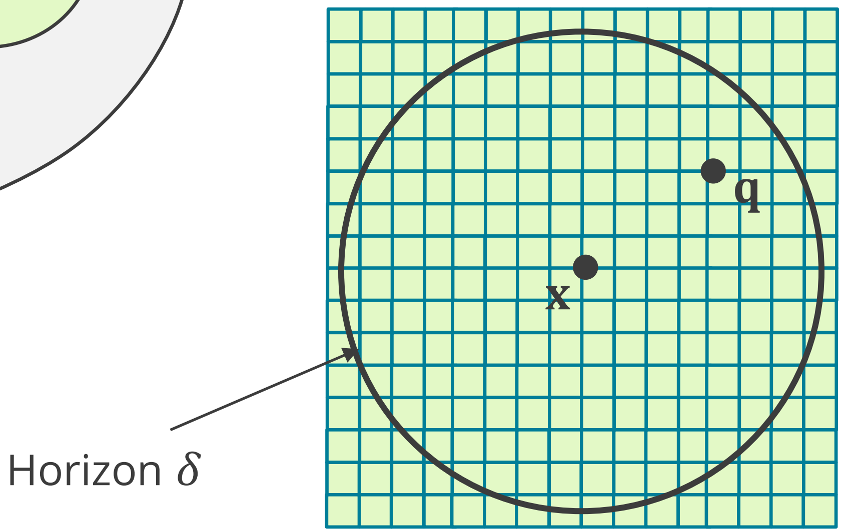
Image: Qian & Zhao, 2017

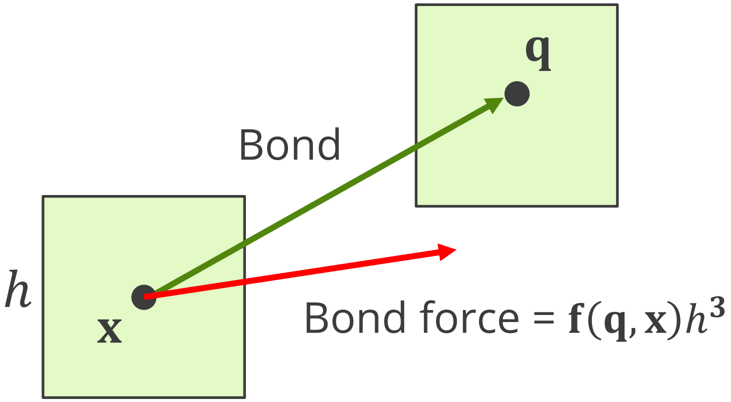
- What would happen if instead we start with more general continuum equations that allow discontinuities?
  - And then discretized these equations?

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.

Continuum equation of motion

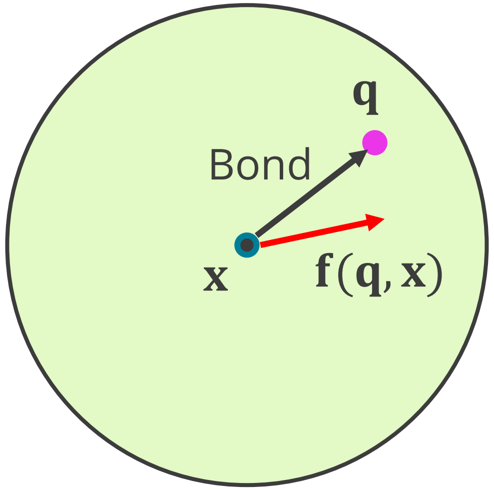
- Sum up the forces on the volume element at $\mathbf{x}$.
- Apply Newton's second law.

$$\rho h^3 \ddot{\mathbf{y}}(\mathbf{x}, t) = \sum_{\mathbf{q} \in \mathcal{H}} \mathbf{f}(\mathbf{q}, \mathbf{x}, t) h^3 + \mathbf{b}(\mathbf{x}, t) h^3$$

where ρ=density, $\mathbf{y}$=deformation map, $\mathbf{b}$=external force density.

- Transition to continuum: $h \to 0$.

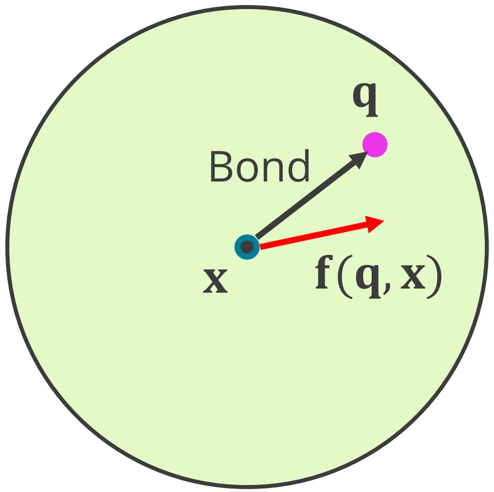
$$\rho \ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{q}, \mathbf{x}, t)\, d\mathbf{q} + \mathbf{b}(\mathbf{x}, t).$$

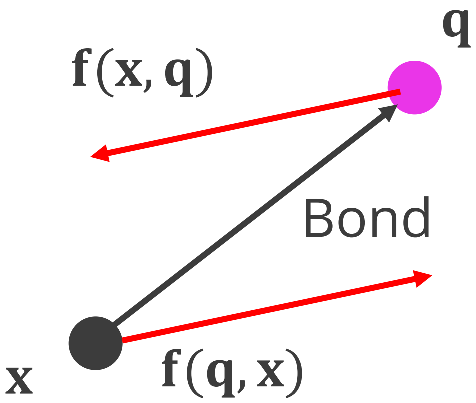


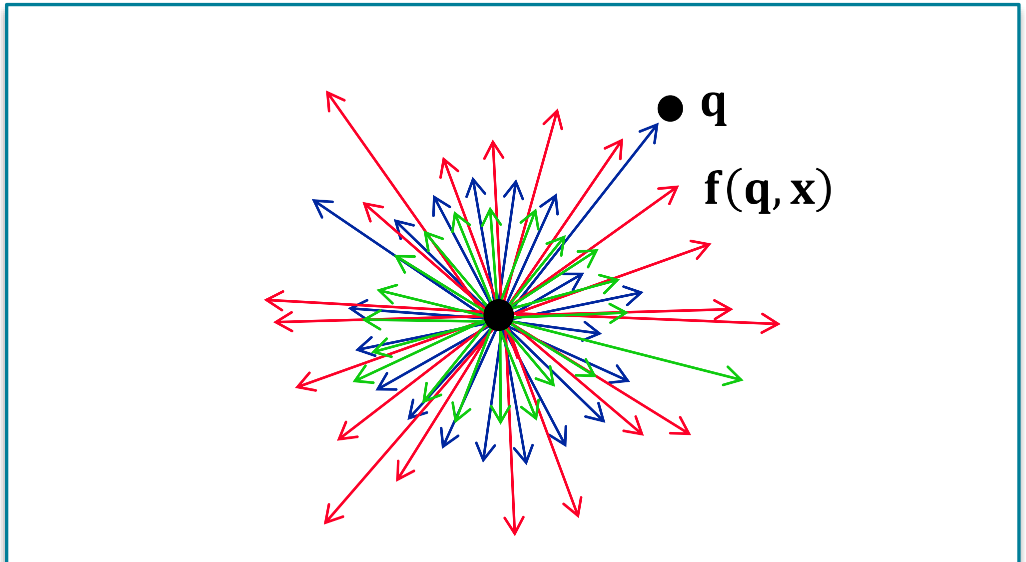
Material modeling

- The material model determines $\mathbf{f}(\mathbf{q},\mathbf{x})$ for every $\mathbf{q}$ in $\mathcal{H}$, for every possible deformation of $\mathcal{H}$.
- Requirement for balance of linear momentum:

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



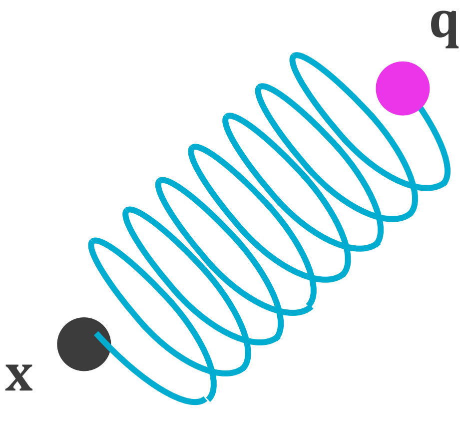


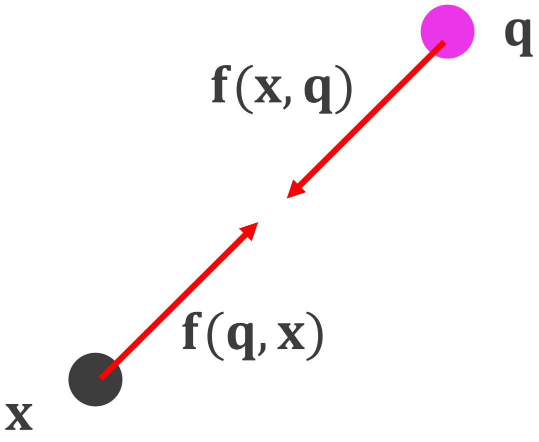


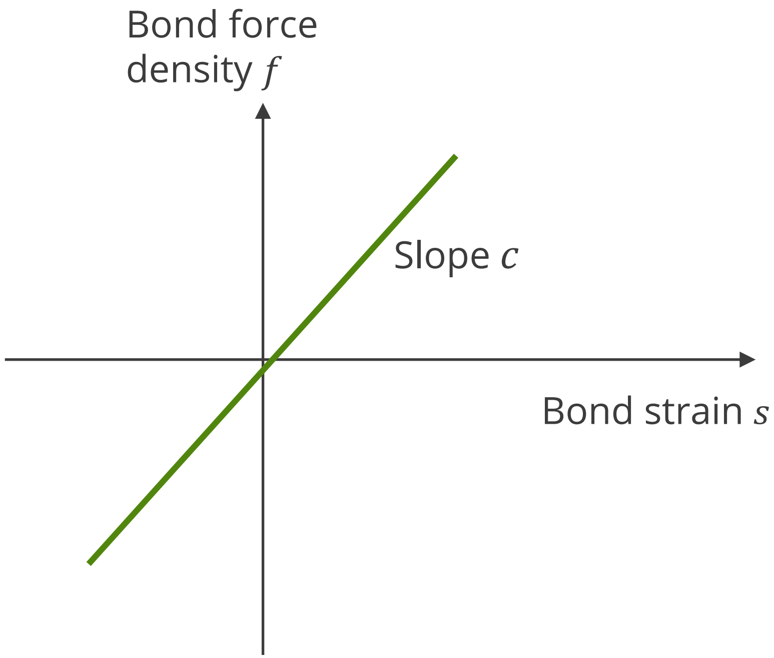
Bond forces

Material modeling: Bond-based vs. state-based

- In a bond-based material, the force density in a bond depends ***only*** on the deformation of that particular bond.
  - Highly restrictive (Poisson's ratio = 1/4 in 3D).
- The alternative assumption is used in ***state-based*** material models.
  - Much more general.
  - Any Poisson ratio.







An elastic bond-based material is a network of springs
(which can be nonlinear)

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.

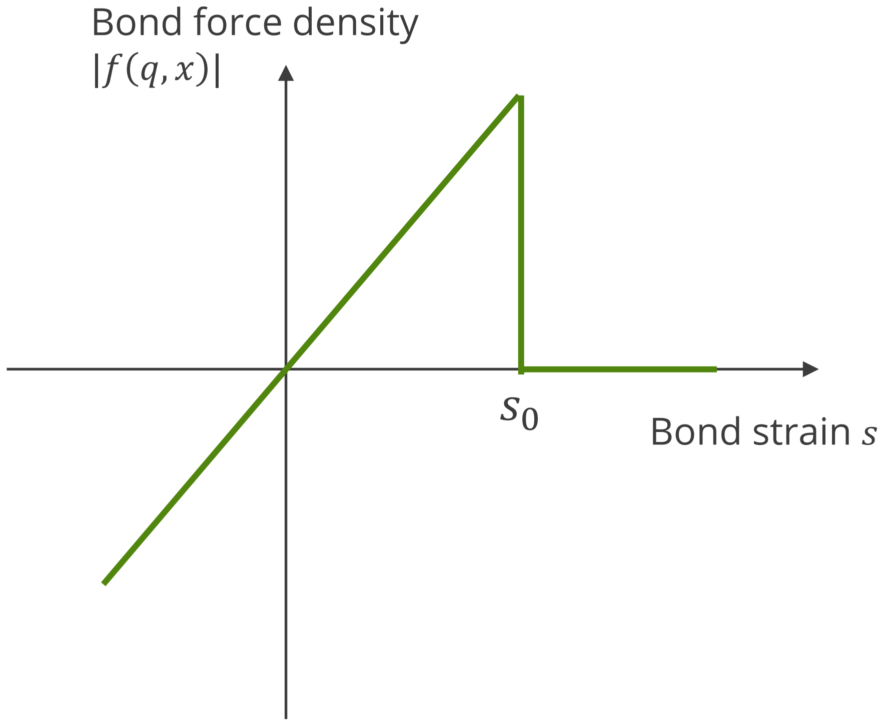
- Units are force/area.

- 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.

Damage: Bond breakage

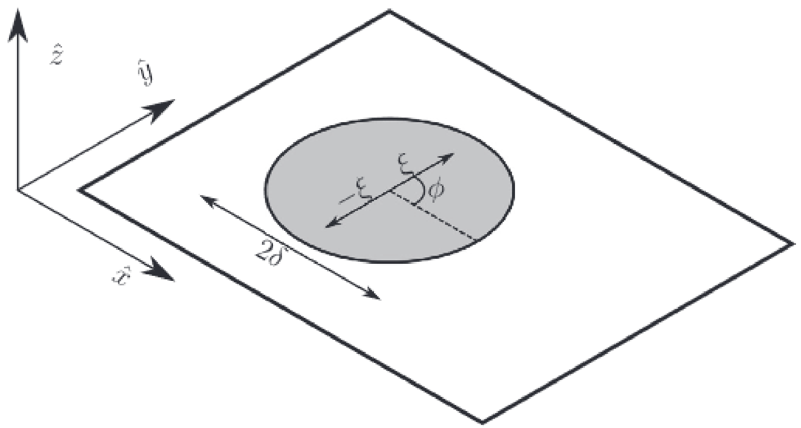
- Bonds can break irreversibly.
- After breakage, a bond cannot carry any tensile load.
- The criterion for bond breakage can be anything you can dream up.
- The simplest criterion is ***critical bond strain***.
- Relation of the critical bond strain to the energy release rate in linear bond-based material:

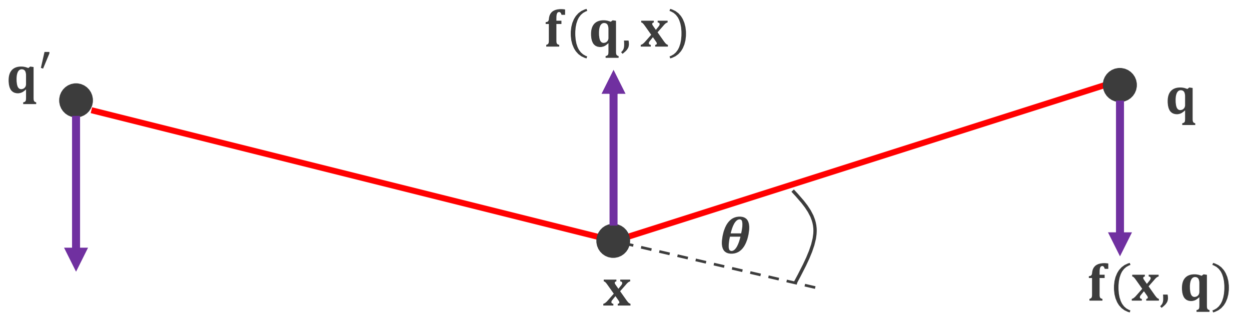
$$s_0 = \sqrt{\frac{5G_0}{9k\delta}}$$



Generality of material models

- Any material model from the local theory can be implemented in state-based peridynamics.
- Also, nonlocality allows material response not possible within the standard continuum PDEs.
  - Example: peridynamic plates and shells*.





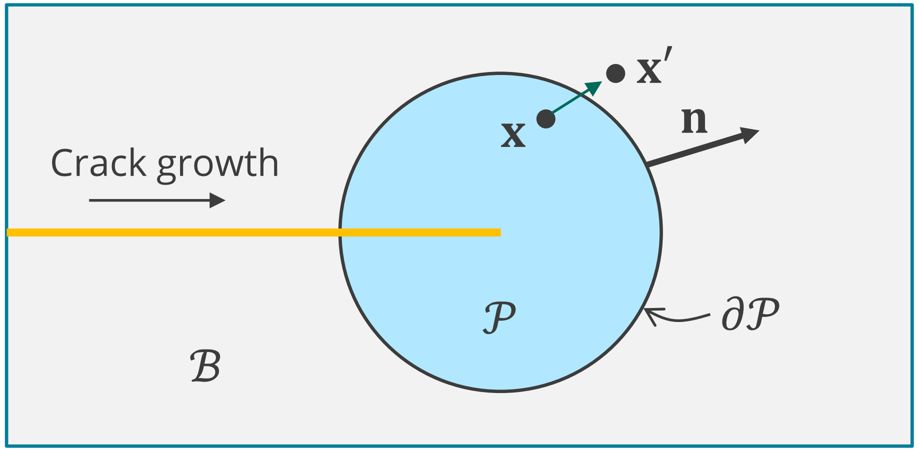
Material model for plates resists angle changes between opposite bonds

*J. O'Grady and J. Foster, 2014. Peridynamic plates and flat shells: A non-ordinary, state-based model. *International Journal of Solids and Structures*, 51(25-26), pp.4572-4579.

Generality of damage models

- Almost any criterion can be used for bond breakage.
- Some damage models that have been implemented:
  - Hashin (composites)
  - Drucker-Prager (granular)
  - Tearing parameter (ductile metals)
  - Johnson-Holmquist-Beissel (ceramics)
  - Nonlocal continuum damage mechanics
  - Fatigue
  - M7 Microplane (concrete)*
  - Nonlocal Rice-Eshelby J-integral**

Nonlocal J-integral



$$\mathbf{J} = \frac{1}{2}\int_{\mathcal{P}}\int_{\mathcal{B}-\mathcal{P}}\left[\left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}(\mathbf{x}')\right)^T - \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}(\mathbf{x})\right)^T\right]\mathbf{f}(\mathbf{x}',\mathbf{x})\, d\mathbf{x}'\, d\mathbf{x} + \int_{\partial\mathcal{P}} W\mathbf{n}\, dA$$

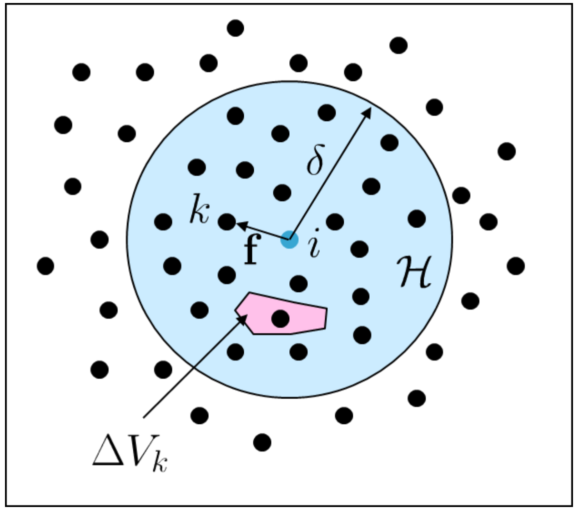
*Y. Bazilevs, M. Behzadinasab, and J.T. Foster, 2022. *Journal of the Mechanics and Physics of Solids*, p.104947.
** W. Hu, Y.D. Ha, F. Bobaru, and SS, 2012. *International journal of fracture*, 176(2), pp.195-206.

Simple particle discretization

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

$$\rho \ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t) \quad \longrightarrow \quad \rho \ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\, \Delta V_k + \mathbf{b}_i^n$$

- Good:
  - Simple.
  - Linear and angular momentum conserved exactly.
- Bad:
  - Not always asymptotically convergent to the right PDE.
  - Fails patch test for irregular grids.

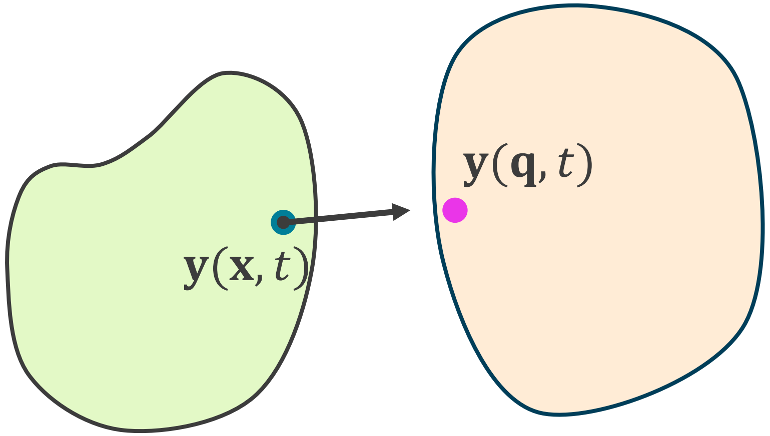


- Discontinuous Galerkin is another viable method (used in LS-DYNA).

- SS & Askari, *Computers and Structures* (2005)
- Bobaru, Yang, Alves, SS, Askari, & Xu, *IJNME* (2009)
- Chen & Gunzburger, *CMAME* (2011)
- Du, Tian, & Zhao, *SIAM J Numerical Analysis* (2013)
- Tian & Du, *SIAM J Numerical Analysis*. (2014)
- Ganzenmüller, Hiermaier, May, in *Meshfree methods for partial differential equations VII,* Springer (2015)
- Seleson & Littlewood, *Computers & Mathematics with Applications* (2016)
- Du, in *Handbook of peridynamic modeling* (2016)

Short-range forces

- These are used for contact between bodies, self-contact, and sometimes for post-failure response within bodies.
- They only depend on the ***current*** (not initial) distance between material points.

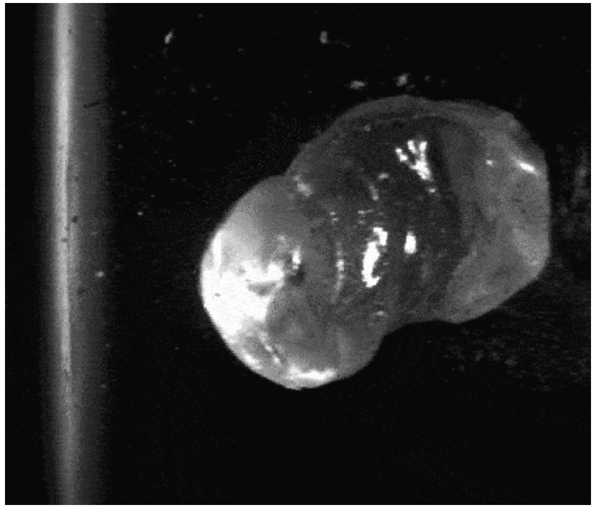


Points repel each other even if they started far apart

We get geometric nonlinearity for free: Bird strike

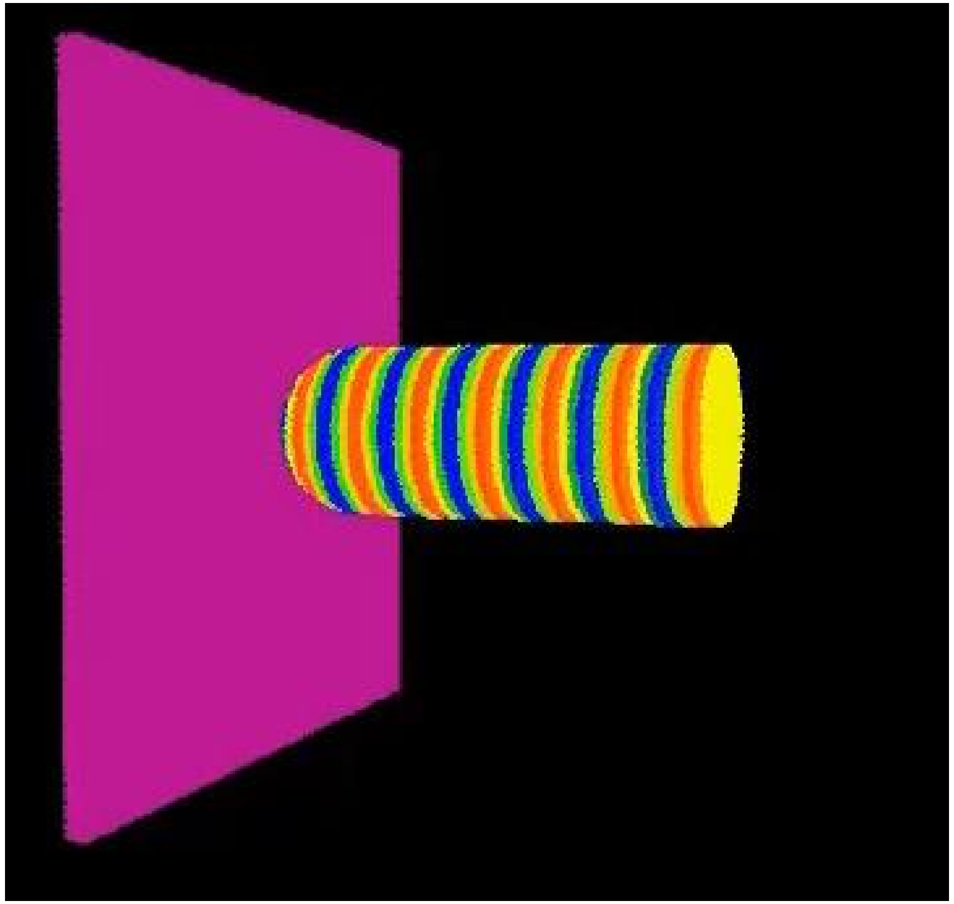
- Bonds can rotate.
- Force vectors rotate with the bonds.
- This holds even if the material model has a linear dependence on strain.

VIDEO



Typical test
(credit: Arthur Core)

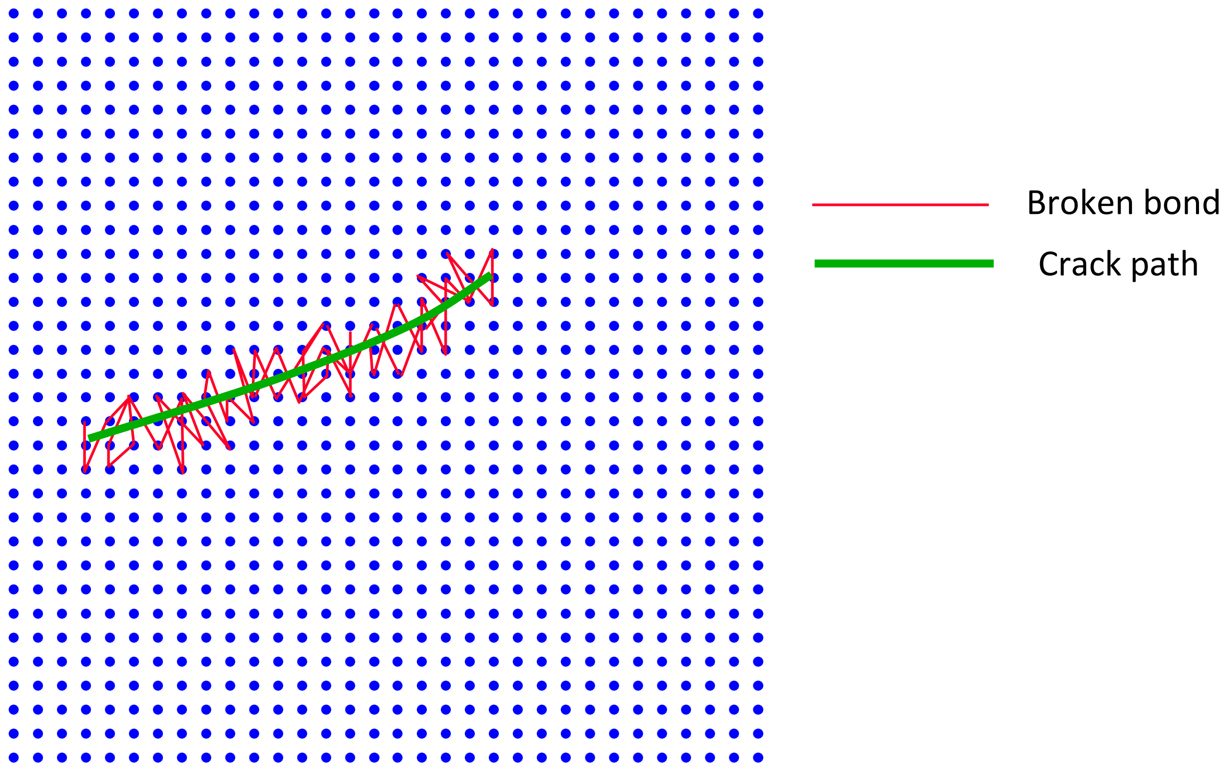
VIDEO



Peridynamic model

Autonomous crack growth

- Bonds break whenever they feel like it.
- When a bond breaks, it becomes more likely that a neighboring bond will also break.



Typical crack growth application

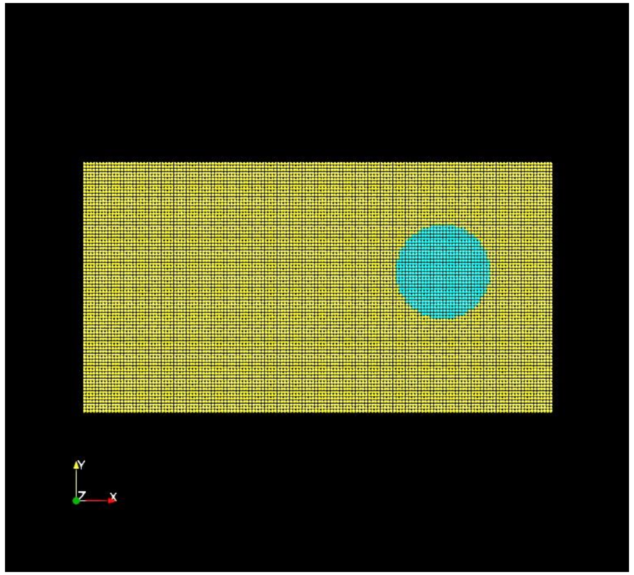
VIDEO

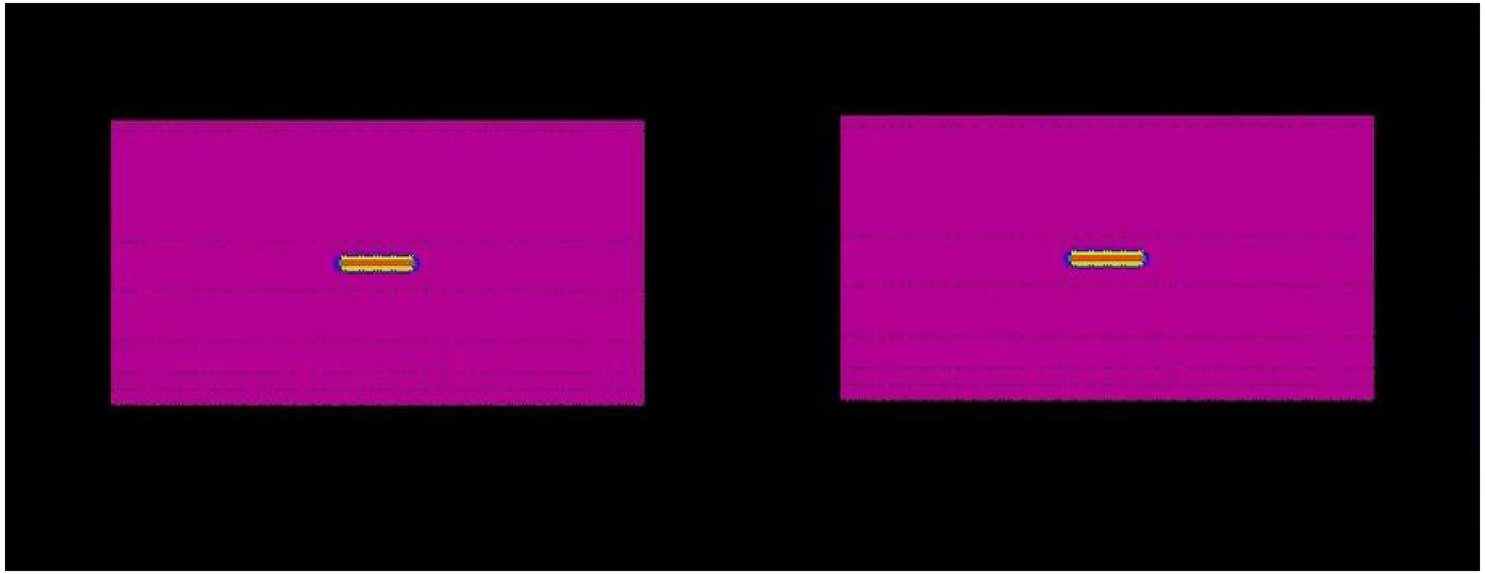
Colors show net damage
Displacements x100

Weak and strong interfaces

- Initial crack grows and encounters a hard inclusion.

VIDEOS

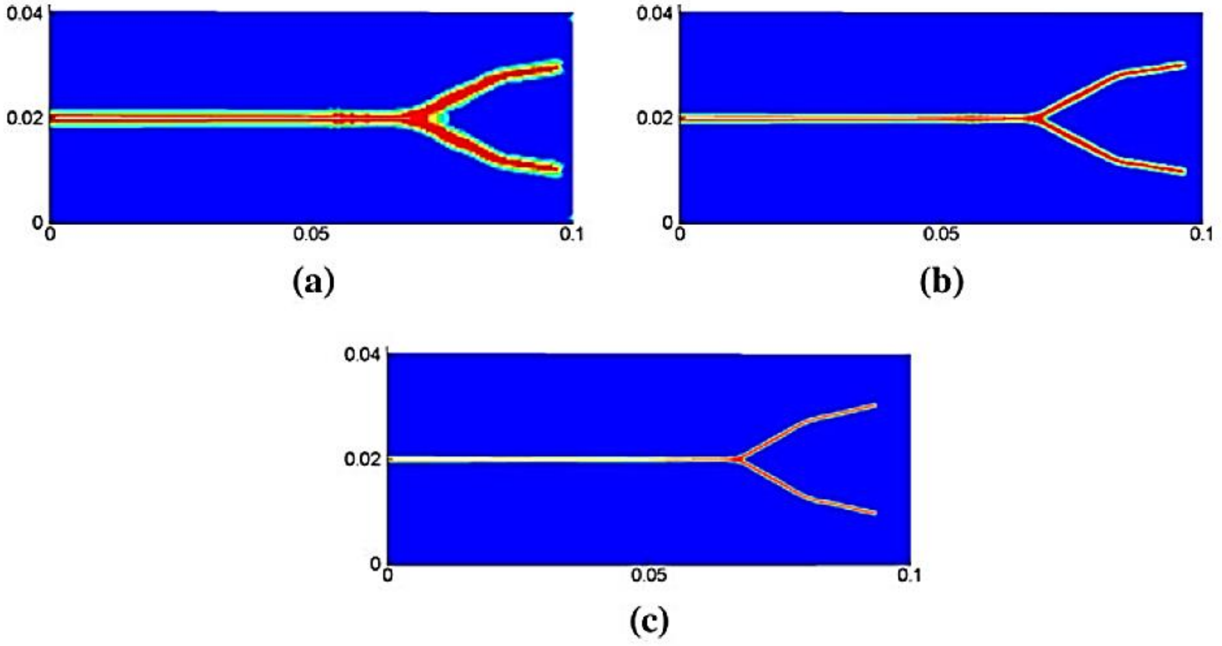


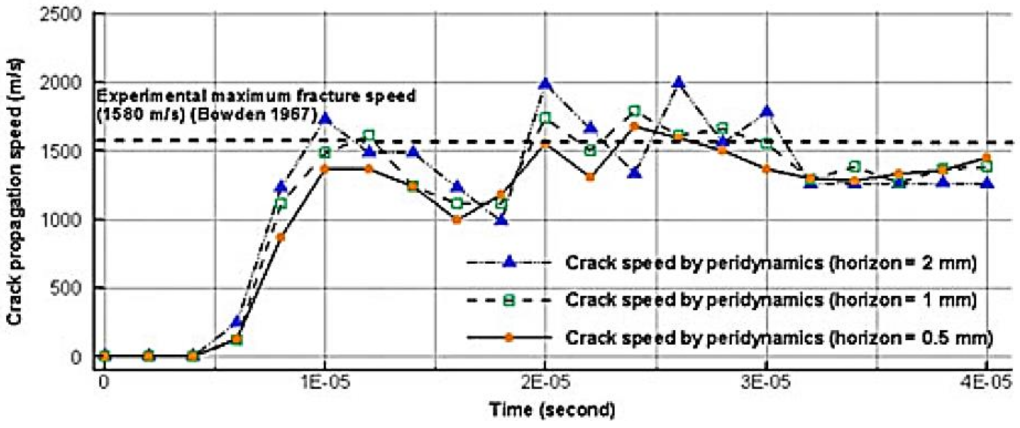


Weak interface Strong interface

Validation of crack speed in glass

- Fracture in soda-lime glass using 3 different grid spacings*.

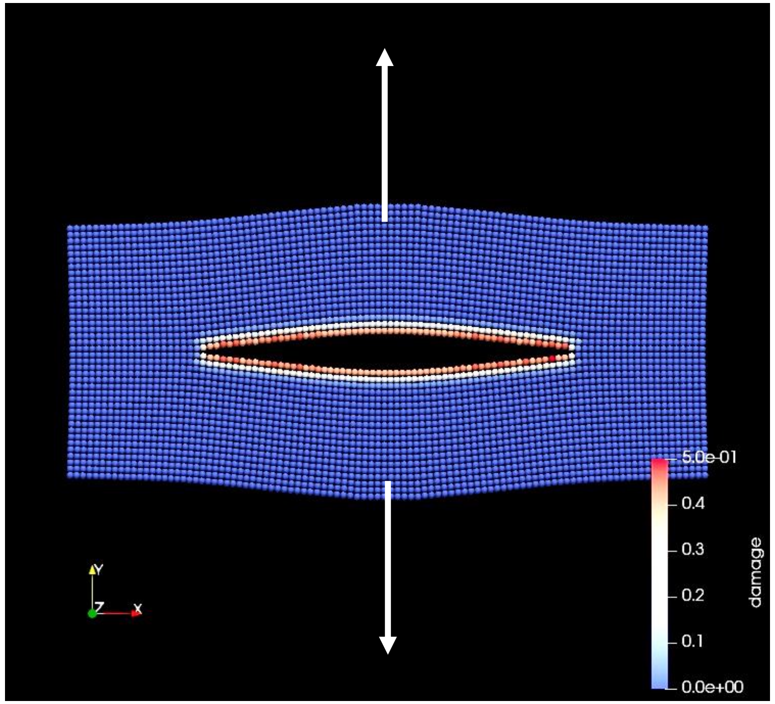


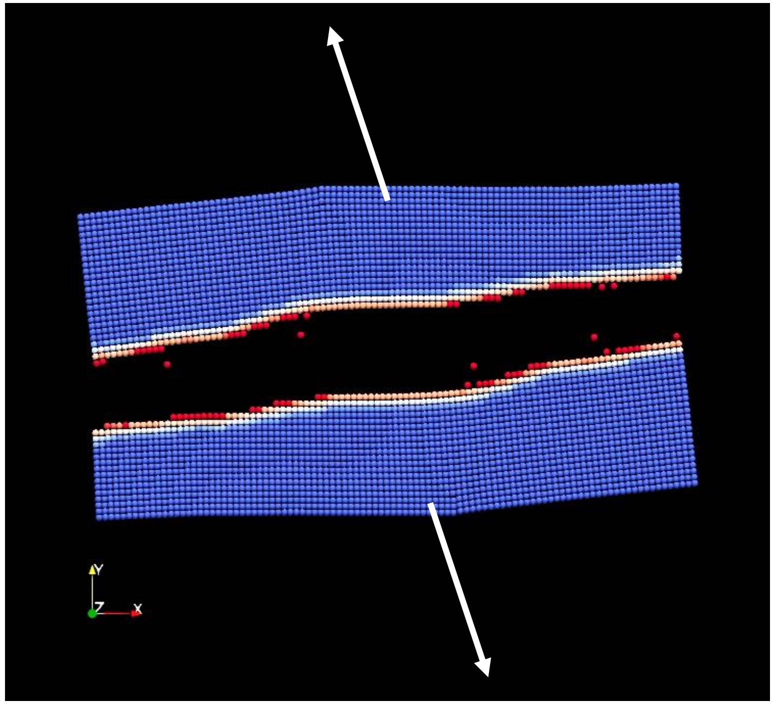


- Ha & Bobaru*, Int J Fracture* (2010)
- *Agwai, Guven, & Madenci*, Int J Fracture* (2011)
- Ha & Bobaru, *Engin Fracture Mech* (2011)
- Dipasquale, Zaccariotto, & Galvanetto*, Int J Fracture* (2014)
- Bobaru & Zhang, *Int. J Fracture* (2015)
- Zhou, Wang, & Qian, *European J Mechanics-A/Solids*. (2016)

Mixed mode fracture

- Crack growth direction changes continuously with load direction.

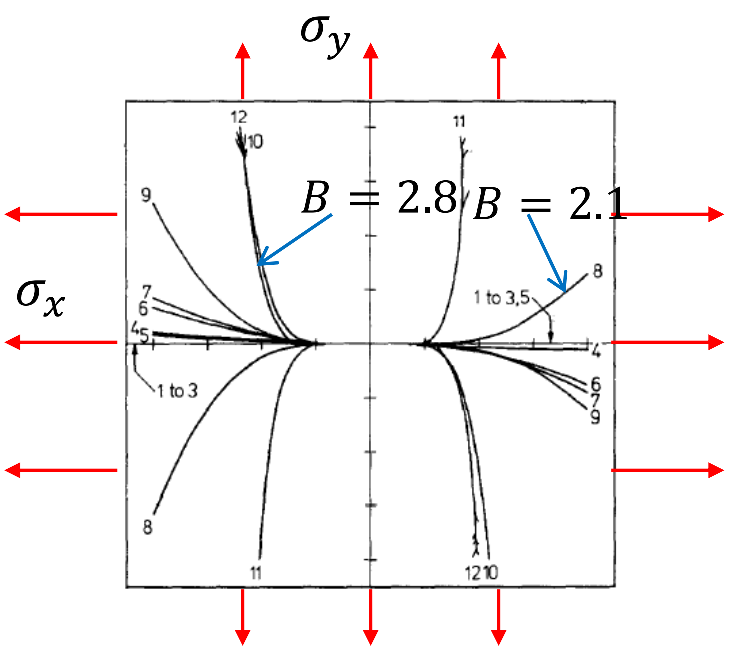




Colors show net damage
Displacements x100

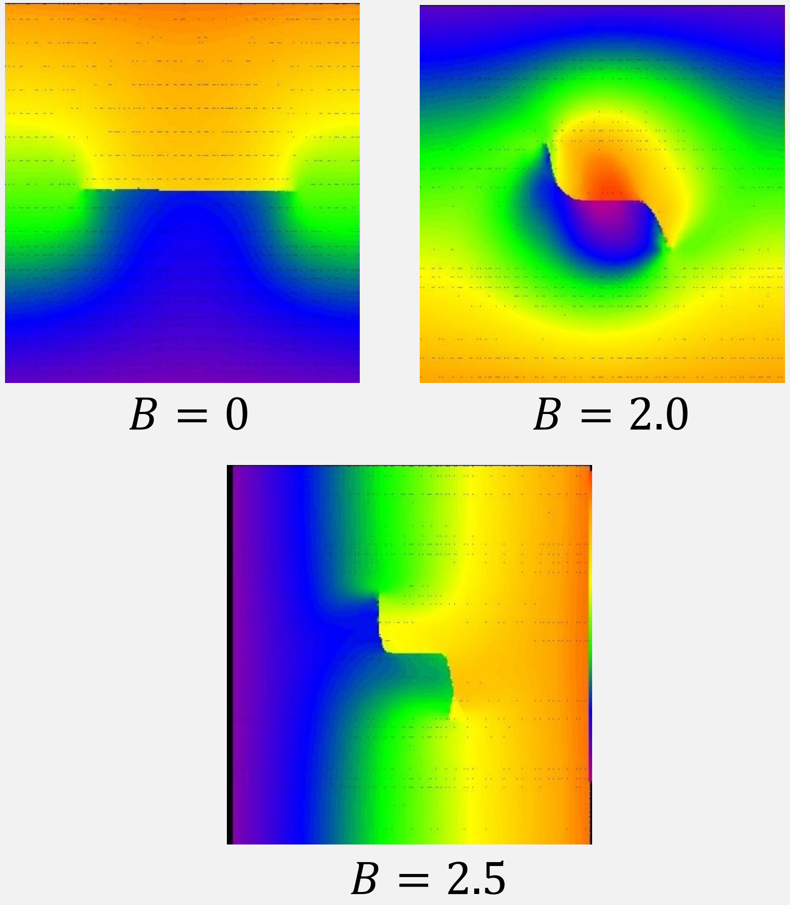
Crack stability and mode transition

- 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*

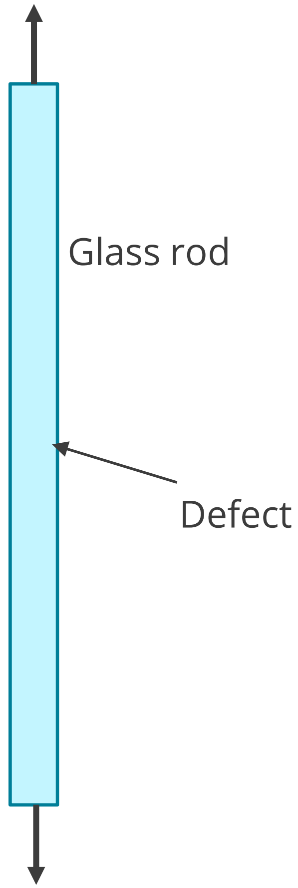
Simulated crack paths

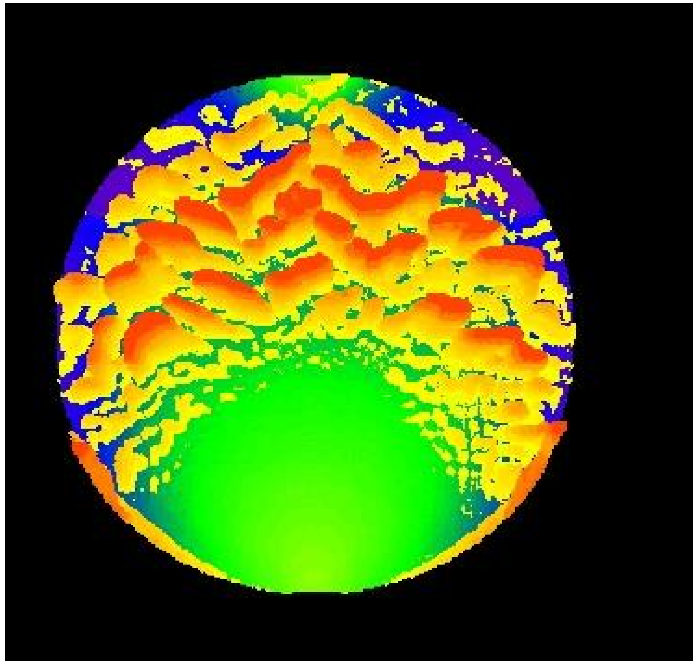


*Leevers, Radon, & Culver JMPS (1976)

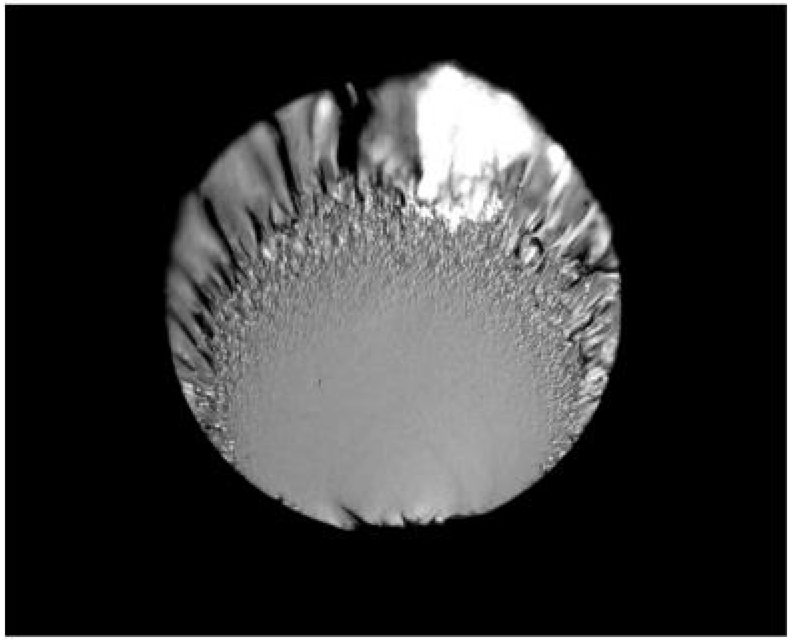
Crack stability: Mirror-mist-hackle transition

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





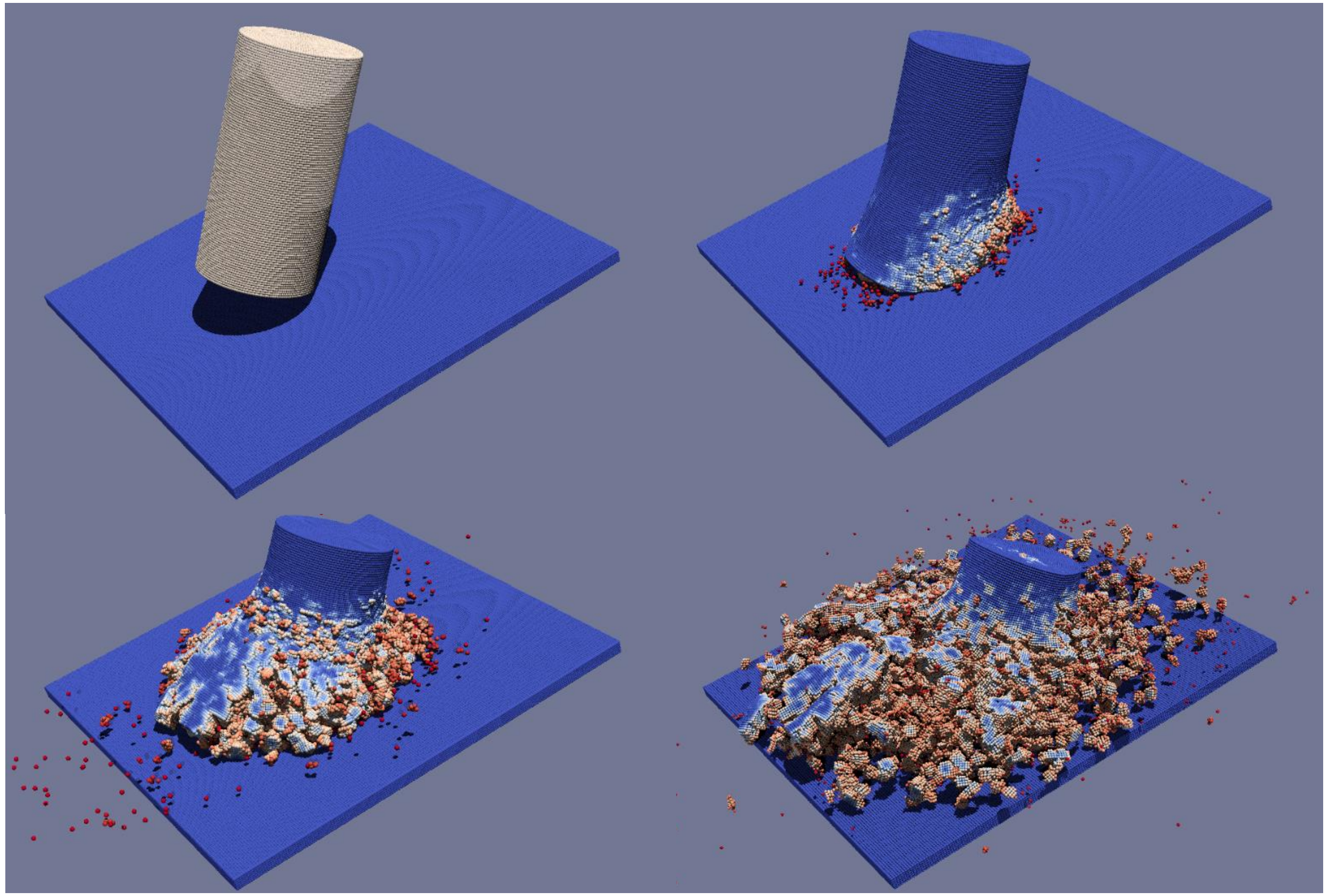
3D peridynamic model
Colors show axial coordinate of damaged nodes.



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

Fragmentation due to impact

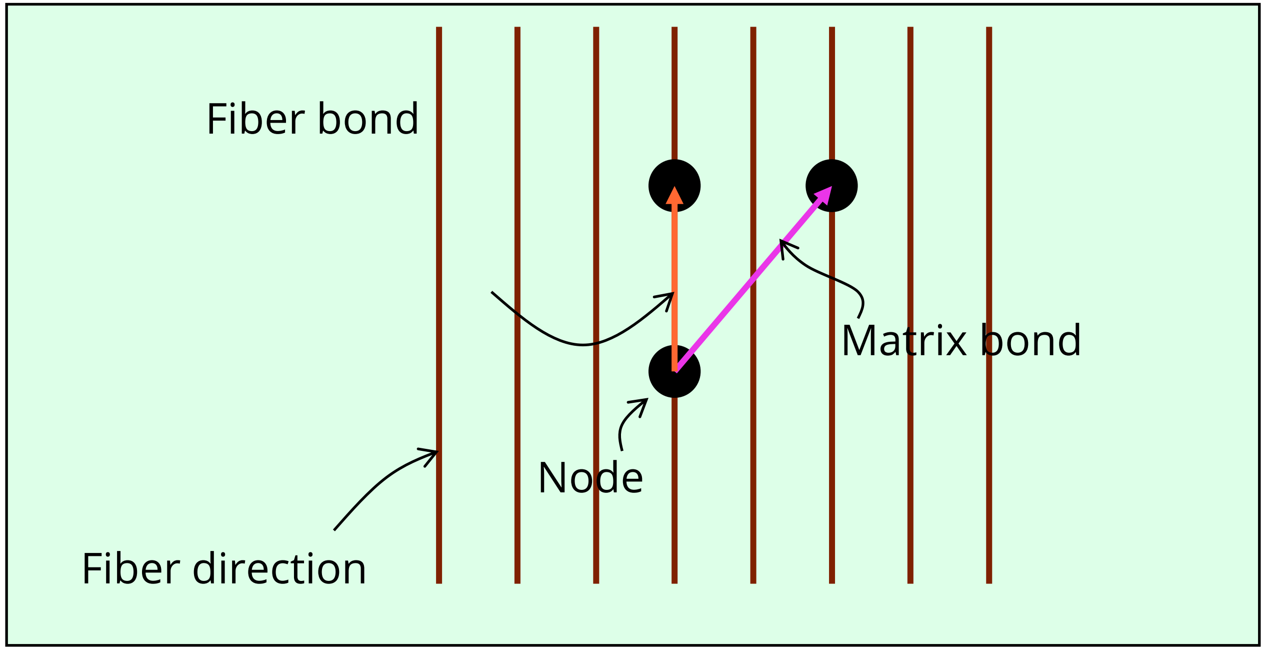
- Brittle cylinder vs. rigid plate at 1km/s.

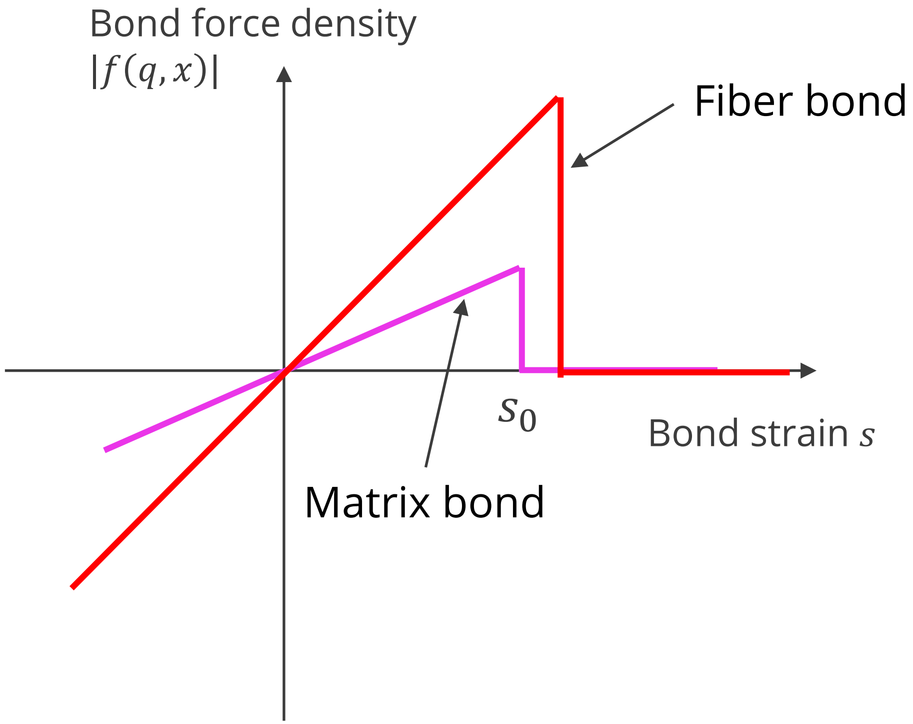


Colors show damage

Anisotropy: Composite lamina

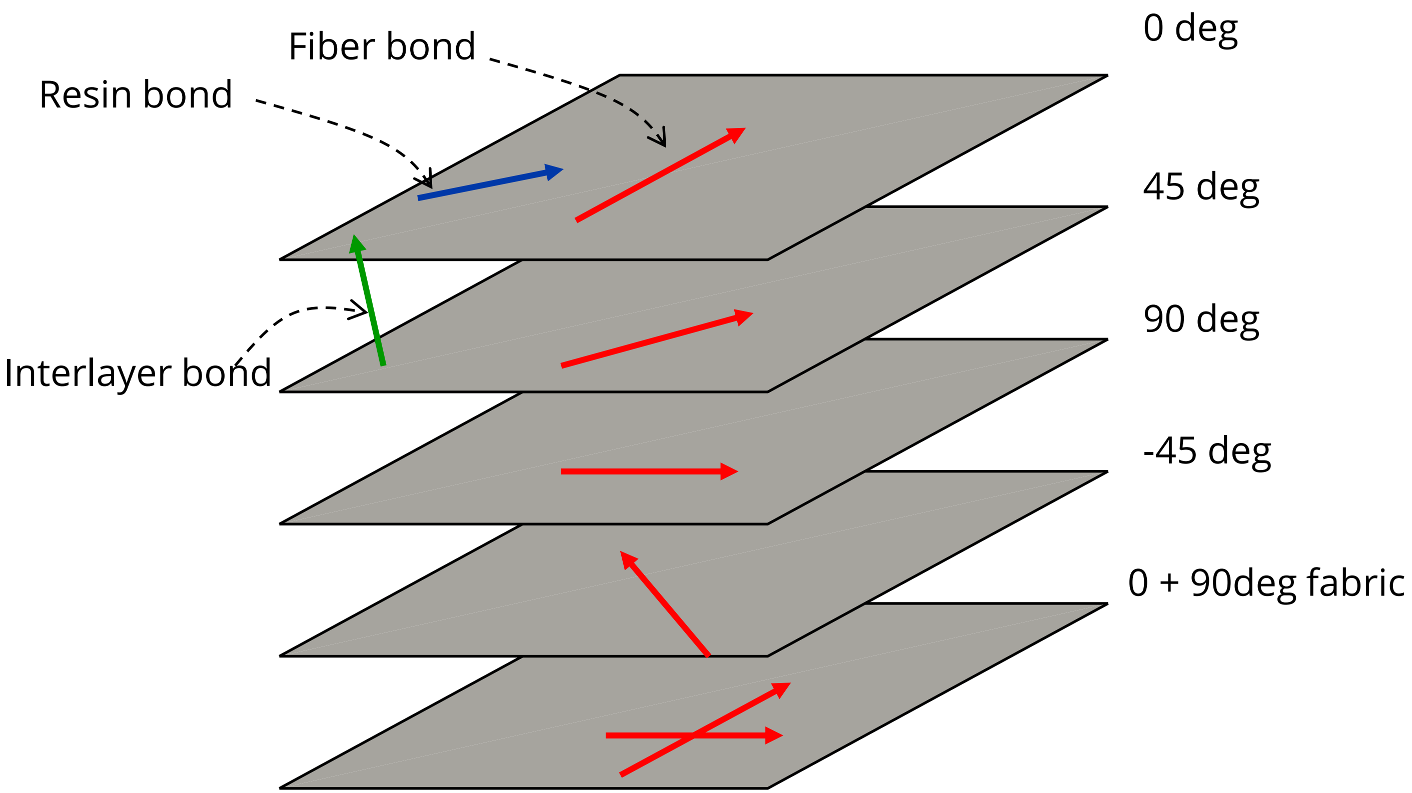
- Bonds in different directions can have different elastic response (c) and critical strain (s_0).





Anisotropy: laminate

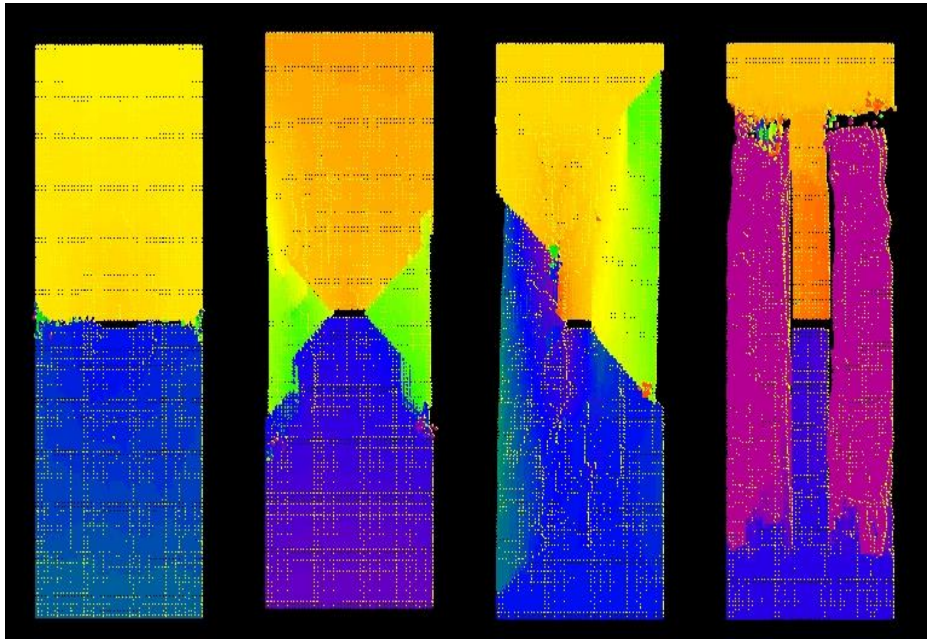
- Stack up laminas, connected by a third type of bond (interlayer).



Effect of composite layup on failure modes

- Large notch tension test.
- Relative numbers of plies in different directions influences the failure mode.
- Harder layups (lots of fibers in the loading direction) often do not fail with a crack straight across the specimen.

Peridynamic simulations of LNT failure modes
Colors show axial displacement in top ply

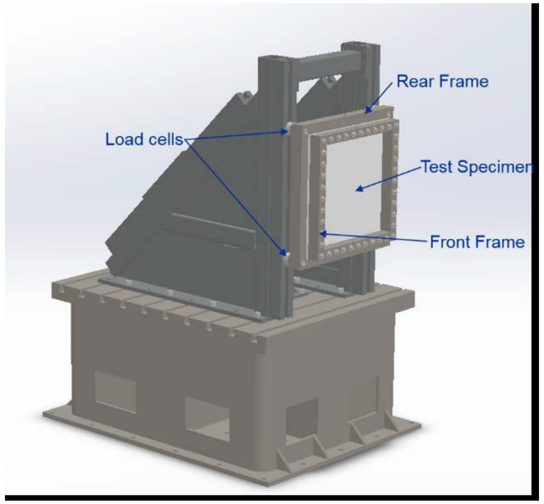


25/50/25 30/60/10 40/50/10 100/0/0

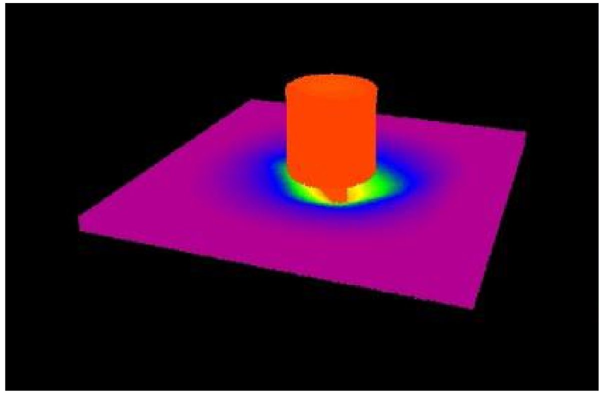
Image: Boeing

Impact on composites: Analysis in predictive mode

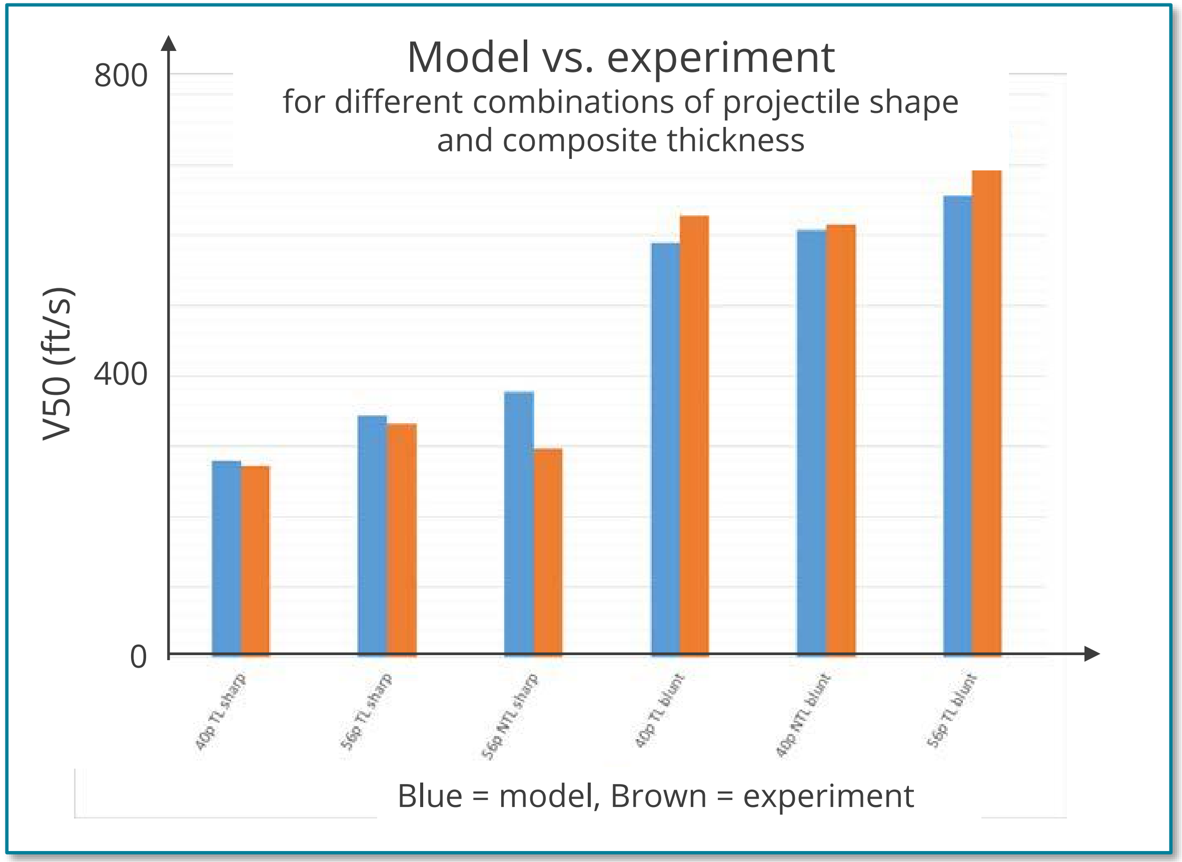
- Deformable projectiles vs. 40 to 56 ply carbon-epoxy laminate (NASA Glenn).
- Try to find V50 (just barely perforate).
- Analysis results were blind predictions – didn't know test data.



Target fixture

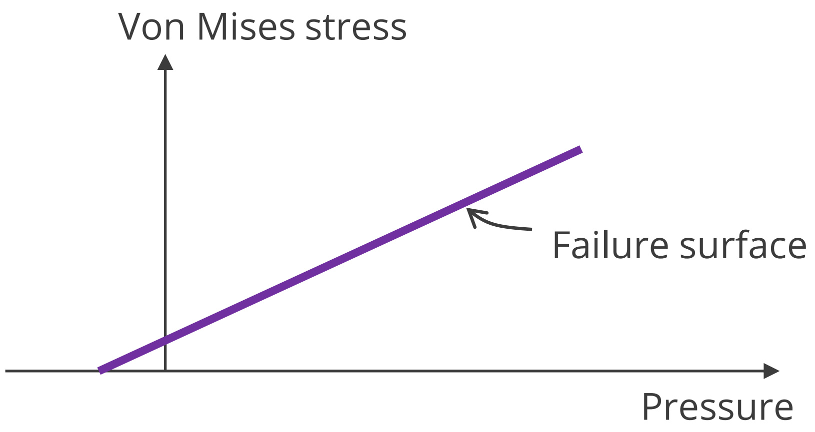


Simulation
Color show displacement



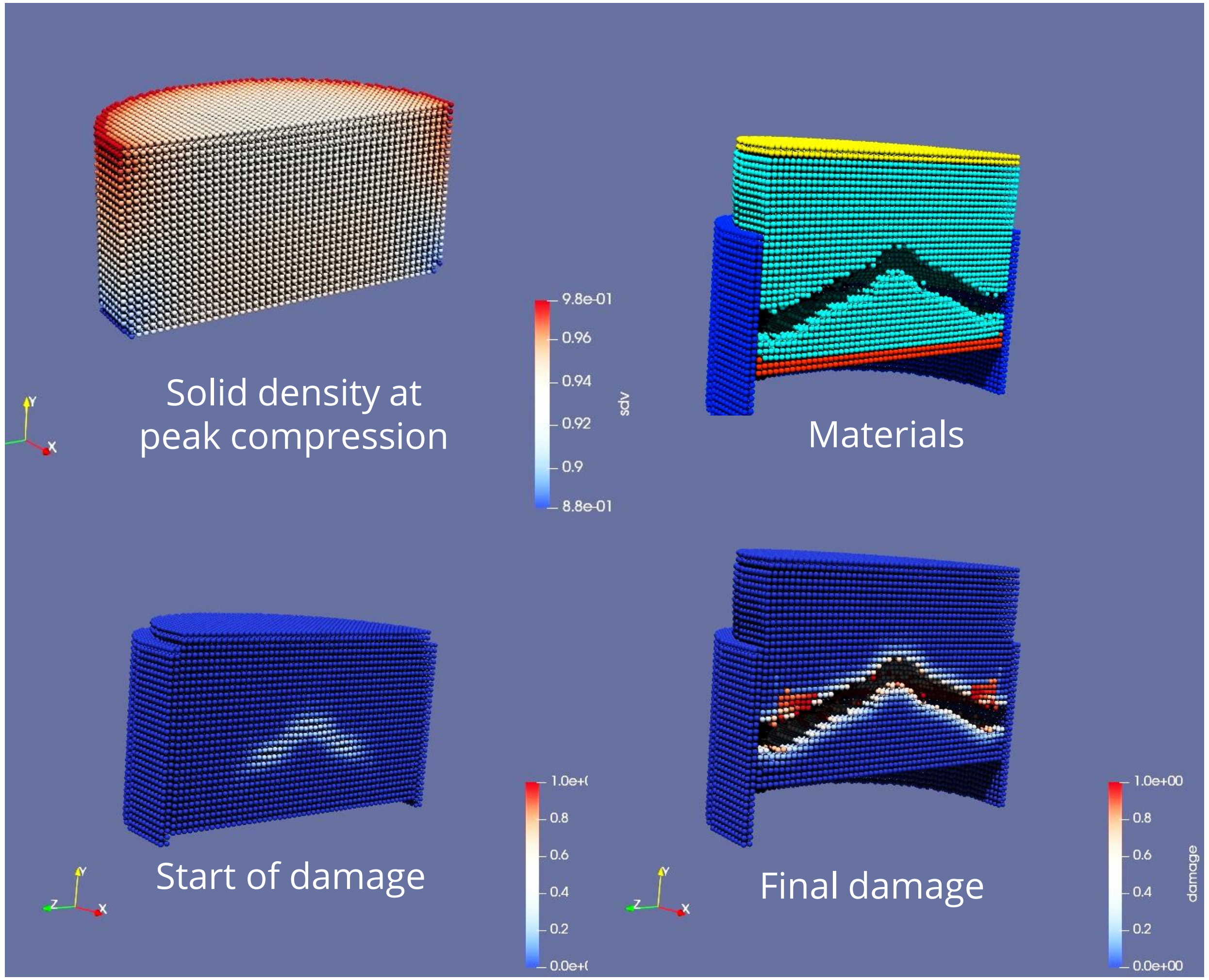
F. Cuenca et al., "Determination of ballistic limit for IM7/8552 using peridynamics." In 2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference (p. 1703).

Special damage criteria: Drucker-Prager*



Tablet “capping” failure
Image: merlin-pc.com

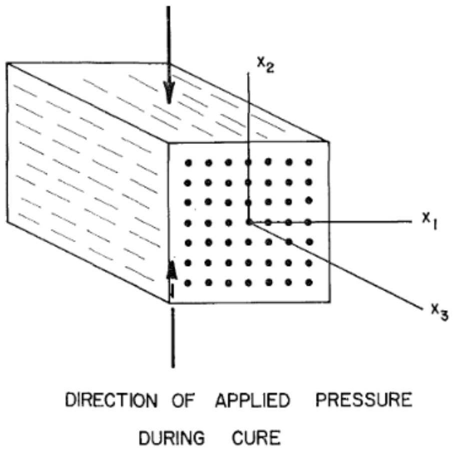
Ejection of a pharmaceutical tablet from a rotary press

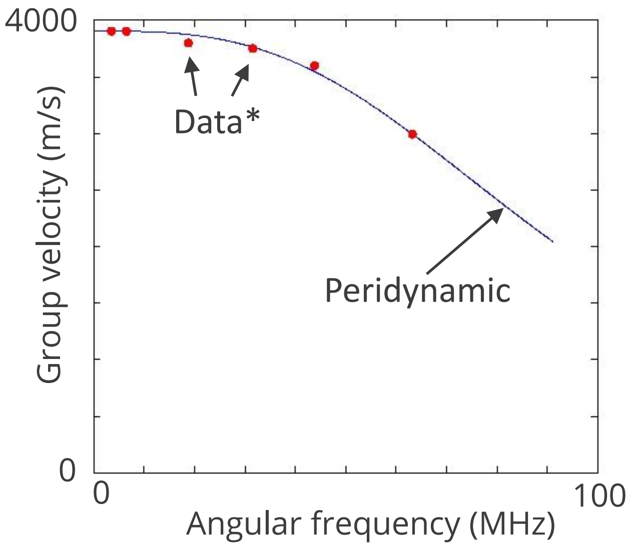


*Joint work with S. Garner, W. Ketterhagen & J. Strong (AbbVie Corp.)

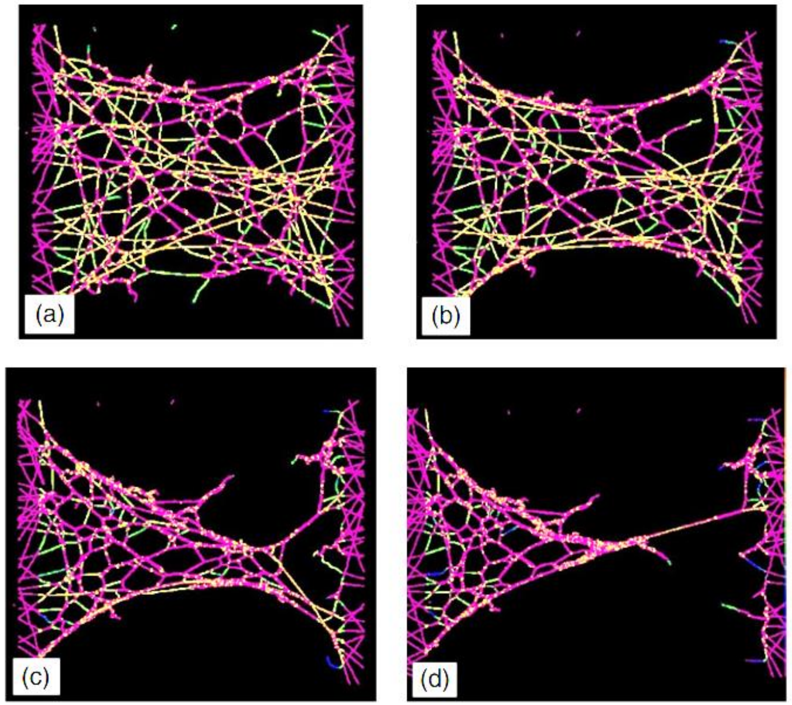
Nonlocality

- All discretized methods are nonlocal.
- Long-range forces are nonlocal (e.g. Van der Waals).
- Heterogeneous materials are nonlocal after homogenization.
- Nonlocality can reproduce wave dispersion.





*Tauchert, Theodore R., and A. N. Guzelsu. "An experimental study of dispersion of stress waves in a fiber-reinforced composite.“ J. Applied Mechanics (1972): 98-102.

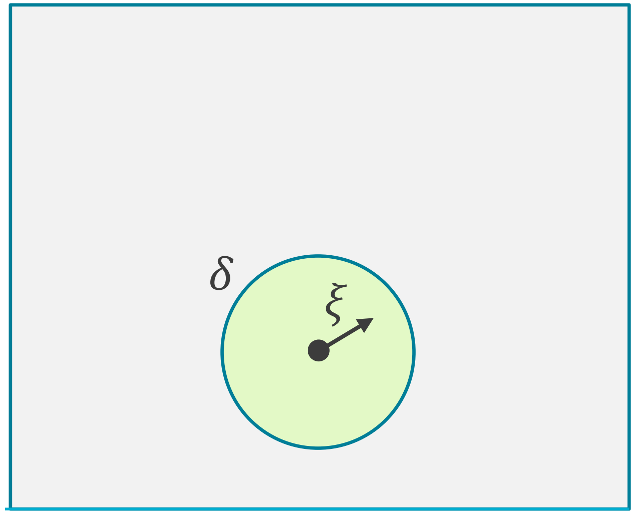


Van der Waals material

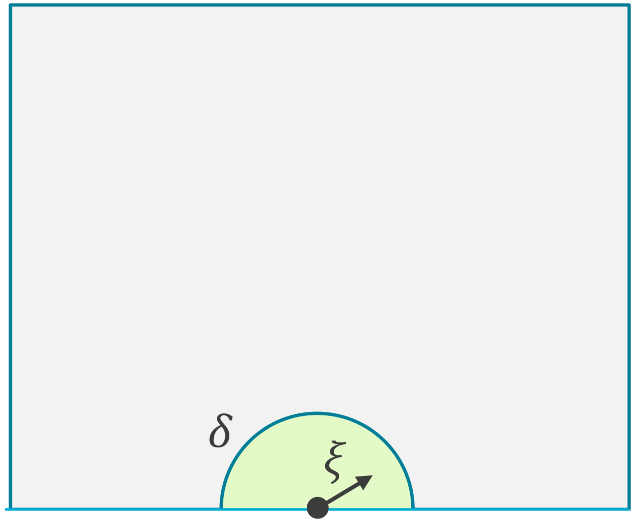
F. Bobaru, *Modelling and Simulation in Materials Science and Engineering* 15, no. 5 (2007): 397.

Some practical challenges

- Boundary conditions with integral equations generally require specifying displacement or external load within a volume, not just on a surface.
  - Lots of fixes for this in the literature.
- Surface effect.
  - Points near a free surface have more compliant elastic properties than in the interior.
  - Many practical fixes available.



Point in the interior

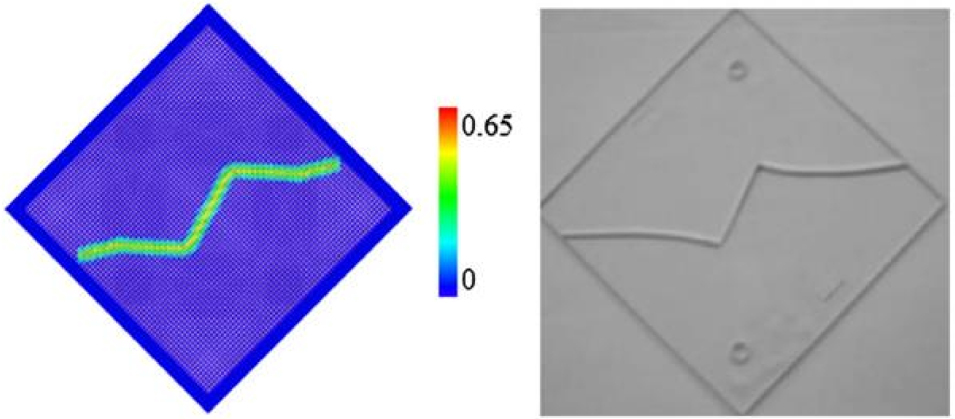


Point near a free surface is missing some bonds

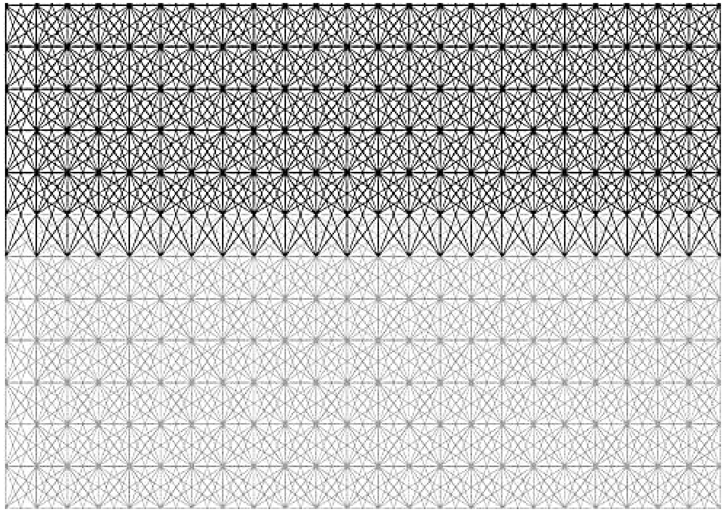
Contours of c which is now position-dependent

Peridynamics with commercial codes: Abaqus

- Peridynamic bond interactions can be included in an Abaqus model as a User Element Library (UEL).



Angled crack growth simulation with PD in Abaqus (image: Huang et al., 2019)

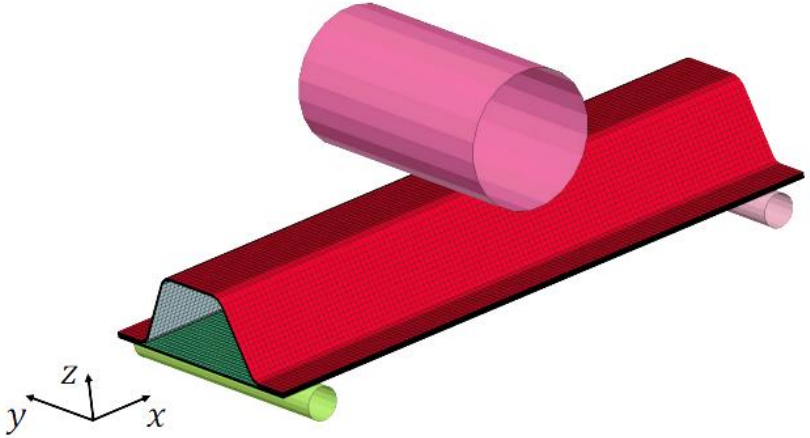


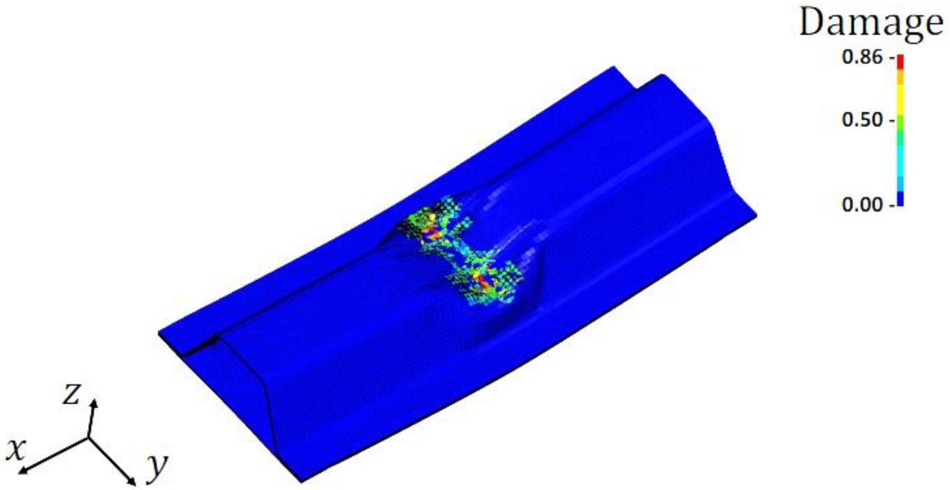
Truss elements (image: Beckmann et al., 2013)

- X.Huang, et al, 2019, *Engineering Fracture Mechanics*, 206, pp.408-426.
- Y. H. Bie, et al, 2020, *Computer methods in applied mechanics and engineering*, 372, p.113398.
- U. Yolum, A. Taştan, and M. A. Güler, 2016. *Procedia Structural Integrity*, 2, pp.3713-3720.
- R. Beckmann, R. Mella, and M. R. Wenman, 2013. *Computer methods in applied mechanics and engineering*, 263, pp.71-80.
- T. A. Haynes, D. Shepherd, and M. R. Wenman, 2020. *Journal of Nuclear Materials*, 540, p.152369.
- R. W. Macek, and S, 2007. *Finite elements in analysis and design*, 43(15), pp.1169-1178.

Peridynamics in commercial codes: LS-Dyna

- Peridynamics was implemented as a user option in LS-Dyna using the Discontinuous Galerkin method.



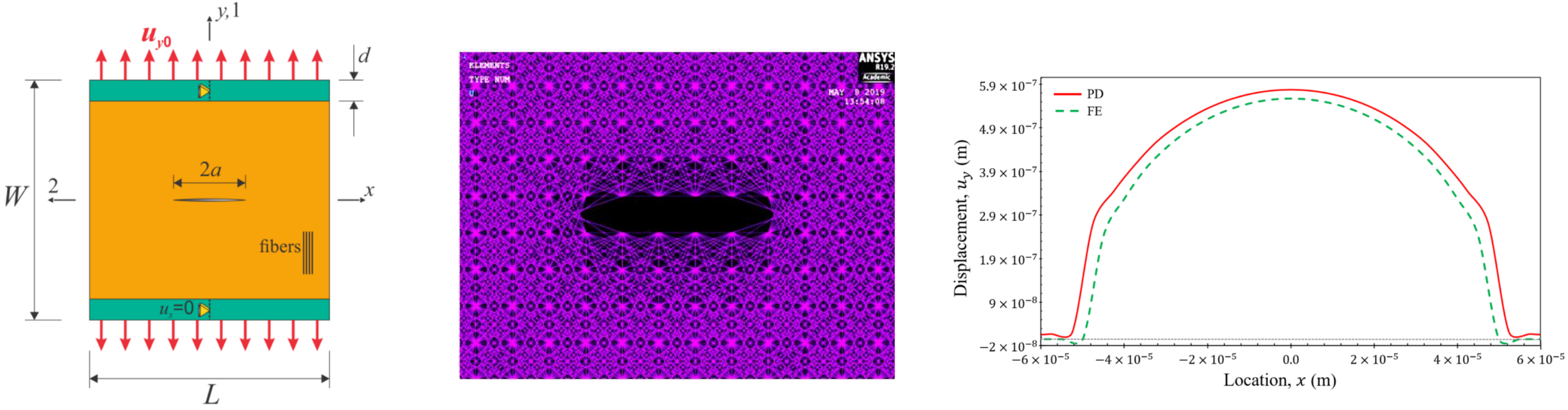


LS-Dyna simulation of a composite laminate (image: Seleson et al. 2022)

- B. Ren, C. T. Wu, and E. Askari, 2017. *International Journal of Impact Engineering*, 99, pp.14-25.
- B. Ren and C. T. Wu, "New Features in LS-Dyna," FEA publications, 2017.
- S. Das et al., 2017, *Journal of Engineering Mechanics* 145(7), p.04019049.
- P. Seleson, B. Ren, C. T. Wu, D. Zeng, and M. Pasetto, M., 2022. ORNL/TM-2022/1826

Peridynamics with commercial codes: ANSYS

- Peridynamics was coupled with Standard ANSYS using MATRIX27 elements and the Peridynamic Differential Operator.

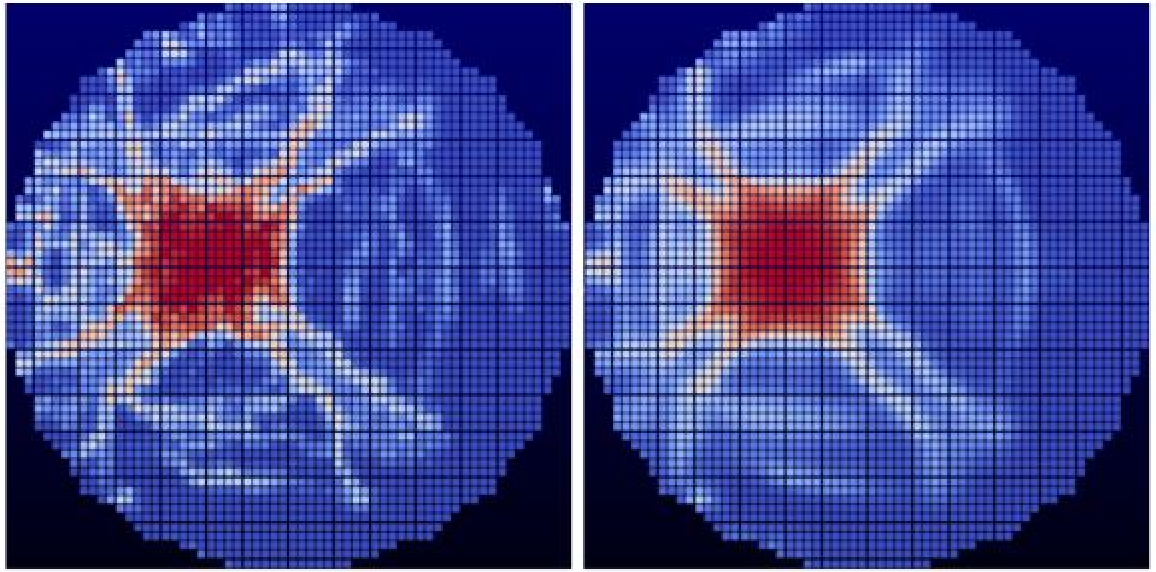


Standard ANSYS model of a notched orthotropic plate (images: Diyaraglu et al., 2019)

- E. Madenci, P. Roy, and D. Behera, 2022. Coupling of Bond-Based Peridynamics with Finite Elements in ANSYS. In *Advances in Peridynamics* (pp. 351-398).
- C. Diyaroglu, E. Madenci, and N. Phan, 2019. Composite Structures, 227, p.111334.

PD and machine learning: Training a neural network

- Peridynamic simulations can be used to train a neural network to predict fracture.



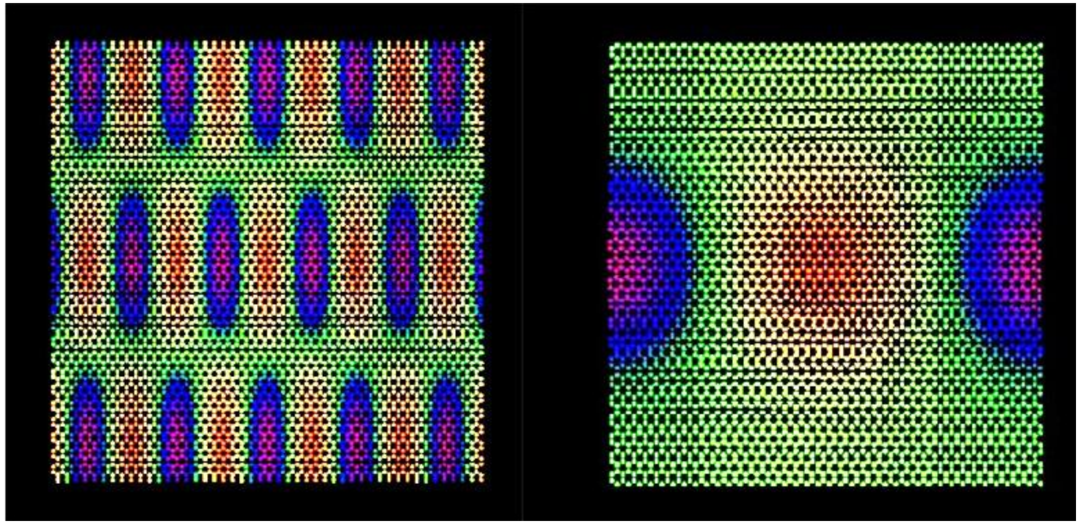
Peridynamics Peri-net NN

Images: Kim et al., 2019

- M. Kim, N. Winovich, G. Lin, and W. Jeong, 2019. *Journal of Peridynamics and Nonlocal Modeling*, 1(2), pp.131-142.

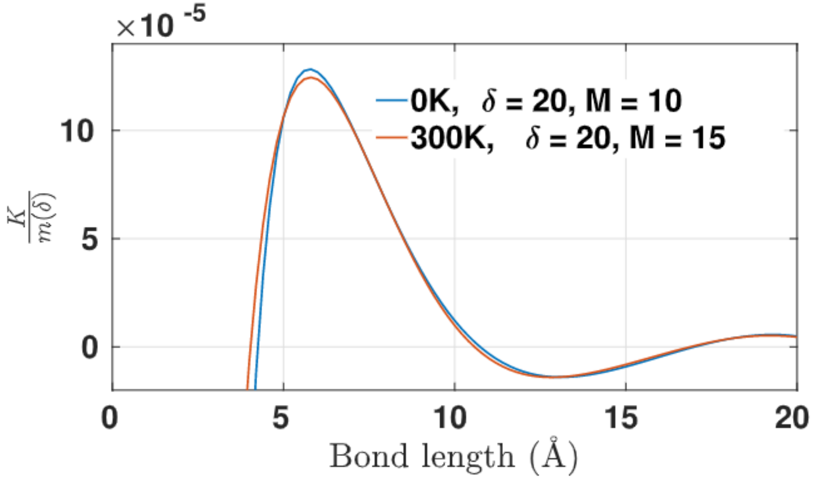
PD and machine learning: Learning a PD material model from molecular dynamics

- Upscale MD to find a peridynamic material model.



MD simulations of graphene under external loading $\mathbf{b}(\mathbf{x})$.
Colors show displacement.

ML



Learned peridynamic kernel

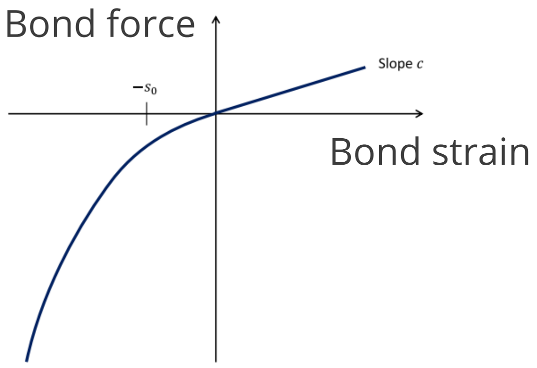
Images: You et al., 2022.

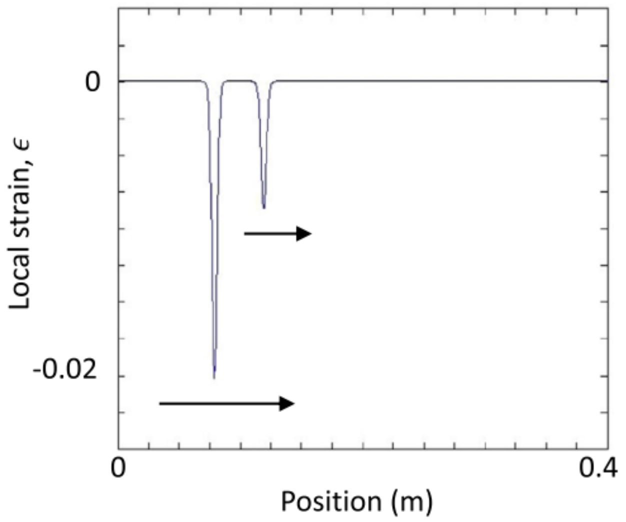
- H. You, Y. Yu, Y., S.S. and M. D'Elia, 2022. *Computer Methods in Applied Mechanics and Engineering*, 389, p.114400.
- X. Xu, M. D'Elia, and J. T. Foster, 2021. *Computer Methods in Applied Mechanics and Engineering*, 386, p.114062.
- C.T. Nguyen, S. Oterkus, and E. Oterkus, 2021. In *Peridynamic Modeling, Numerical Techniques, and Applications* (pp. 419-435).

Discovering a PDE vs. learning a kernel

- People try to discover new PDEs from data.
  - Sometimes a new peridynamic kernel acts like a new PDE.
- Example: Solitary waves.
  - It may be possible to discover the Korteweg–De Vries (KdV) equation.
- But there is a peridynamic material model that generates similar solutions:

$$\frac{\partial u}{\partial t} + \frac{\partial^3 u}{\partial x^3} - 6u\frac{\partial u}{\partial x} = 0$$





Nonlinear peridynamic material model predicts solitary waves.

- S.S., 2016. *Journal of the Mechanics and Physics of Solids*, *96*, pp.121-132.
- R. L. Pego and T.S. Van, 2019. *Journal of Elasticity*, 136(2), pp.207-236.

Summary

- Peridynamics is a continuum theory that allows for cracks within the basic equations.
- Any material model and damage criterion can be included.
- It lends itself to a straightforward meshless discretization.
- It is gradually being incorporated into commercial codes.
- It may offer opportunities in AI.

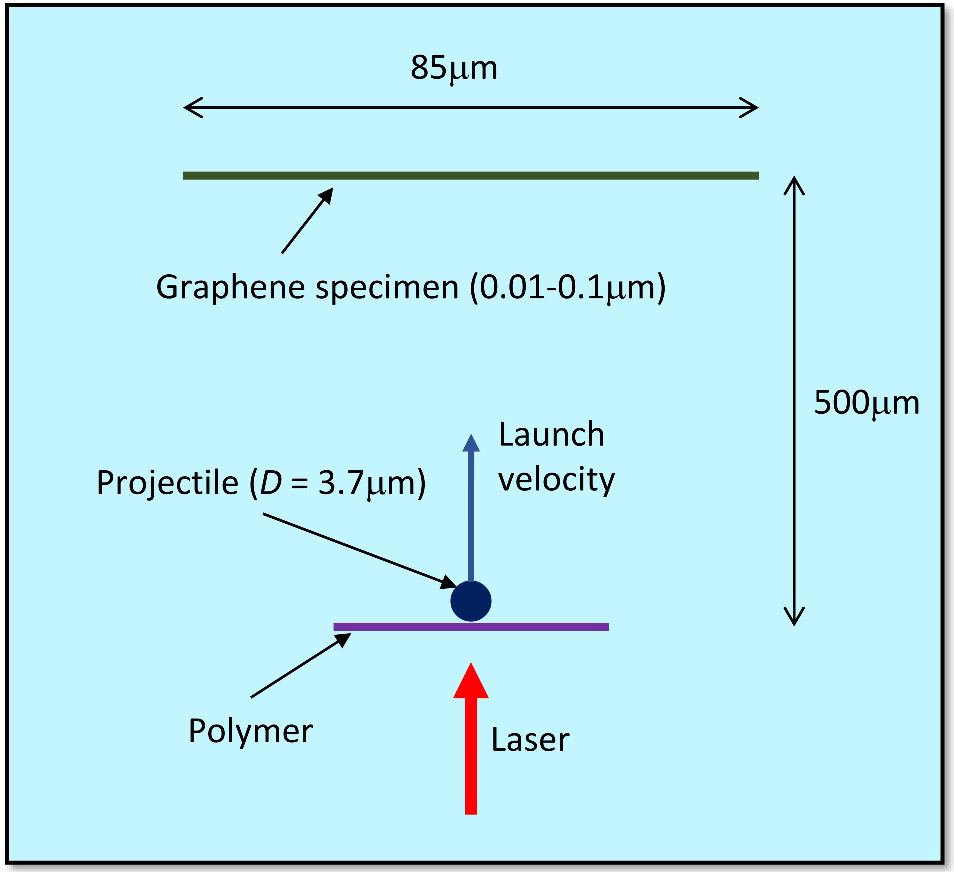
Sandia's open source peridynamic code: ***Peridigm***
peridigm.sandia.gov

Thank you!

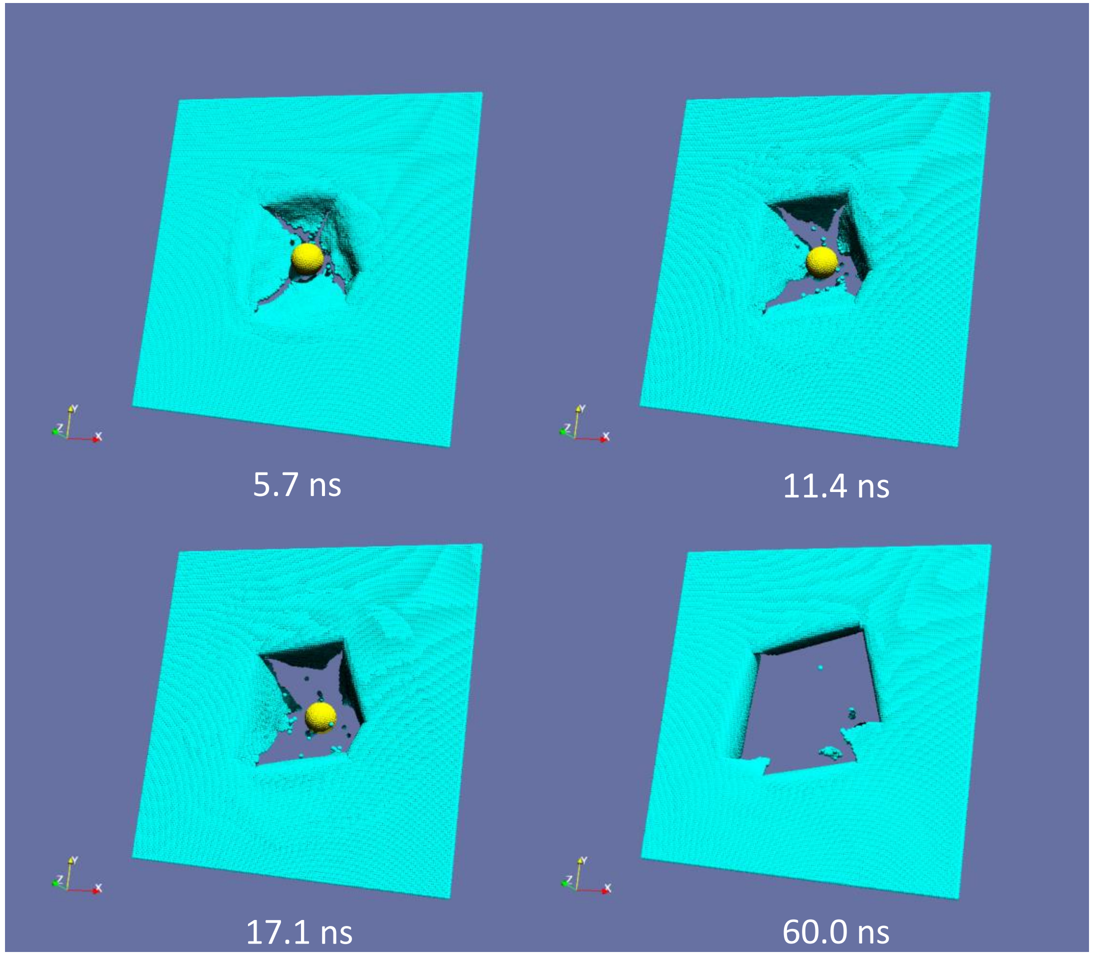
Conclusion: Some research areas in peridynamics

- Local-nonlocal coupling.
- Multiphysical modeling & nonlocal diffusion chemistry, and heat transport.
- Implicit solvers.
- Relation to AI & ML.
- Nonlocal & nonlinear wave motion.
- Post-failure material modeling.
- Ductile failure.
- Better meshless discretizations including RKPM.
- Integration into FEM tools.
- Isogeometric analysis.
- Boundary condition implementation.
- Nanoscale material modeling, self-assembly, self-shaping of structures.
- Material stability.
- Phase transitions.

Microballistic perforation of multilayer graphene



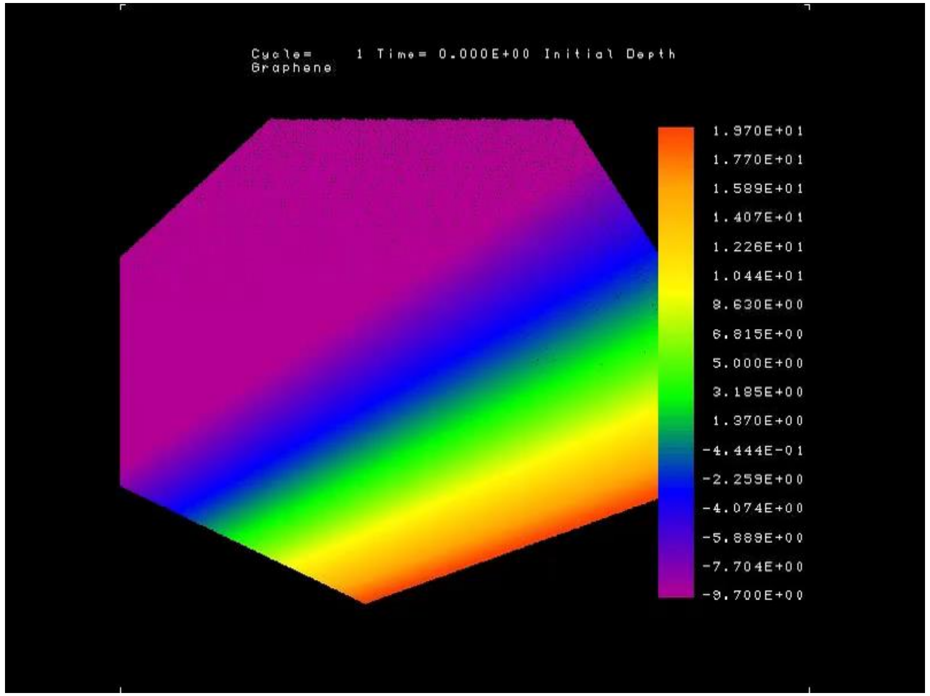
Microballistic experiment*

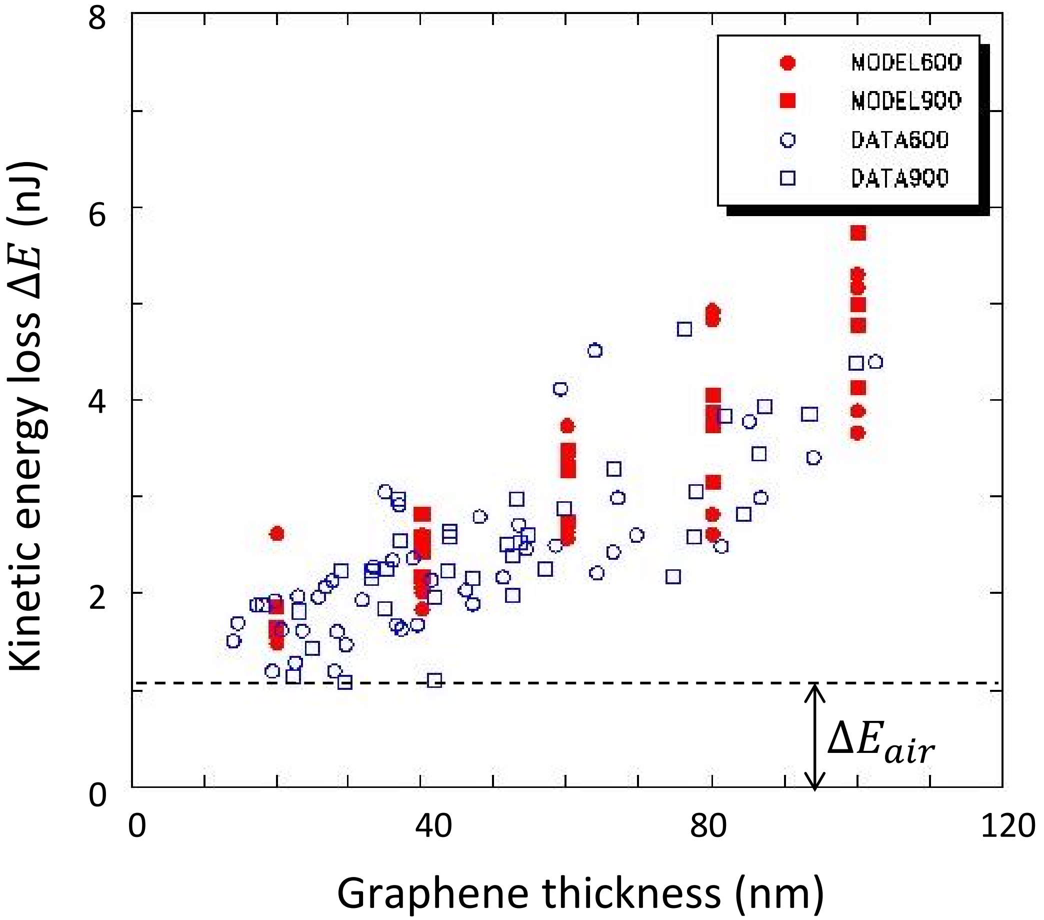


*J-H Lee et al, Dynamic mechanical behavior of multilayer graphene via supersonic projectile penetration, *Science* (2014)

Microballistic perforation of multilayer graphene

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

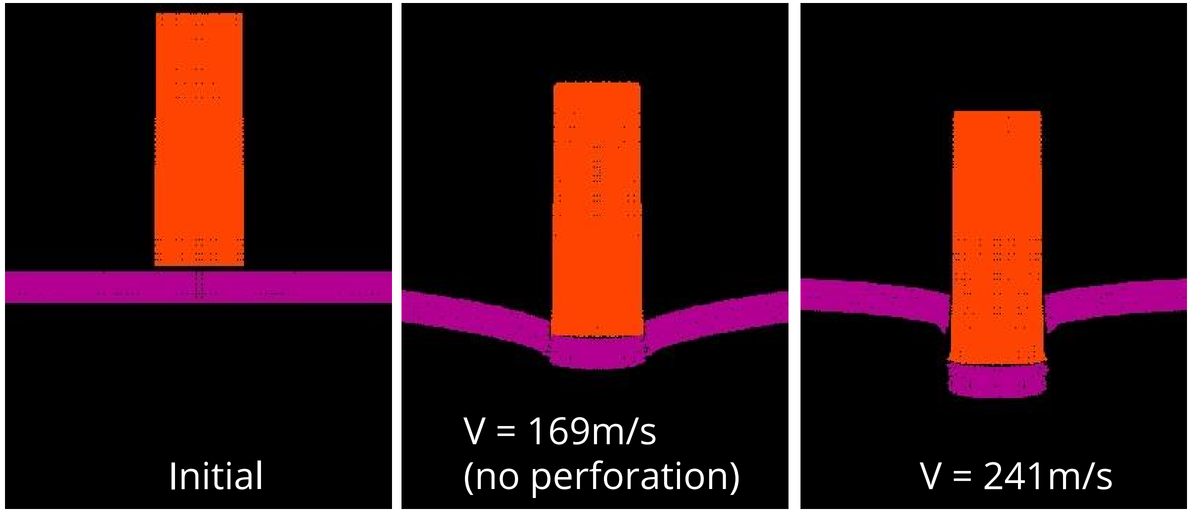


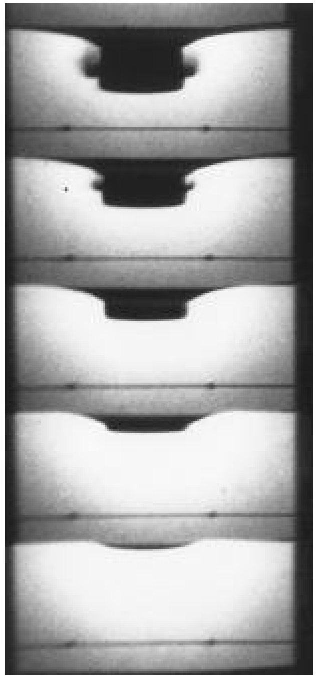


- J-H Lee et al, “Dynamic mechanical behavior of multilayer graphene via supersonic projectile penetration”, *Science* (2014)
- SS & M Fermen-Coker, “Peridynamic model for microballistic perforation of multilayer graphene.” *Theoretical and Applied Fracture Mechanics*. 2021 Jun 1;113:102947.

Blunt projectile vs. steel plate

- 30mm diameter 4340 steel cylinder onto 10.5mm thick HY-100 steel plate.
- Failure mode is plugging.
- Both materials use Johnson-Cook plasticity.

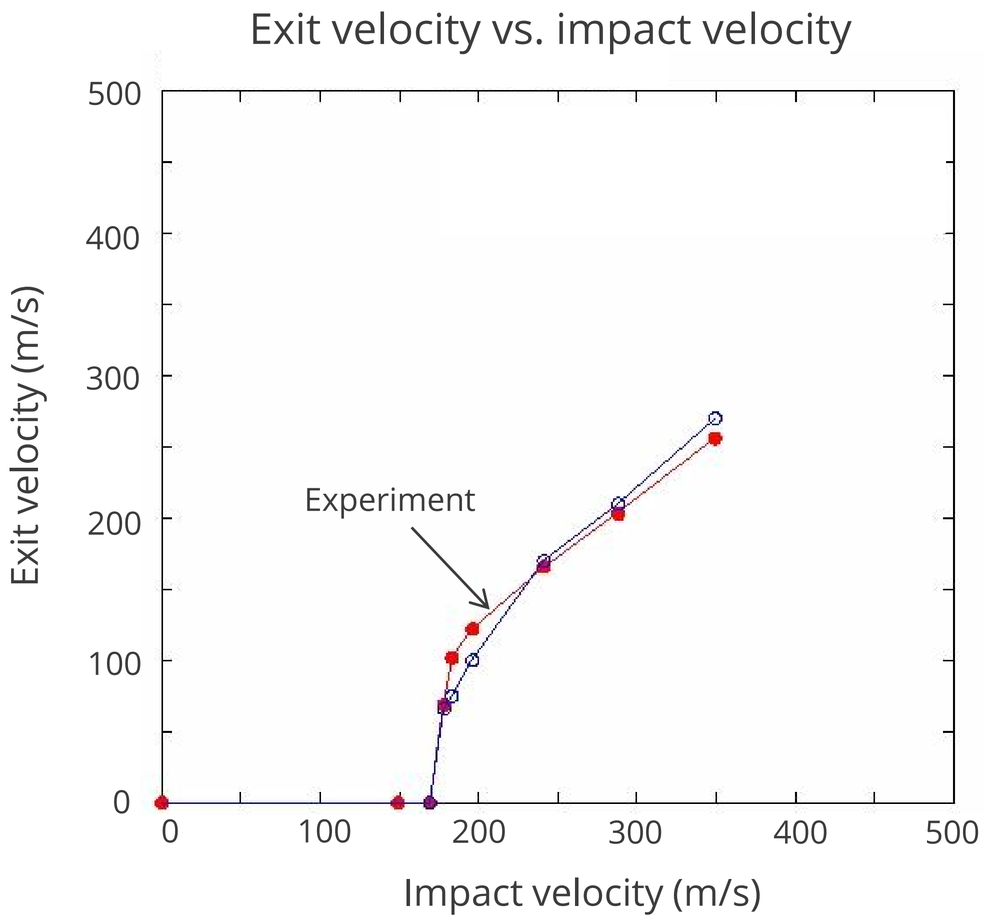


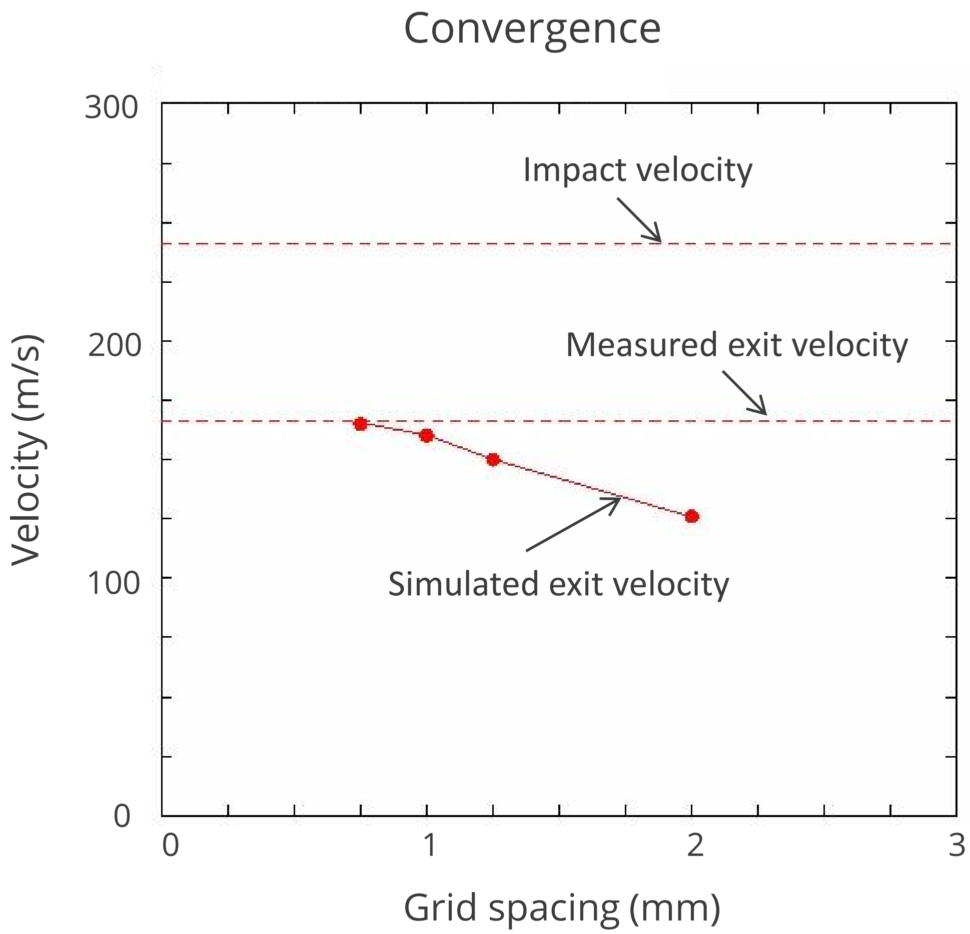


V = 246 m/s
Experiment

- Forrestal & Hanchak, Int. J. Impact Eng. (1999)

Blunt projectile vs. steel plate,ctd.

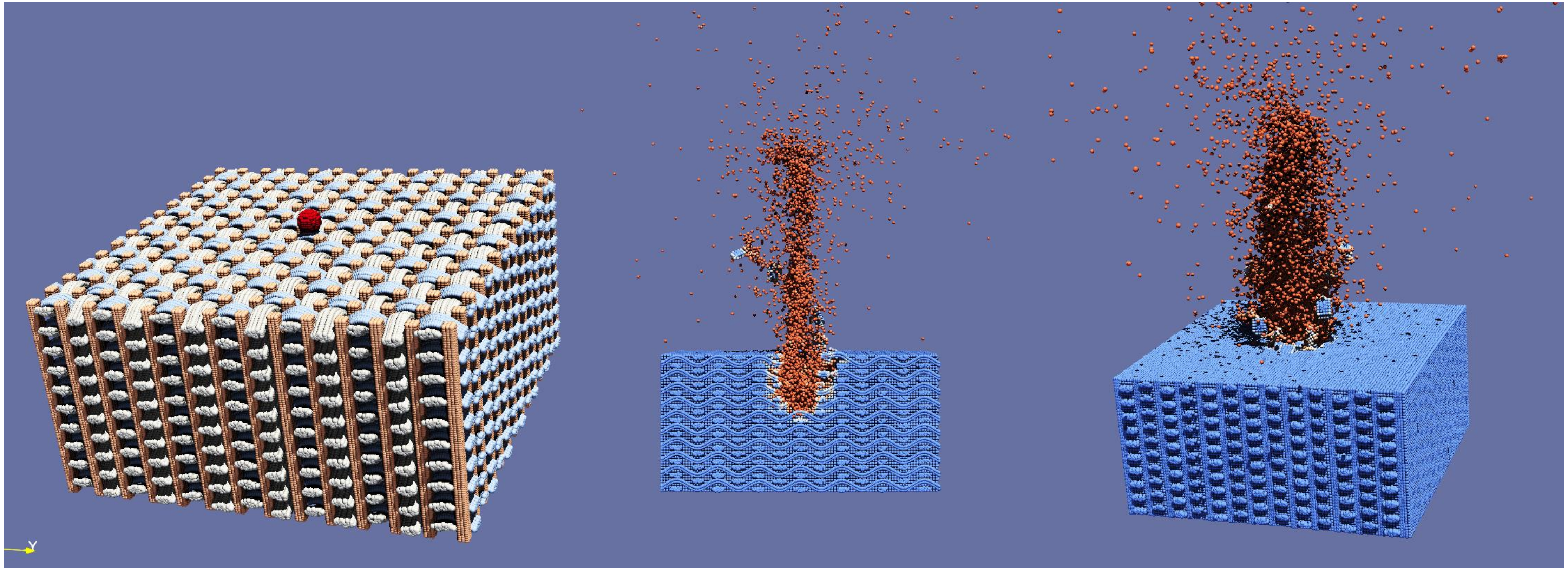




- Forrestal & Hanchak, Int. J. Impact Eng. (1999)

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

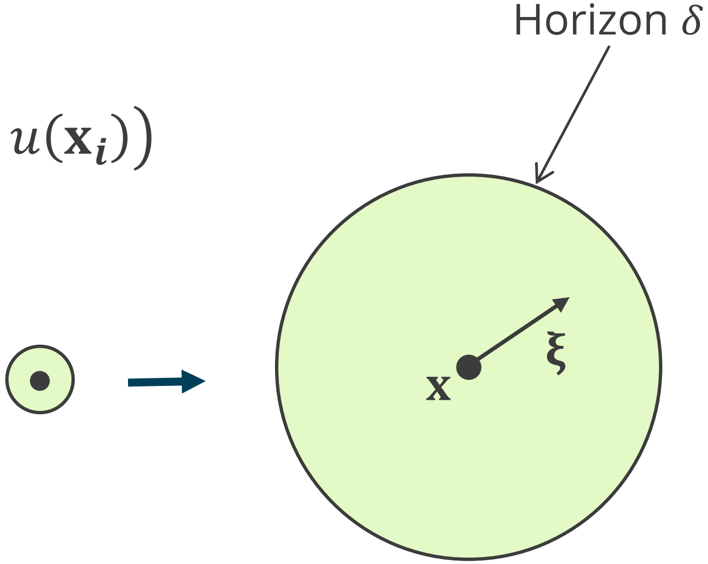
Local operator can be represented as nonlocal operator

- Sort of a converse to the previous result:
- We can approximate partial derivatives by peridynamic-type integrals that are then discretized.
  - Peridynamic differential operator*.
  - Example: Laplacian:

$$\nabla^2 u \approx \int_{\mathcal{H}_x} w(\boldsymbol{\xi})\big(u(\mathbf{x}+\boldsymbol{\xi}) - u(\mathbf{x})\big)|\boldsymbol{\xi}|^2 d\boldsymbol{\xi} \approx \sum_{\boldsymbol{k}} g_{\boldsymbol{ki}}\big(u(\mathbf{x}_{\boldsymbol{k}}) - u(\mathbf{x}_{\boldsymbol{i}})\big)$$

where the $g_{ki}$are weights that can vary with position.

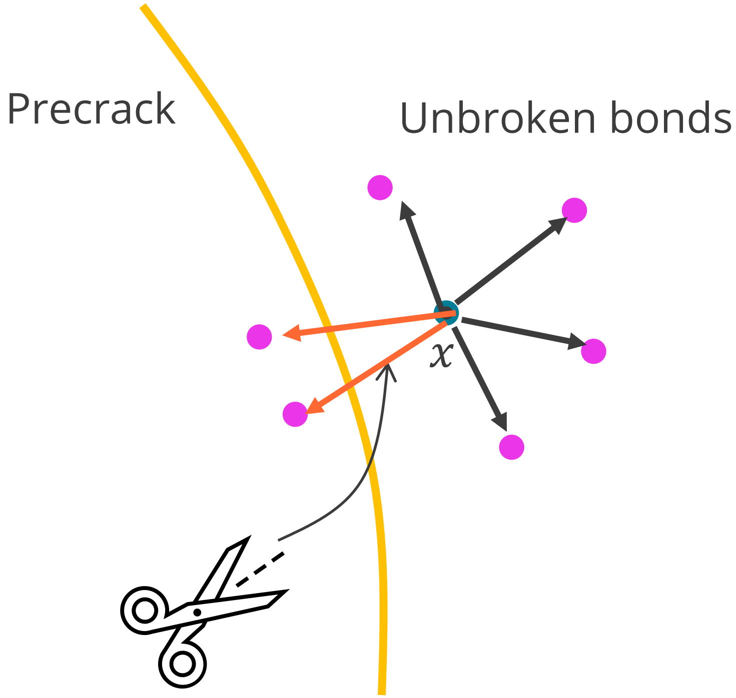
- Related to RKPM & other ideas, see ** for discussion.

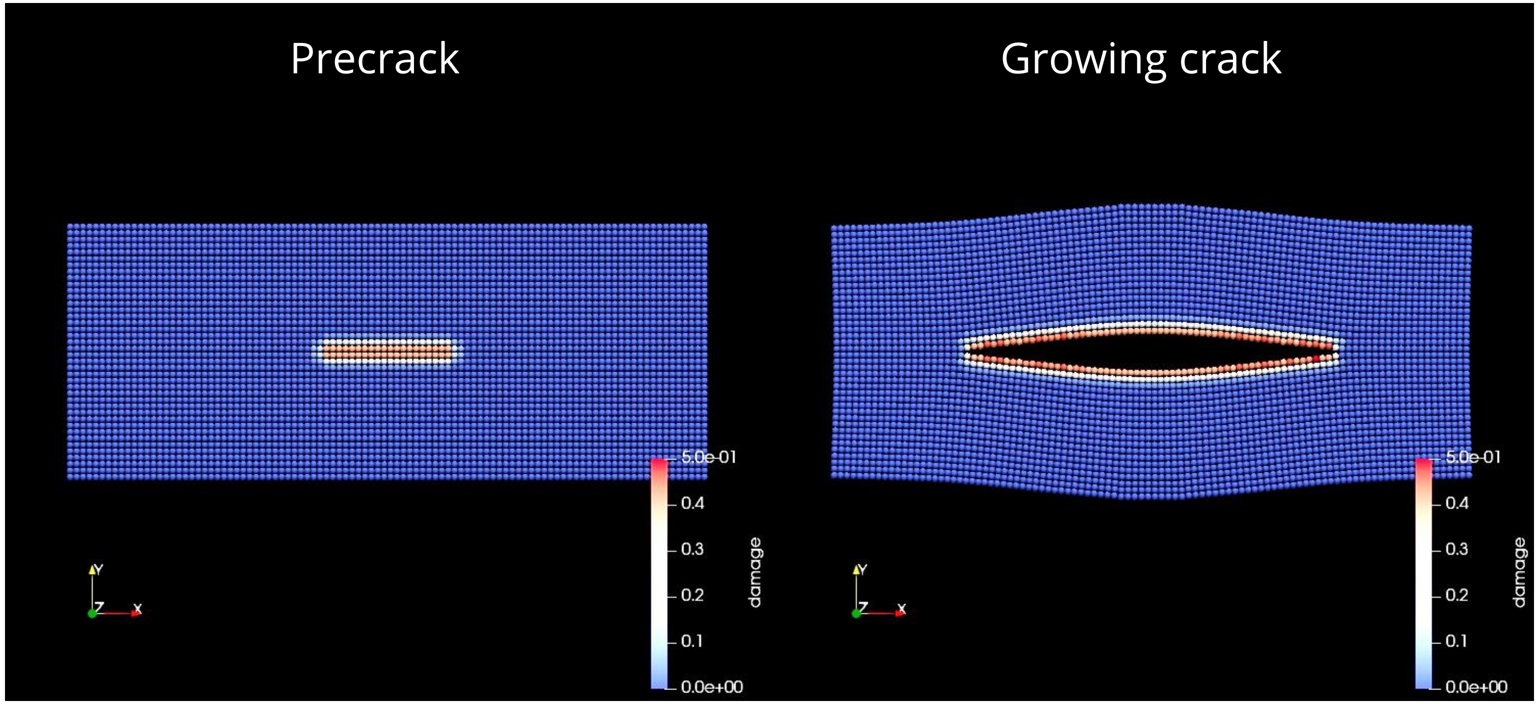


- * E. Madenci, A. Barut, and M. Futch, 2016. Peridynamic differential operator and its applications. *Computer Methods in Applied Mechanics and Engineering*, 304, pp.408-451..
- ** X. Kan, J. Yan, S. Li, and A. Zhang, 2021. On differences and comparisons of peridynamic differential operators and nonlocal differential operators. *Computational Mechanics*, 68(6), pp.1349-1367.

Precracks

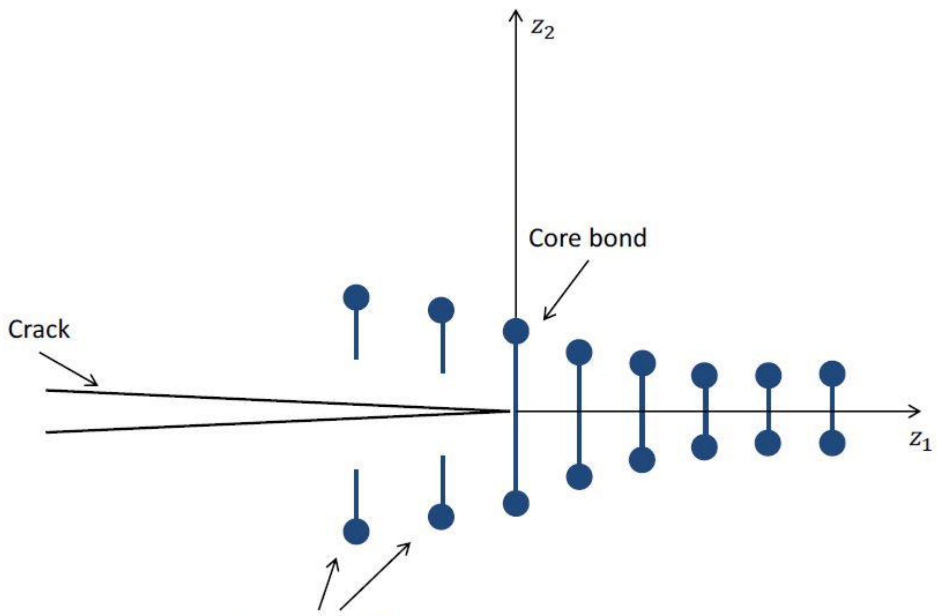
- How to create a pre-existing crack?
- Cut all the bonds across the surface where you want the crack.



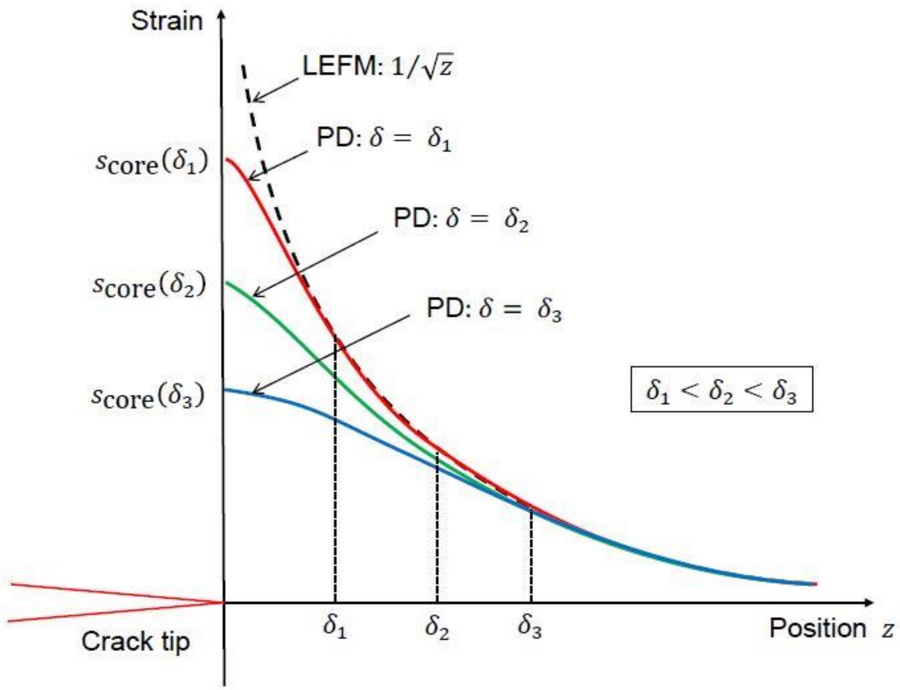


Colors show net damage
Displacements x100

What does a crack tip strain field look like?



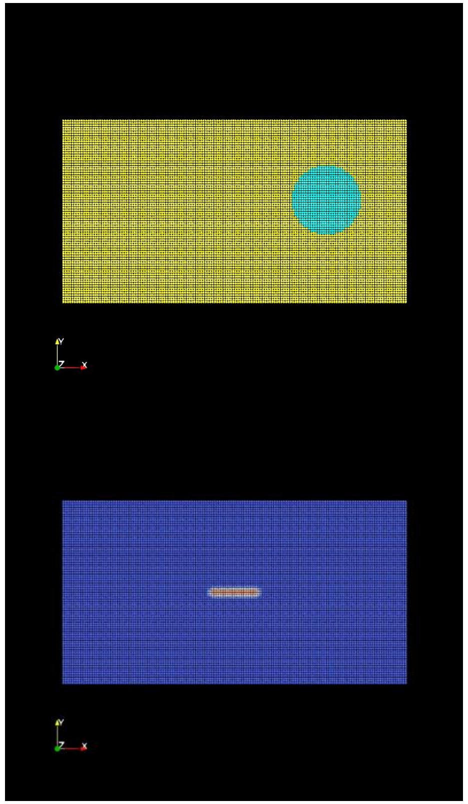
Bonds break as a crack approaches

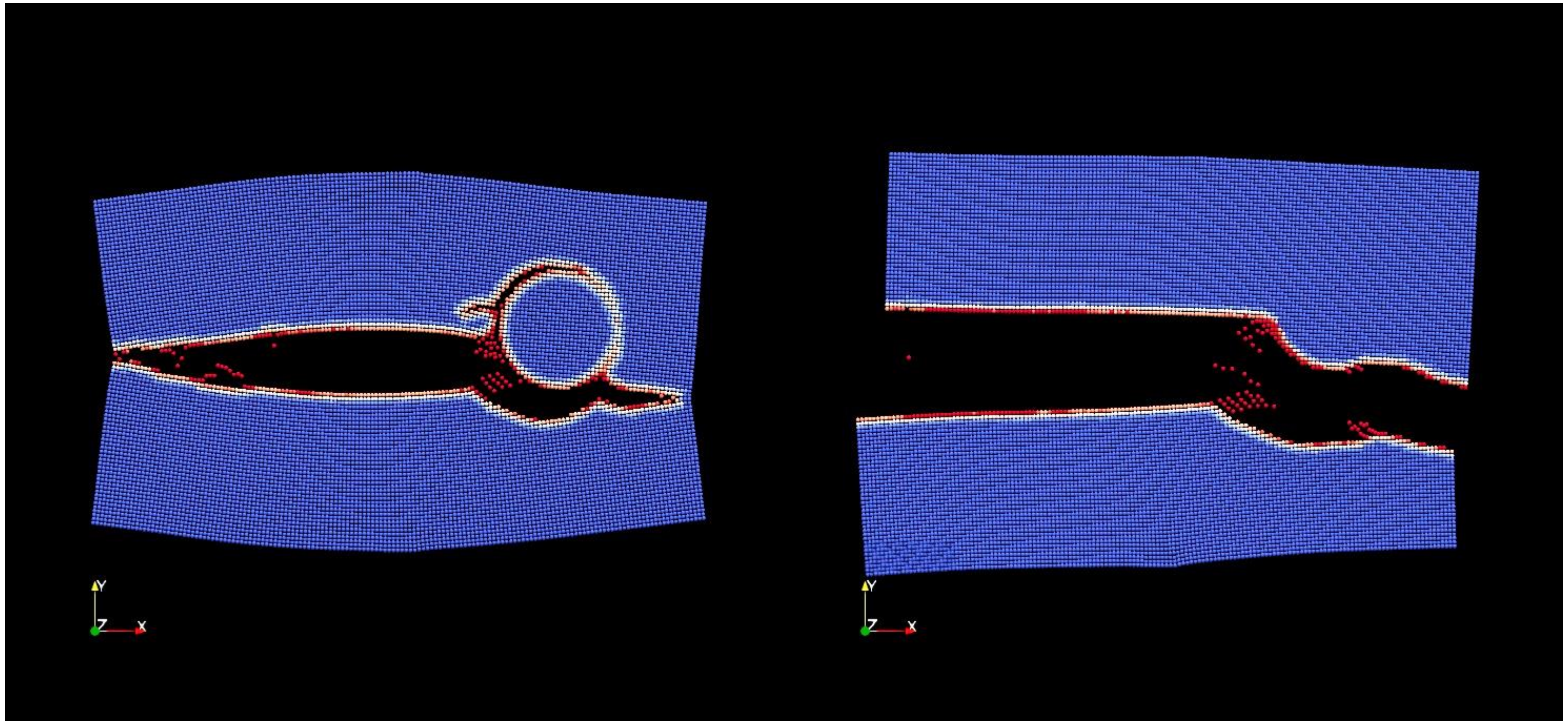


Strain approached LEFM solution away from a crack tip

Weak and strong interfaces

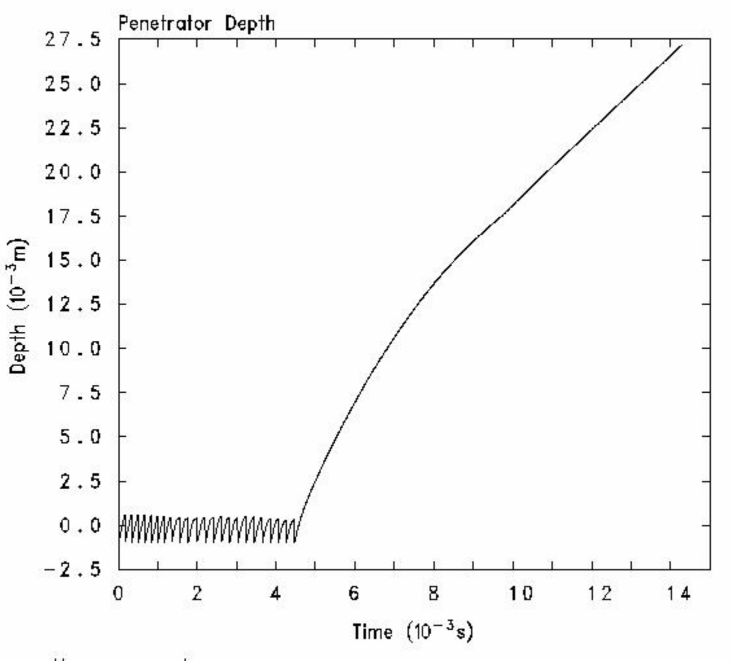
- Bonds from one material to another can be stronger or weaker than internal bonds.





Weak interface Strong interface

Accumulation of damage: Hammering on a block

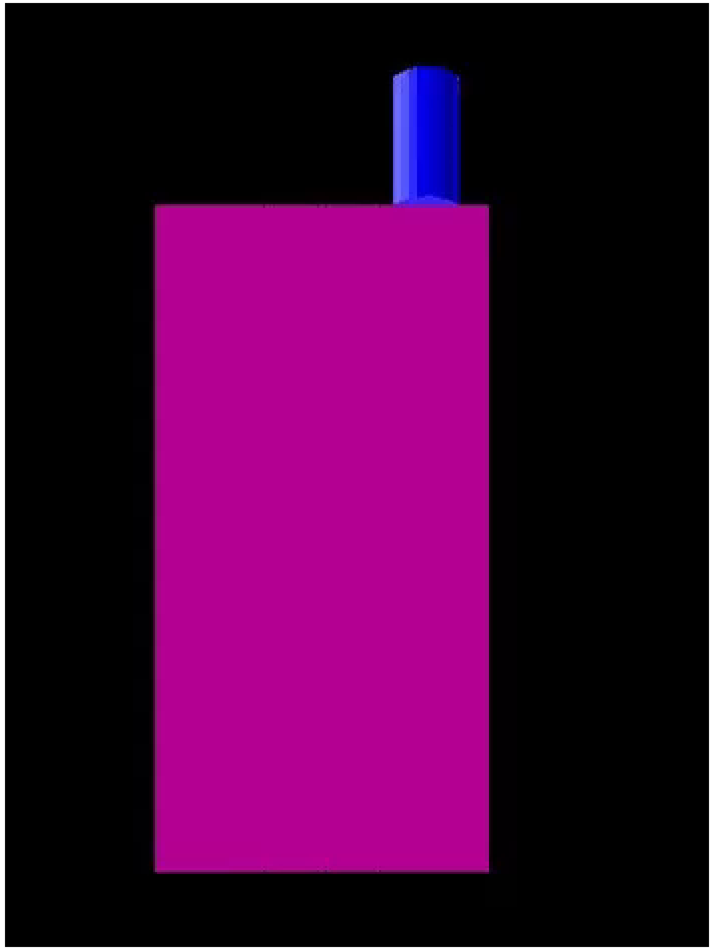


Penetration depth vs. time

Each peak is a strike.

Break through at 24 strikes.

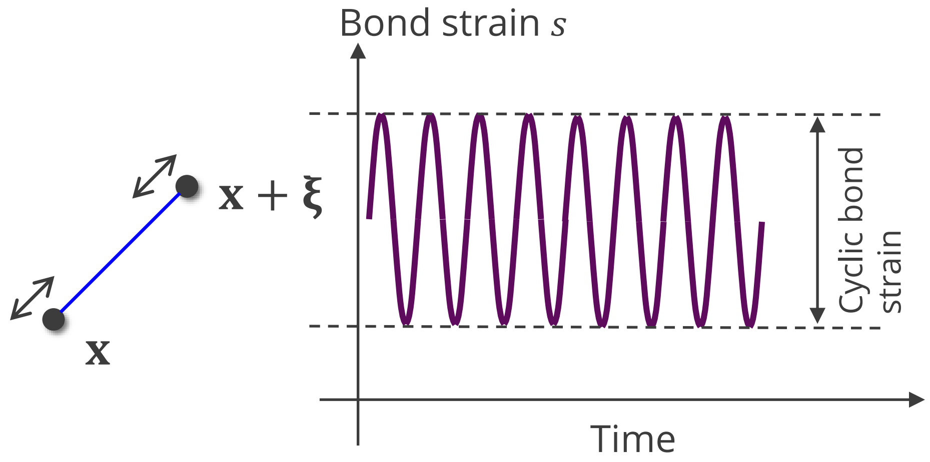
VIDEO

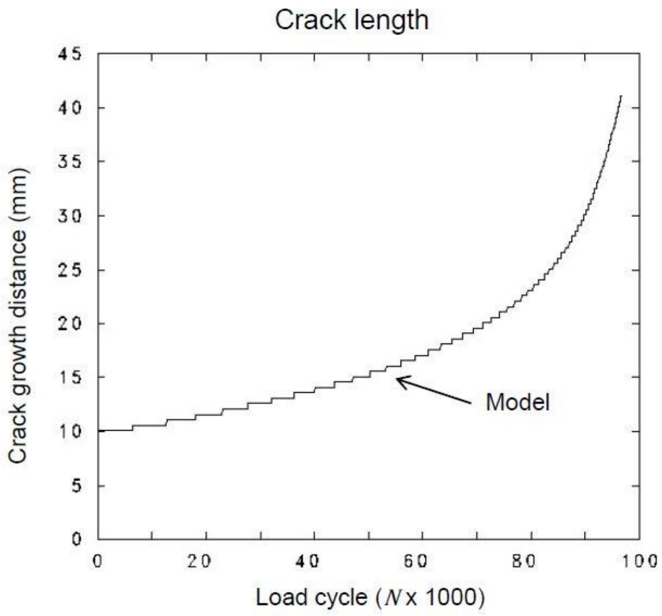


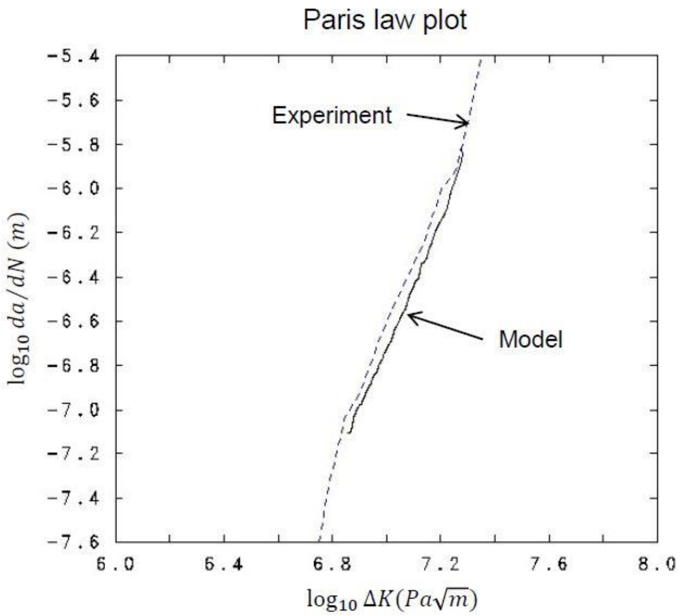
Colors show damage

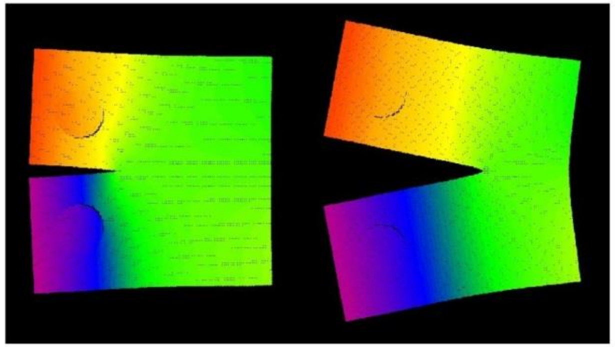
Special damage criteria: Fatigue

- Bond breakage criterion depends on cyclic loading in the bond and number of loading cycles.









Simulation of fatigue in an aluminum coupon
Colors show displacement (x100)

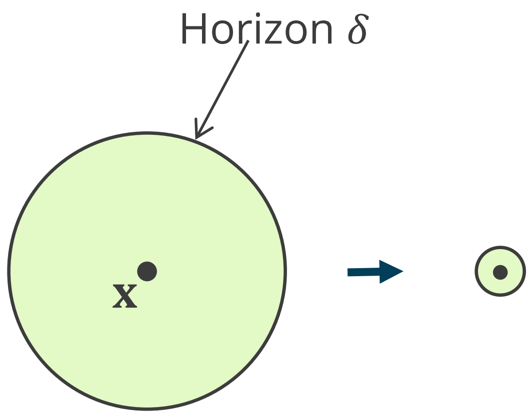
- Test data: T. Zhao, J. Zhang, and Y. Jiang. A study of fatigue crack growth of 7075-T651 aluminum alloy. *International Journal of Fatigue,* 30 (2008) 1169-1180.
- G. Zhang, et al., 2016. Validation of a peridynamic model for fatigue cracking. *Engineering Fracture Mechanics*, 162, pp.76-94.

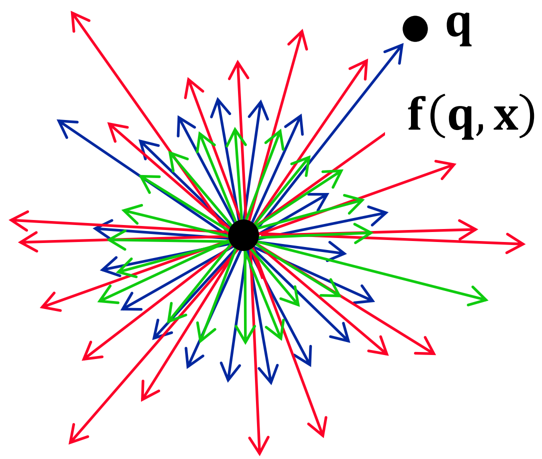
Peridynamics approaches classical theory as $\delta \to 0$

- In the above we let $h \to 0$ but δ was fixed.
- Now let $\delta \to 0$.
- Can show there is a tensor field $\boldsymbol{\sigma}$ such that

$$\lim_{\delta \to 0} \int_{\mathcal{H}} \mathbf{f}(\mathbf{q}, \mathbf{x}, t)\, d\mathbf{q} = \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t)$$

if $\boldsymbol{\sigma}$ is differentiable (i.e. not on a crack).





Bond forces have no required smoothness.
Big mess.

R.B. Lehoucq and SS, 2008. Force flux and the peridynamic stress tensor. *Journal of the Mechanics and Physics of Solids*, 56(4), pp.1566-1577.

Some good and bad features of peridynamics based on experience

- Good
  - Autonomous crack growth.
  - Simple meshless discretization and treatment of contact.
  - Allows long-range nanoscale forces.
    - Nonlocality provides opportunities in material modeling.
  - Post-failure meshless nodes act like classical particles.
  - Seems to interface well with AI & ML.
  - Can easily adapt material & damage models from the local theory.
- Bad
  - “Feels different” to users than traditional analysis methods (exception: LS-Dyna).
    - Boundary conditions are weird.
    - Need to adjust material properties from point to point.
  - Generally slower than FEM due to nonlocality.
    - Sometimes need a finer discretization than one would like to use.