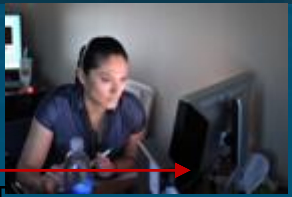
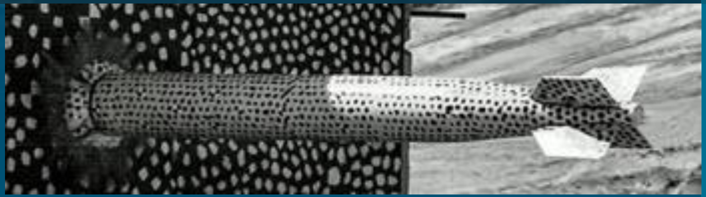
SAND2024-04870C

Climbing higher and digging deeper





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Stewart Silling

Quarter Century of Peridynamics
Tucson, AZ
April 25, 2024

SANDxxxx

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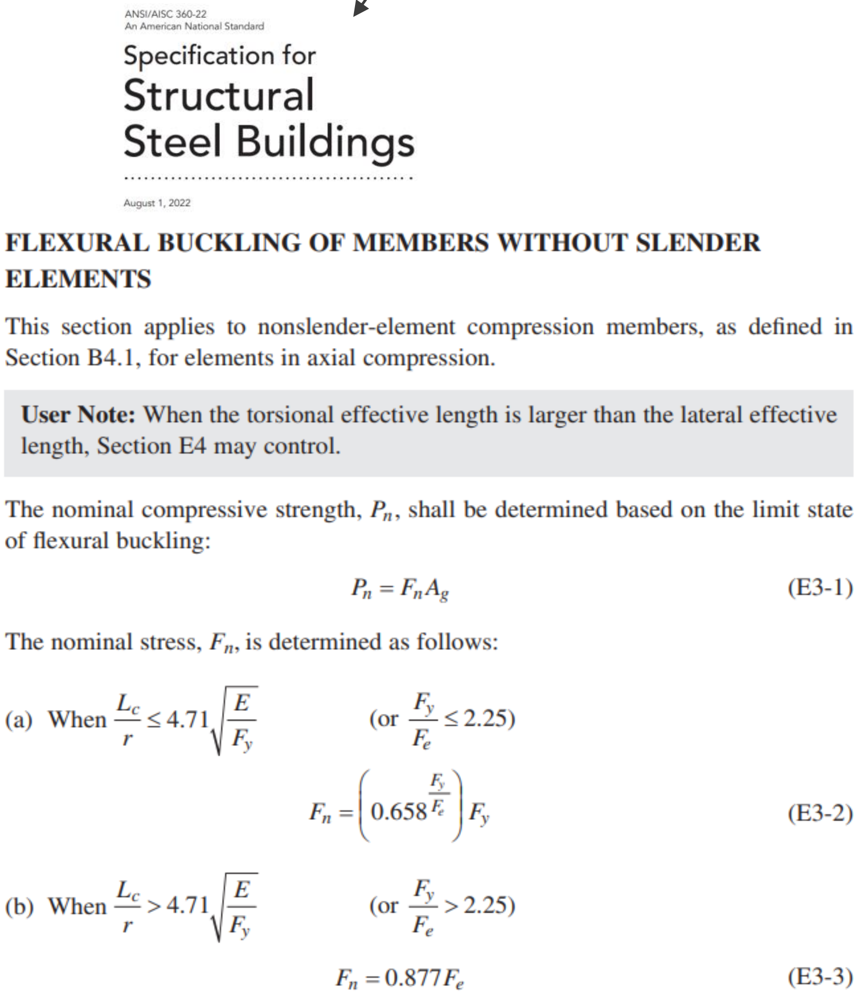
Outline: Get fired up about the future of peridynamics

- Mechanics is changing.
- Fundamental soundness of PD: What is known?.
- Where do we stand?
- Some areas for growth beyond fracture:
  - PD as a surrogate for complex systems.
  - Microstructure evolution.
  - PD as a way of getting reduced order models.
  - Digital twins.
  - Additive manufacturing.
  - Digital engineering.
  - Effective use of full field test data (e.g. Digital Image Correlation)
  - Social systems
  - Nanoscale and biological materials
  - Multiphysics
  - Artificial intelligence and machine learning

Why are some “simple” things so hard to model on a computer?

- To design **this**, engineers use **this**. Not **this**.

www.directorsteelstructure.com



ANSI/AISC 360-22
An American National Standard

Specification for
Structural
Steel Buildings

August 1, 2022

FLEXURAL BUCKLING OF MEMBERS WITHOUT SLENDER ELEMENTS

This section applies to nonslender-element compression members, as defined in Section B4.1, for elements in axial compression.

User Note: When the torsional effective length is larger than the lateral effective length, Section E4 may control.

The nominal compressive strength, P_n, shall be determined based on the limit state of flexural buckling:

$$P_n = F_n A_g \quad \text{(E3-1)}$$

The nominal stress, F_n, is determined as follows:

(a) When $\frac{L_c}{r} \leq 4.71\sqrt{\frac{E}{F_y}}$ (or $\frac{F_y}{F_e} \leq 2.25$)

$$F_n = \left(0.658^{\frac{F_y}{F_e}}\right) F_y \quad \text{(E3-2)}$$

(b) When $\frac{L_c}{r} > 4.71\sqrt{\frac{E}{F_y}}$ (or $\frac{F_y}{F_e} > 2.25$)

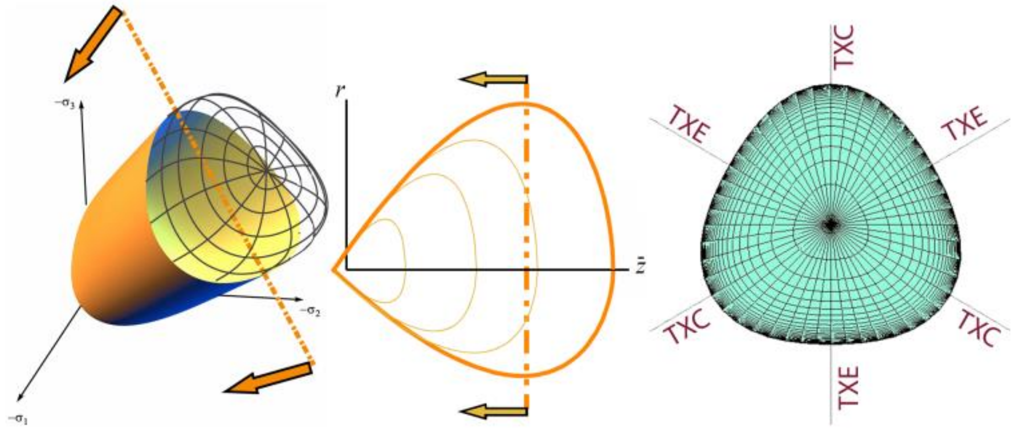
$$F_n = 0.877 F_e \quad \text{(E3-3)}$$

Trinity supercomputer, Los Alamos National Laboratory
https://deixismagazine.org

McDonald’s, Los Alamos NM
Hard to get away from Oppy up there

Mechanics is changing

- Research 60 years ago:
  - Cauchy's equations (and assumptions) were treated as fact.
    - Fracture was treated as a separate science.
  - Most research focused on:
    - Solution methods.
    - Material models.
      - Emphasis on complete generality.
  - "Mature field"
- Now:
  - "Discover" new field equations.
  - Reduced order modeling.
  - Involve artificial intelligence.
  - Directly incorporate full-field test data.



Yield surface in the Kayenta* material model.
Kayenta uses 67 input parameters, 50 internal state variables.

- *R.M. Brannon et al., KAYENTA: Theory and User's Guide, SAND2015-0803 (revised 2015)
- S.H. Rudy et al., Data-driven discovery of partial differential equations. *Science advances*. (2017).

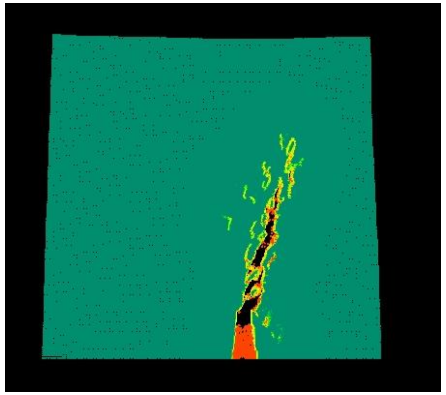
What does peridynamics seek to accomplish?

- We treat fracture and long-range forces within the basic field equations.
  - …while satisfying all the requirements of classical mechanics.

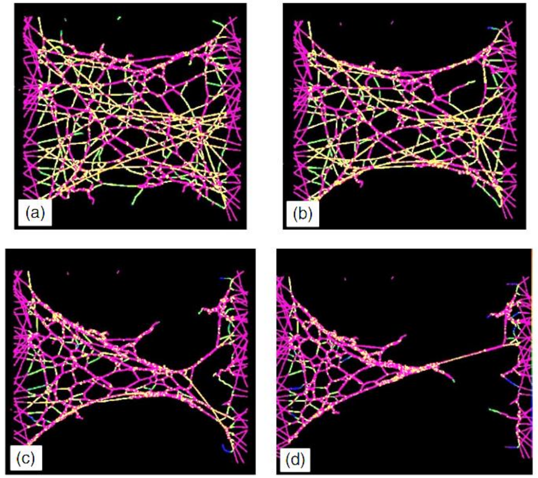
Why do this?

- Autonomous fracture
  - Freedom from special techniques for discontinuities implemented at the discretized level.
- Consistent way to include nanoscale forces.
- Incorporate material length scales without representing them explicitly.

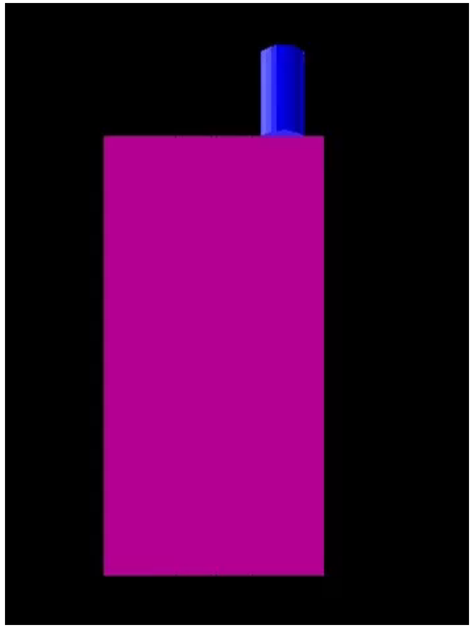
VIDEO



Seamless transition from continuous to discontinuous deformation



Fracture of nanofiber network held together by Van der Waals forces*.



Multiple impacts on a block
Colors show damage

*F. Bobaru, *Modelling and Simulation in Materials Science and Engineering* (2007).

Fundamental mechanics

- There is no doubt that PD is consistent with classical mechanics.
- Linear momentum balance is always satisfied.
- Angular momentum balance & objectivity require restrictions on the material model.
- Galilean invariance is always satisfied.
- Energy balance is satisfied for elastic materials.
- First law of thermodynamics is expressed in nonlocal form.
- Second law leads to restrictions on the material model.

- S.S. & R. B. Lehoucq RB. Peridynamic theory of solid mechanics. *Advances in applied mechanics*. (2010)

Relation to PDE theory

- Convergence of the field equations as $\delta \to 0$ has been shown in many cases (if the deformation is smooth enough).

$$\int \mathbf{f} \to \nabla \cdot \sigma$$

  - Convergence of solutions has also been shown in some important cases: $u_{PD} \to u_{Local}$
  - Elastic PD models converge to conventional stress-strain material models.
  - Results include aspects of nonlocal boundary conditions.

- Well-posedness with growing fractures has been shown in some important cases.

- Peridynamic differential operator further establishes close connection between PD and PDEs.

- Relation to higher-order PDEs has been studied.

- T. Mengesha & Q. Du*, Journal of Elasticity*. (2014).
- E. Emmrich & O. Weckner, *Communications in Mathematical Sciences* (2007).
- Q. Du et al., M. Gunzburger, *Journal of Elasticity* (2013).
- Q. Du & K. Zhou, *ESAIM: Mathematical Modelling and Numerical Analysis*. (2011).
- J. Scott, thesis, University of Tennessee (2020).
- T. Mengesha & J. Scott. *Journal of Mathematical Analysis and Applications*. (2020).
- M. Foss, P. Radu, & Y. Yu, *Journal of Peridynamics and Nonlocal Modeling*. (2023).
- R. Lipton*, Journal of Elasticity*. (2014).
- E, Madenci, A. Barut, & M. Futch, *CMAME* (2016).
- B. Aksoylu & T. Mengesha T. *Numerical functional analysis and optimization*. (2010).
- M. D'Elia & Y. Yu, *Research in Mathematics of Materials Science* (2022).
- P. Seleson, M.L. Parks, M.L. Gunzburger, & R. B. Lehoucq, *Multiscale Modeling & Simulation* (2009).

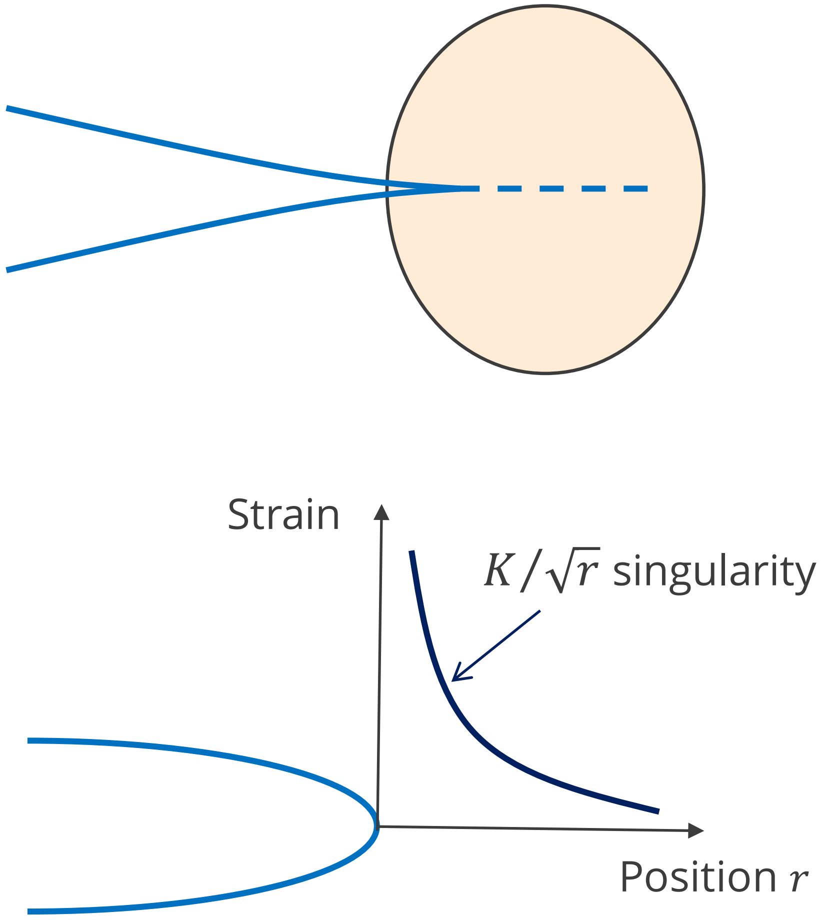
Numerical discretizations and solvers

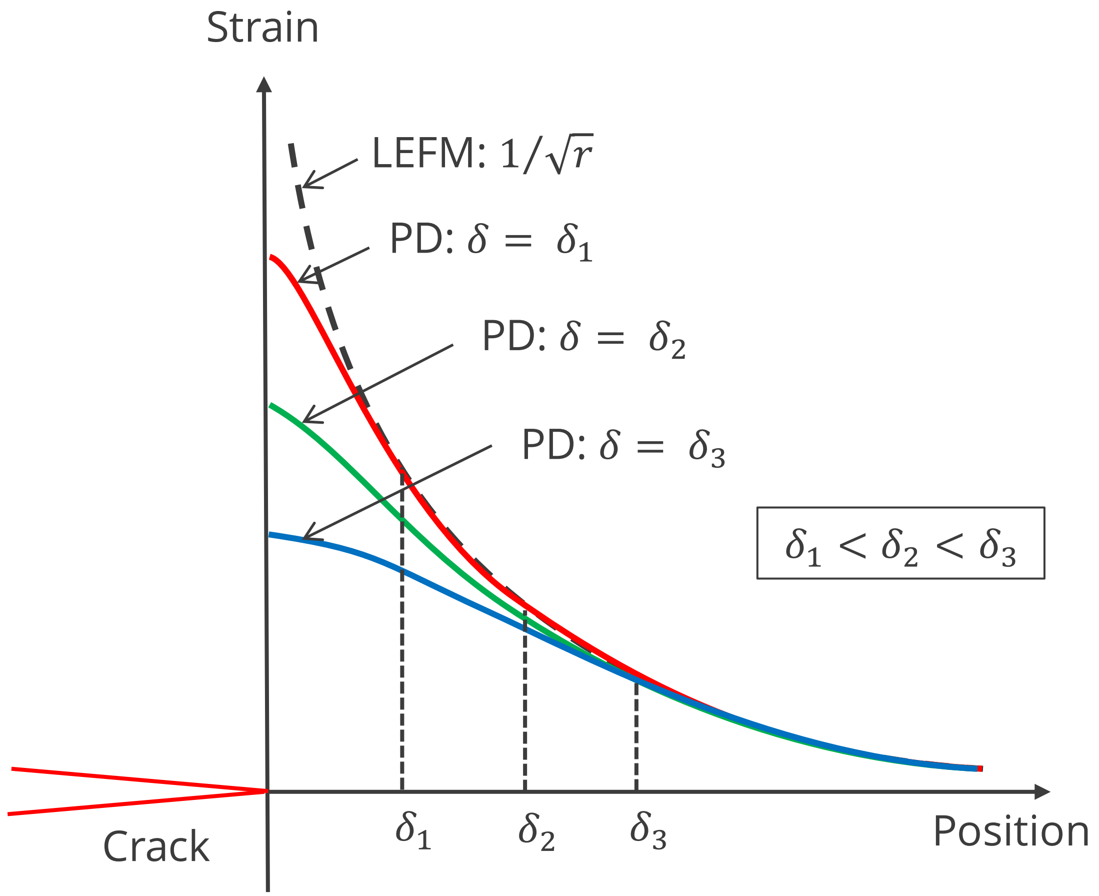
- Midpoint quadrature has some great properties but doesn't converge very well.
  - The discretized model **exactly** satisfies the PD continuum equations (although it only approximates the continuum).
  - Doesn't converge to the PDEs in the expected way (fails asymptotic convergence).
  - Very easy to program and implement fracture models.
  - Sometimes creates discontinuities abnormally.
- Newer discretizations avoid some of these problems and have good ways of treating boundary conditions.
- Explicit dynamics works very well.
- Implicit solvers are available (including Peridigm).
- Large scale parallelism, GPUs, spectral methods, other methods can greatly speed up numerical solutions.

- S. Jafarzadeh et al., *CMAME* (2022).
- A. Alali & N. Albin, *Journal of Peridynamics and Nonlocal Modeling* (2020).
- Y. Yu, H. You, & N. Trask, *CMAME* (2021).
- P. K. Jha & R. Lipton, *CMAME* (2019).
- X. & Q. Du,Tian X, Du Q. *SIAM Journal on Numerical Analysis* (2014).
- S. Reeve & P. Seleson, "CabanaPD", Oak Ridge National Laboratory (2022).

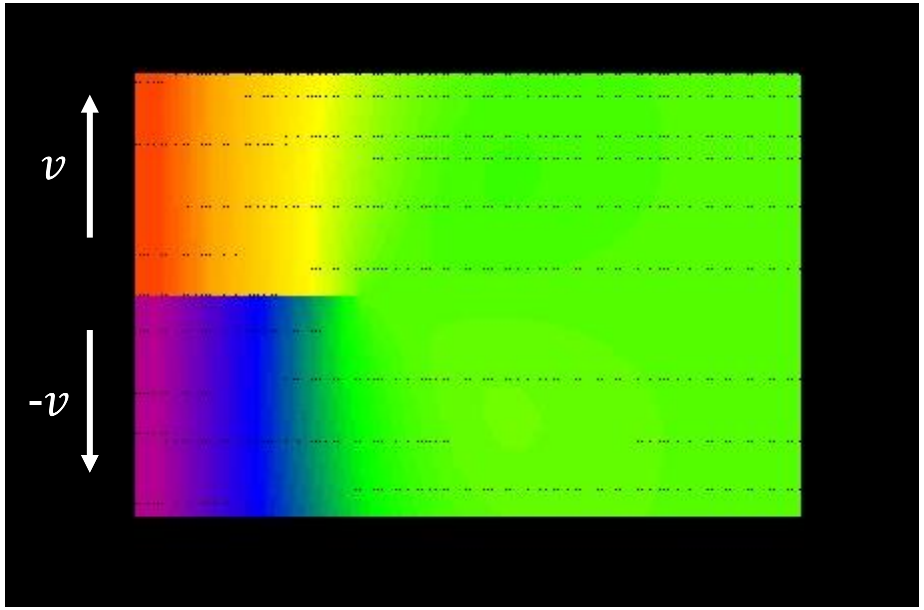
Fracture: PD vs. linear elastic fracture mechanics (LEFM)

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

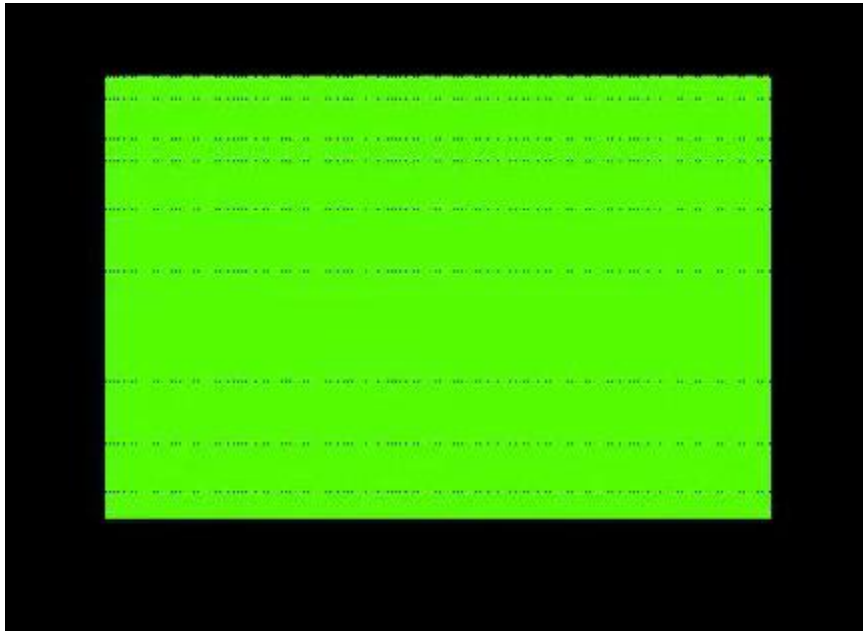




Fracture: Simulated PD crack growth in a plate: Mode I



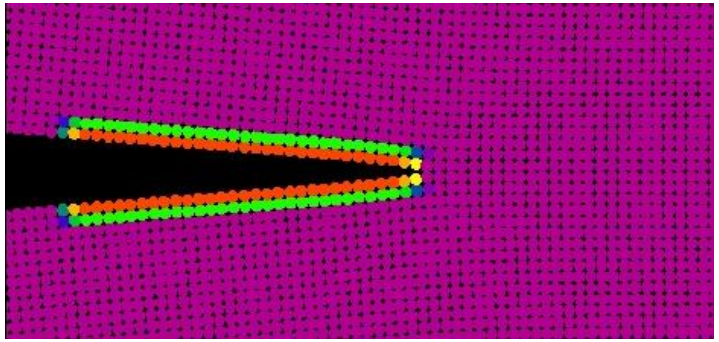
VIDEO



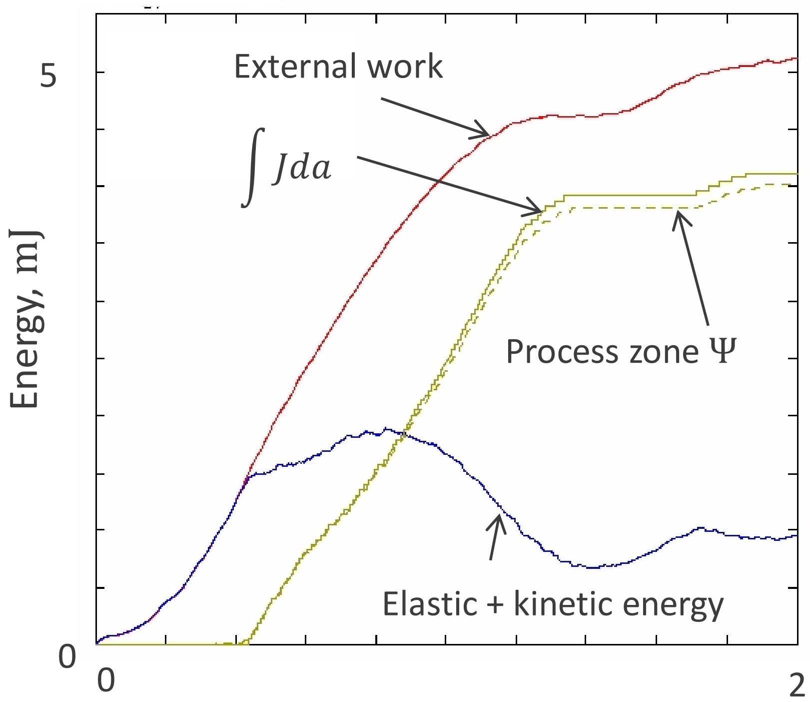
Colors show vertical displacement

Fracture: Energy balance agrees with LEFM, Griffith theory

Work done through boundaries closely matches current value of stored energy + kinetic energy + dissipated energy



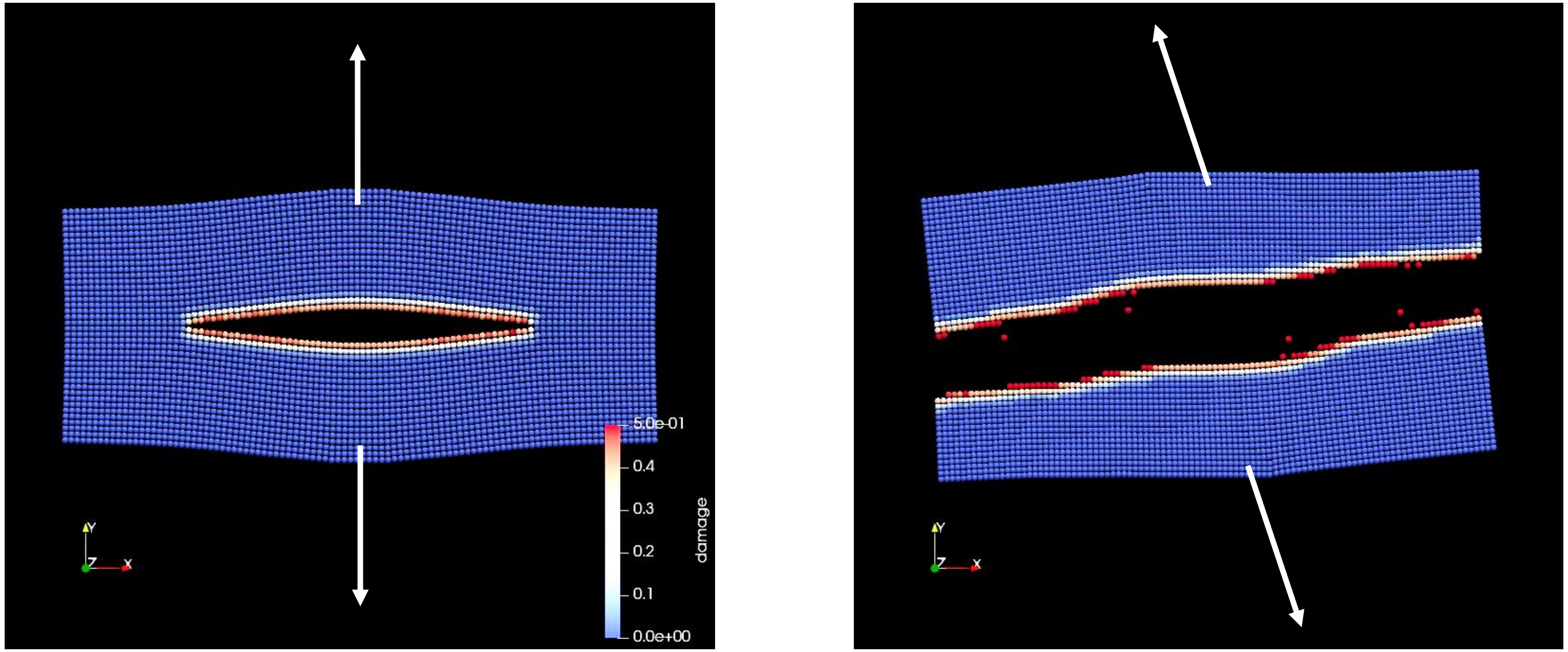
Colors show energy dissipated energy at each node



- 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)
- R.P.Lipton, R.B. Lehoucq, & P.K. Jha*, Journal of Peridynamics and Nonlocal Modeling* (2019).

Mixed mode fracture

- Crack growth direction changes continuously with load direction (good).

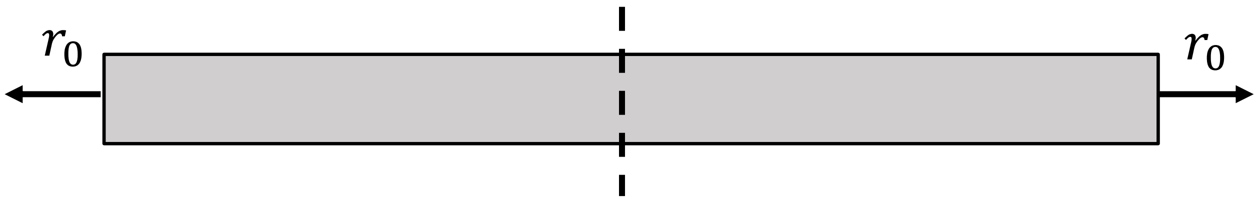


Colors show net damage
Displacements x100

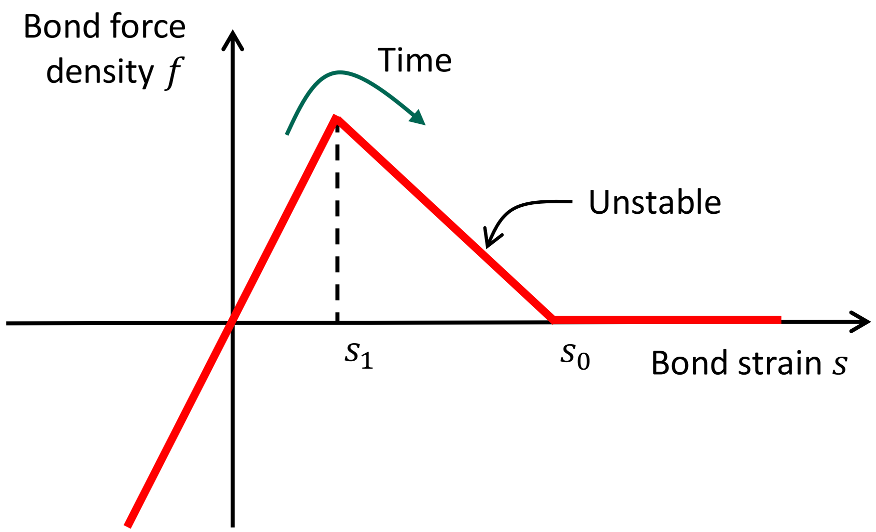
Where do we stand?

Crack nucleation as an outcome of material instability

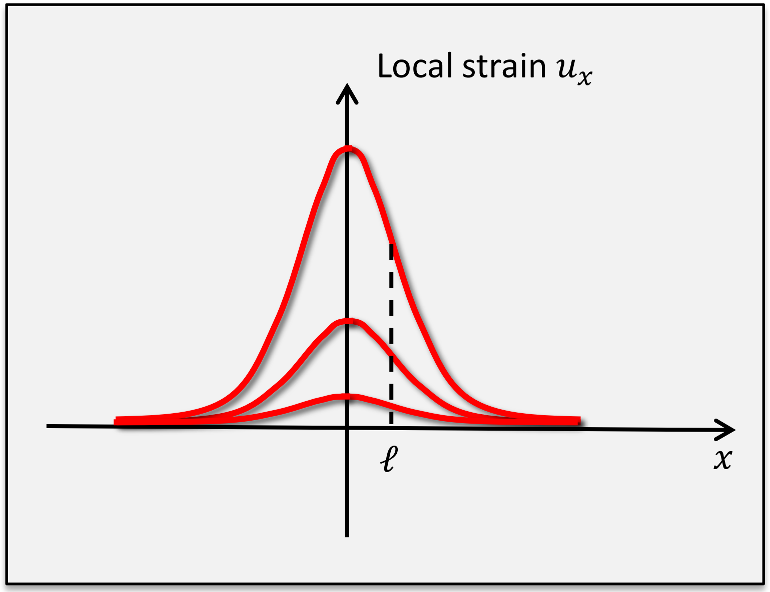
- A weak spot opens up as a bar is stretched at a constant strain rate.
- Instability comes from a nonconvex elastic material model or from a bond damage variable.



Nonmonotonic material model



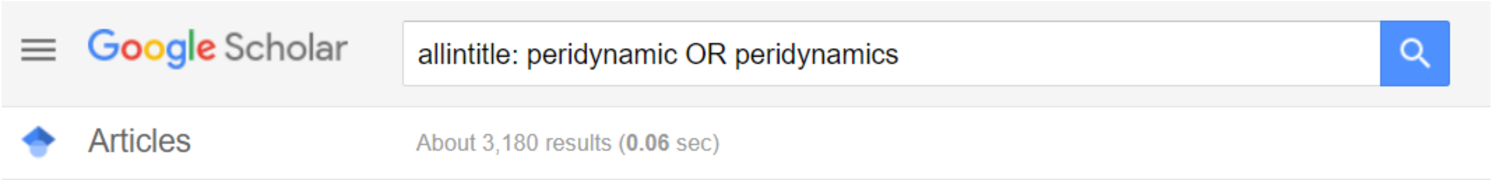
Evolution of strain



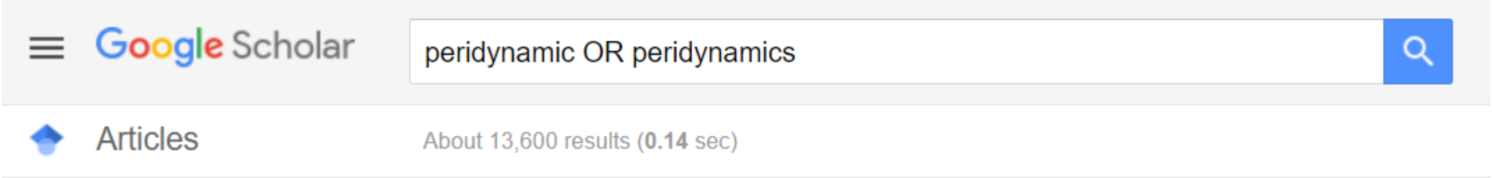
- R.P Lipton, R.B. Lehoucq & P.K. Jha. *Journal of Peridynamics and Nonlocal Modeling* (2019).
- SS, *Journal of Peridynamics and Nonlocal Modeling* (2021).

Are these ideas accepted?

- Number of papers with peridynamic(s) in the title = 3180



- Number of papers with peridynamic(s) anywhere = 13,600

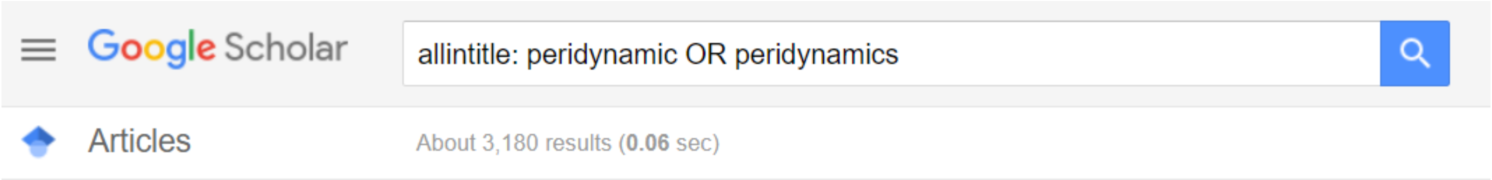


- We're in the conversation.

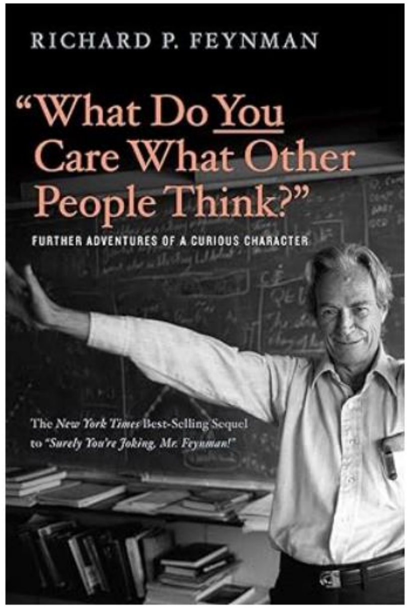
- BTW: Number of papers with XFEM or "extended finite element" in the title: _____?_____

Are these ideas accepted?

- Number of papers with peridynamic(s) in the title = 3180



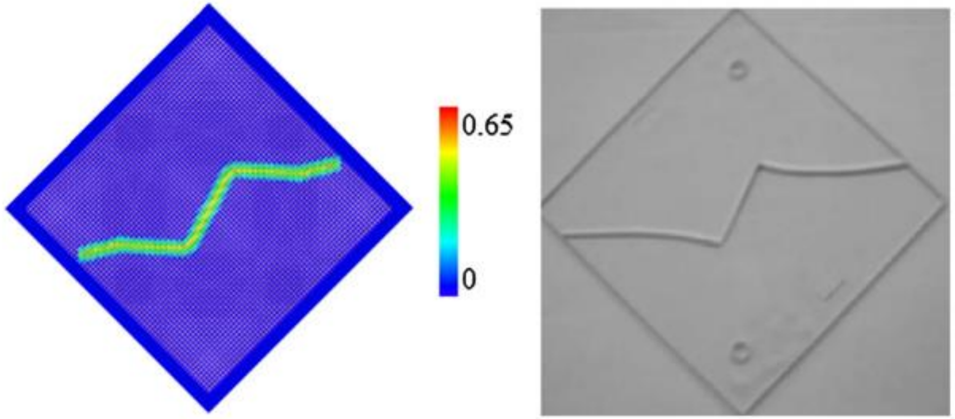
- Number of papers with XFEM or “extended finite element” in the title: 174



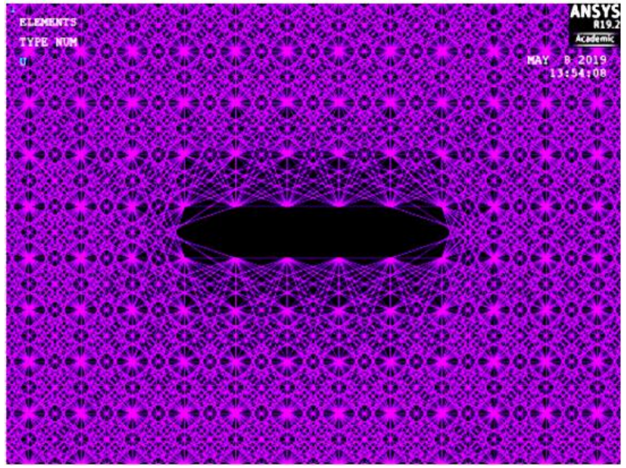
Autobiographical book by a Nobel Prize winner.
Great title!

Peridynamics in commercial codes

- Abaqus: Peridynamic bond interactions available as a User Element Library (UEL).
- LS-Dyna: Available in the production code using the Discontinuous Galerkin method.
- ANSYS standard: New interface with FEM soon to be available using PDDO & dual-horizon PD as a transition region.



Angled crack growth simulation with PD in Abaqus*

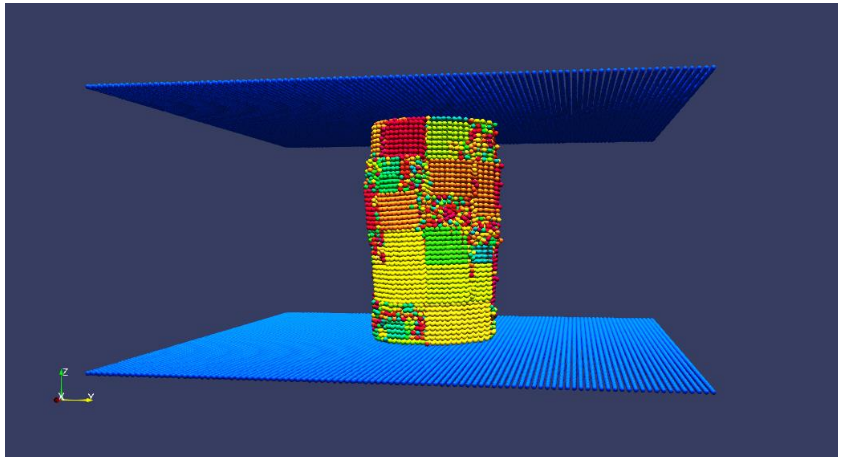


Standard ANSYS model of a notched orthotropic plate**

- * X.Huang, et al, *Engineering Fracture Mechanics*, (2019)
- B. Ren, C. T. Wu, and E. Askari, *International Journal of Impact Engineering* (2017)
- E. Madenci, P. Roy, and D. Behera, Coupling of Bond-Based Peridynamics with Finite Elements in ANSYS. In *Advances in Peridynamics* (2022).
- **C. Diyaroglu, E. Madenci, and N. Phan, *Composite Structures* (2019).

Some technical areas for exploration in PD fracture modeling

- Not clear how to define a damage model that allows both K_Ic and K_IIc to be specified independently.
- How does the damage model affect the predicted crack growth?
- How do free surface and interfaces affect cracks in PD?
- Does the bond breakage concept need updating?
- How to treat post-failure behavior?
- How to implement ductile failure criteria?
- Elastic stability and convexity.



PD simulation of a drop weight test on a rock sample
How to treat recompression after fracture?

Building trust in PD fracture modeling

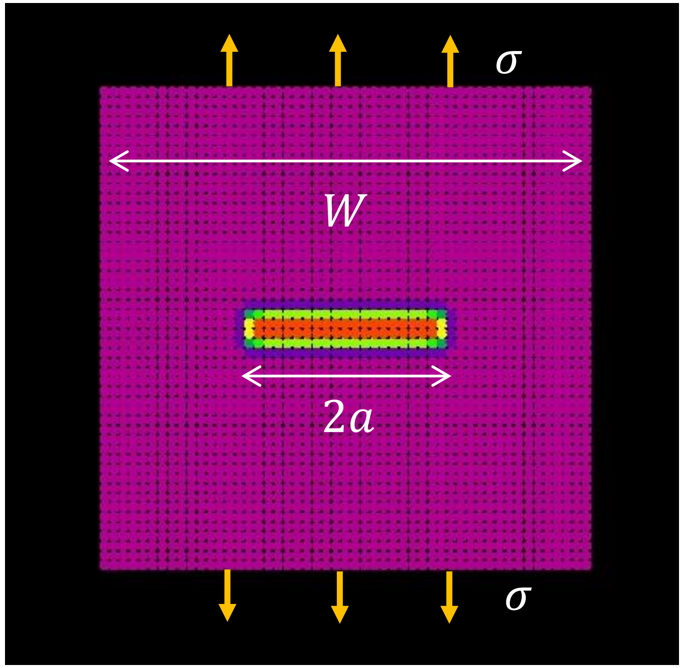
- Engineers need to trust the methods they use – not the same as accuracy.
- Need confidence they can:
  - Set up and run a model without a lot of special fixes.
  - Interpret the results and present them to others.
  - Get reasonable answers.
  - Results are not super-sensitive to discretization, other details.
- We're not quite there yet with PD.
  - Need to get it into the hands of end users.
  - Need to make its use more automated.
  - Need to build a set of test problems for training.

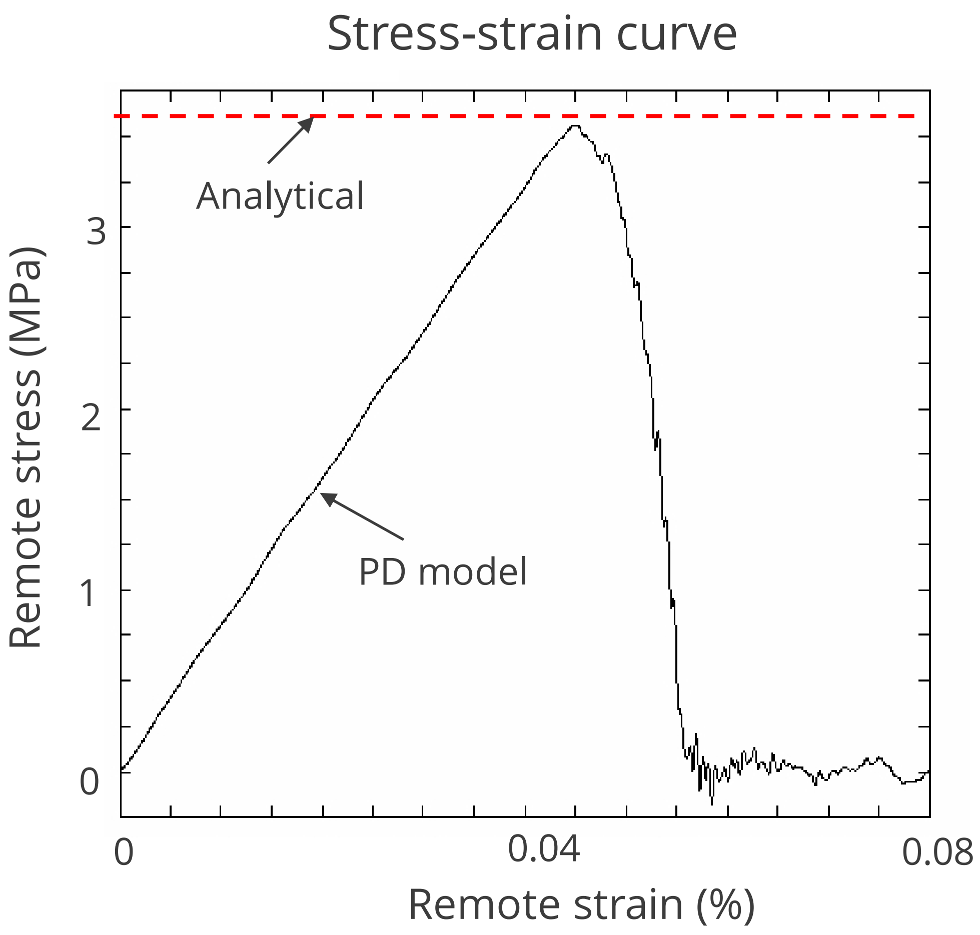
Example of what helps build trust: Classical fracture problem

- 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.

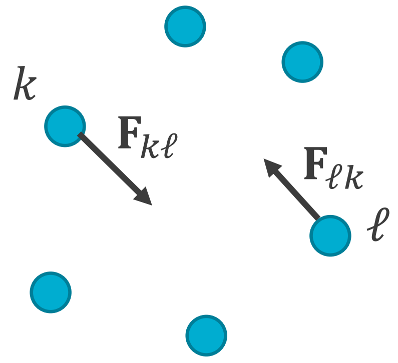




Why PD is the right way to model the real world

- Consider a set of discrete particles that exert forces $\mathbf{F}_{k\ell}(t)$ on each other,

$$\mathbf{F}_{\ell k}(t) = -\mathbf{F}_{k\ell}(t).$$



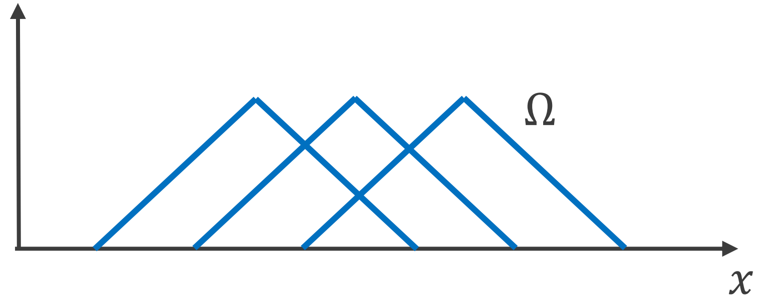
- Particles are subjected to external forces $\mathbf{B}_k(t)$.
- The particles obey Newton's second law,

$$M_k \ddot{\mathbf{u}}_k(t) = \sum_{\ell} \mathbf{F}_{k\ell}(t) + \mathbf{B}_k(t).$$

- Define smoothing functions $\Omega(\mathbf{x}, \cdot)$ normalized such that

$$\int \Omega(\mathbf{x}, \mathbf{p})\, \mathrm{d}\mathbf{x} = 1 \qquad \forall \mathbf{p}.$$

Center of smoothing function → $\mathbf{x}$; Atom position → $\mathbf{p}$



- This derivation: SS, Chapter 1 in *Peridynamic Modeling, Numerical Techniques, & Applications*, E. Oterkus, ed., Elsevier (2021).
- Statistical physics derivation: R. B. Lehoucq & M. P. Sears, *Physical Review E* (2011).

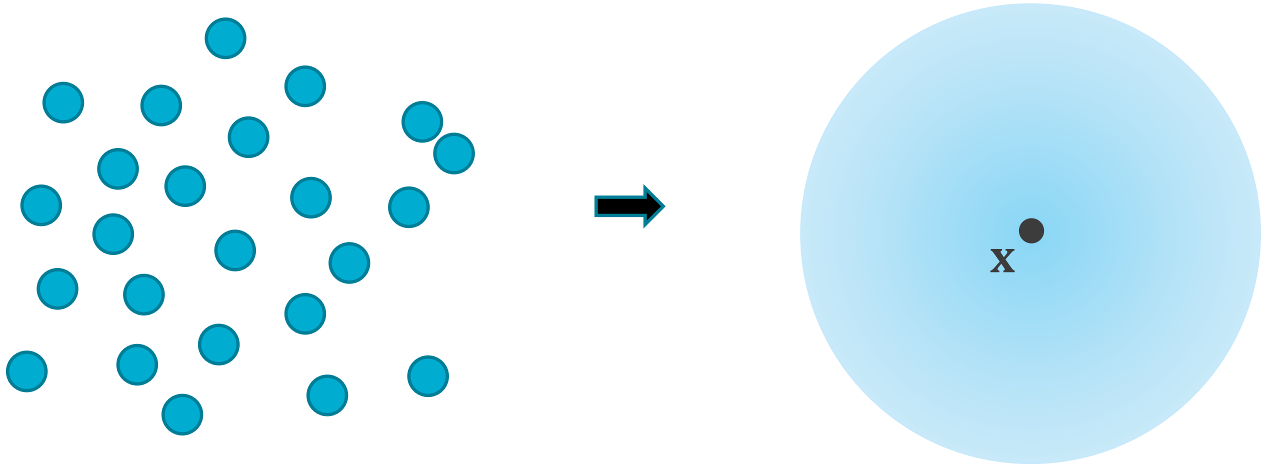
Continuous density, external force, and displacement

- Define the smoothed mass density and body force density fields by

$$\rho(\mathbf{x}) = \sum_k \Omega(\mathbf{x}, \mathbf{x}_k) M_k, \qquad \mathbf{b}(\mathbf{x}, t) = \sum_k \Omega(\mathbf{x}, \mathbf{x}_k) \mathbf{B}_k(t).$$

- Define the smoothed displacement field by

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x})} \sum_k \Omega(\mathbf{x}, \mathbf{x}_k) M_k \mathbf{u}_k(t).$$



Atoms

Each $\mathbf{u}(\mathbf{x})$ represents a weighted average of atomic displacements

Smoothed displacements obey the PD equation of motion

- Combine all of the above, find

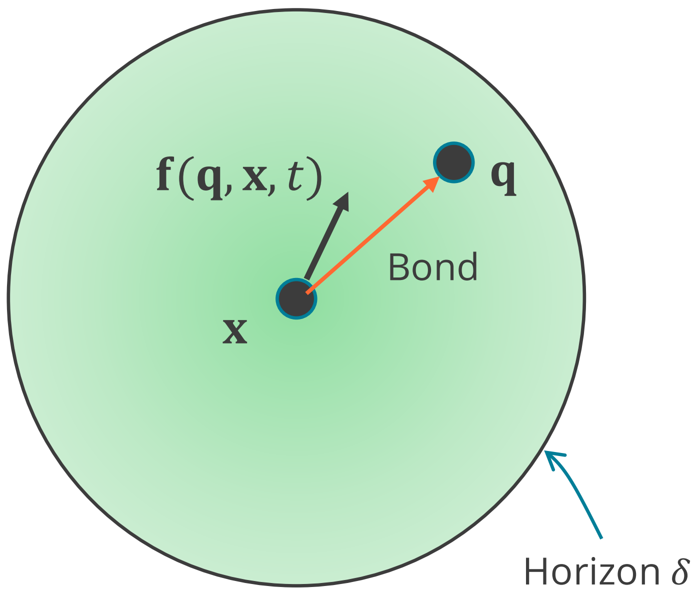
$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}_\mathbf{x}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\mathrm{d}\mathbf{q} + \mathbf{b}(\mathbf{x},t)$$

where

$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = \sum_k \sum_\ell \Omega(\mathbf{x},\mathbf{x}_k)\Omega(\mathbf{q},\mathbf{x}_\ell)\mathbf{F}_{k\ell}(t).$$

- Observe

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



Peridynamics as a reduced order model for complex systems

- Recall that PD is the result of coarse graining a small-scale system.
- Nonlocality always arises from the use of homogenized degrees of freedom.

- The small-scale system can be almost anything:
    - Molecular dynamics (MD)
    - Detailed local model
    - Potts or Monte Carlo
    - Random walk
    - Agent based
    - (Not sure about DFT.)

Many types of small-scale systems can be coarse grained too

- Example: Upscale a heterogeneous model in the local theory.
- $\boldsymbol{\sigma}$=stress in the small-scale model.
- The CG bond forces turn out to be

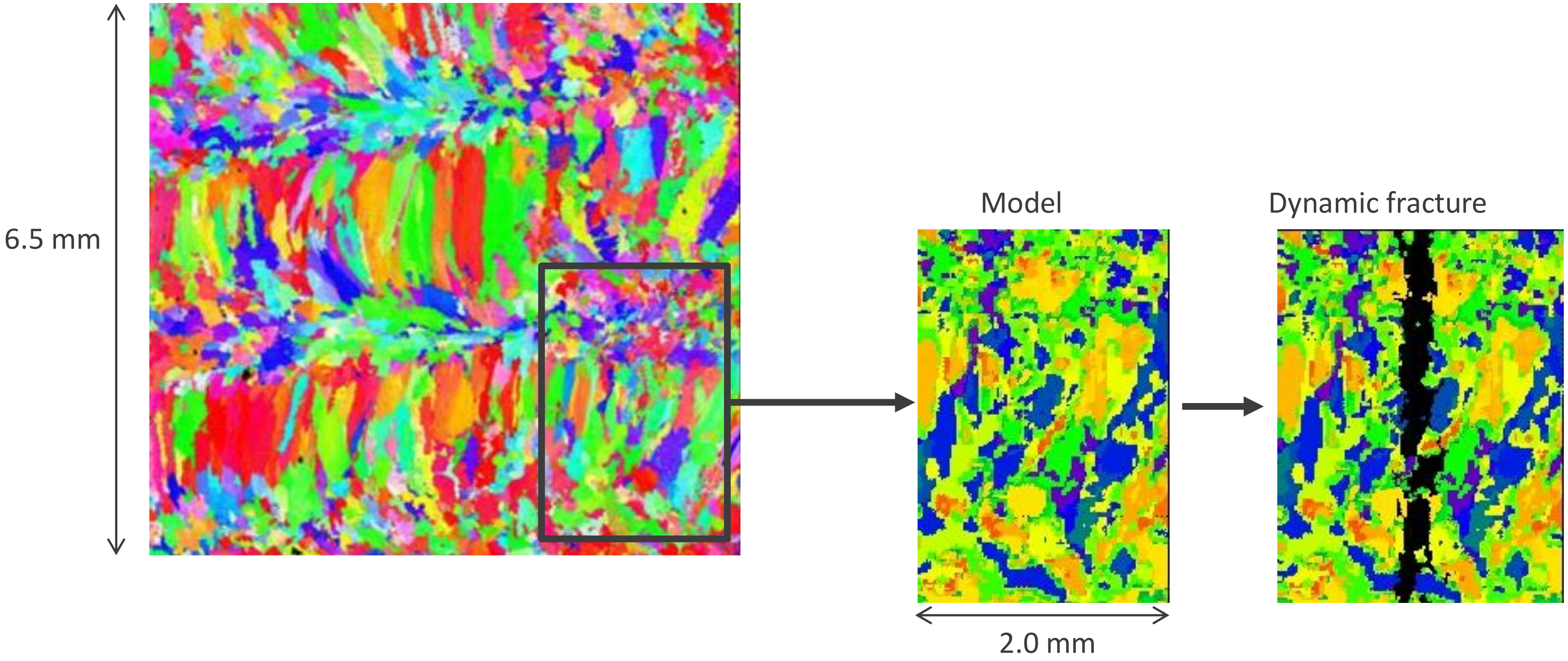
$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = \int \boldsymbol{\sigma}(\mathbf{z},t)\Big[\Omega(\mathbf{z},\mathbf{x})\nabla_{\mathbf{z}}\Omega(\mathbf{z},\mathbf{q}) - \Omega(\mathbf{z},\mathbf{q})\nabla_{\mathbf{z}}\Omega(\mathbf{z},\mathbf{x})\Big]\,\mathrm{d}\mathbf{z}$$

instead of

$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = \sum_k \sum_\ell \Omega(\mathbf{x},\mathbf{x}_k)\Omega(\mathbf{q},\mathbf{x}_\ell)\mathbf{F}_{k\ell}(t).$$

We can import a microstructure and upscale it

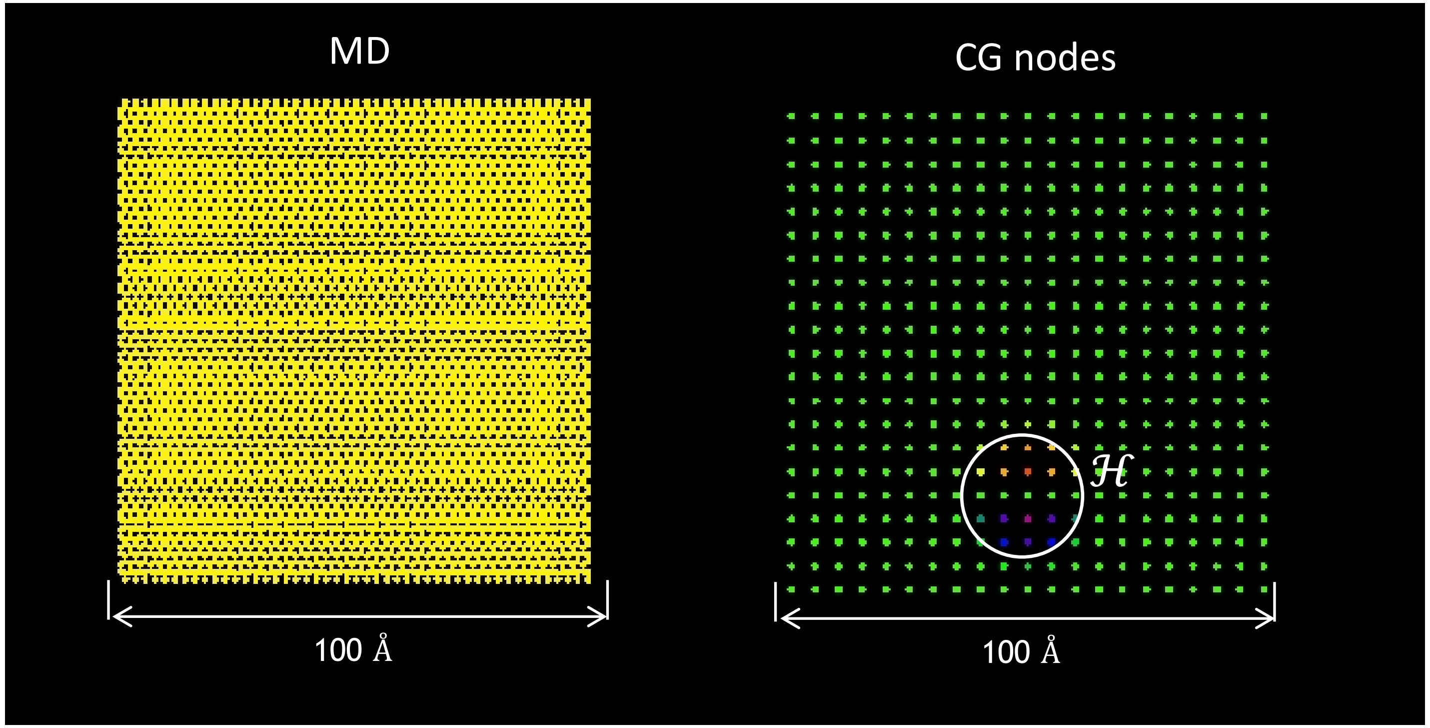
Electron backscattering diffraction (EBSD)
image of 304L stainless steel



- S.S., D.P. Adams, & B.A Branch, Mesoscale Model for Spall in Additively Manufactured 304L Stainless Steel. *International Journal for Multiscale Computational Engineering.* (2023).

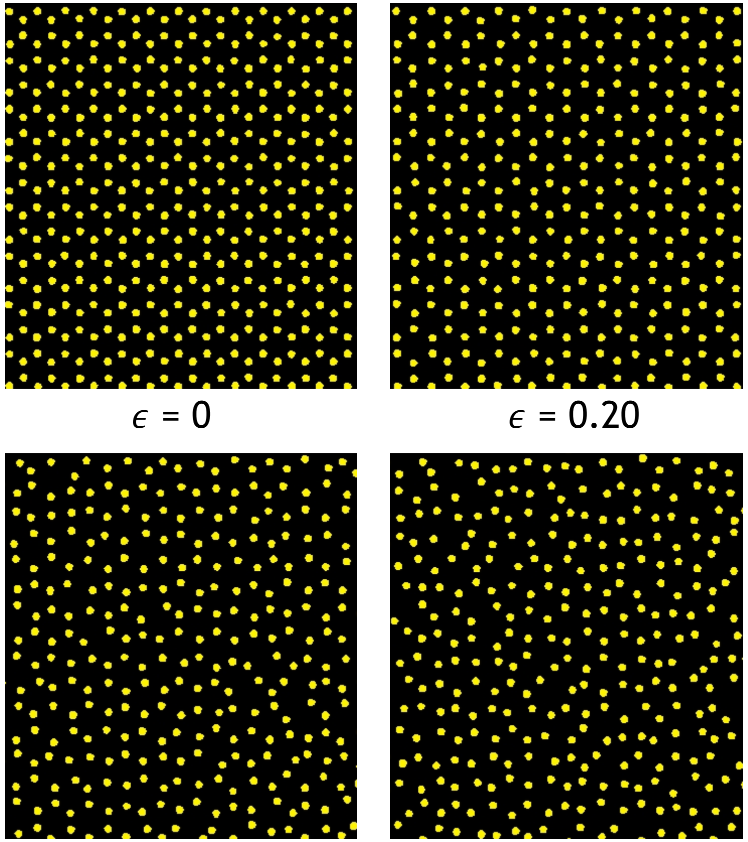
Example: PD model from MD in graphene

- Perform MD modeling of a perfect graphene sheet under isotropic extension and uniaxial strain.
- Compute the coarse grained forces and displacements.
- Fit the parameters in an OSB peridynamic model to the CG forces.
- OSB model is like LPS but with nonlinear terms for strain softening.



Graphene peridynamic bond response

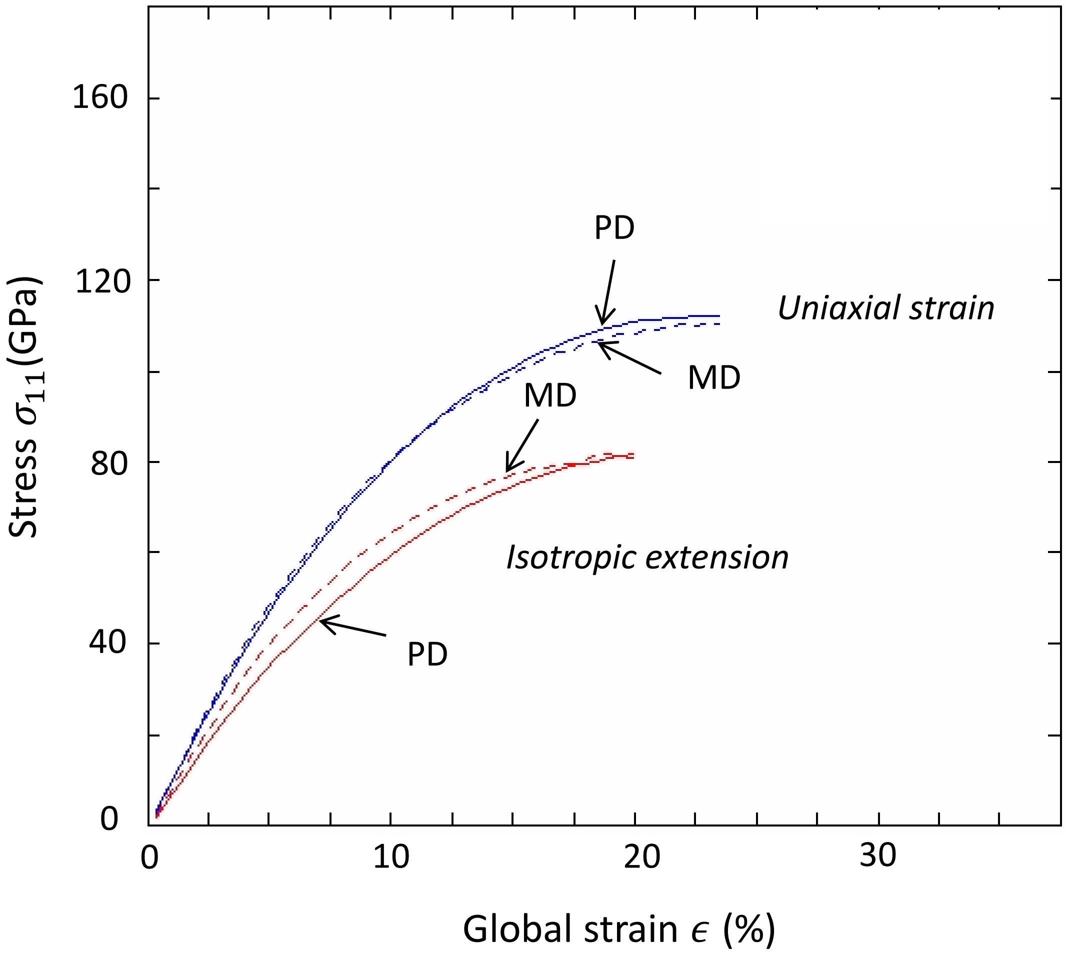
MD



ϵ = 0 ϵ = 0.20

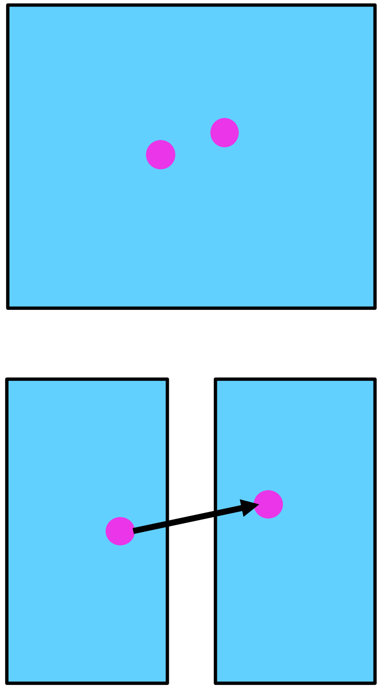
ϵ = 0.29 ϵ = 0.30

Stress-strain curves from PD bonds
Comparison with MD



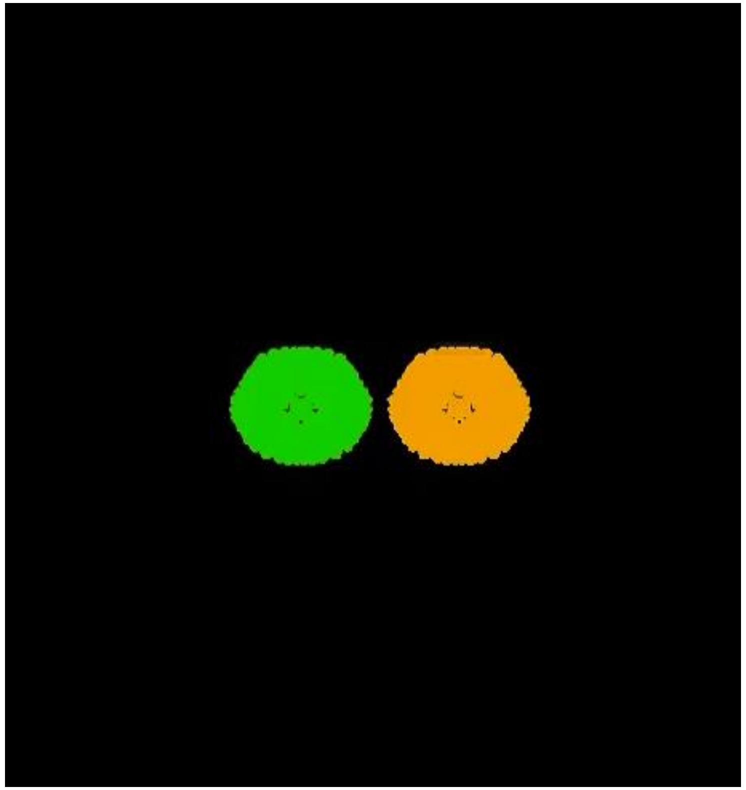
Surface energy and microstructure evolution

- In metals, the microstructure is strongly influenced by the surface energy of grain boundaries.
- Nonlocality offers a way to treat surface energy without mathematically defining a surface.
- Analogous to autonomous fracture.

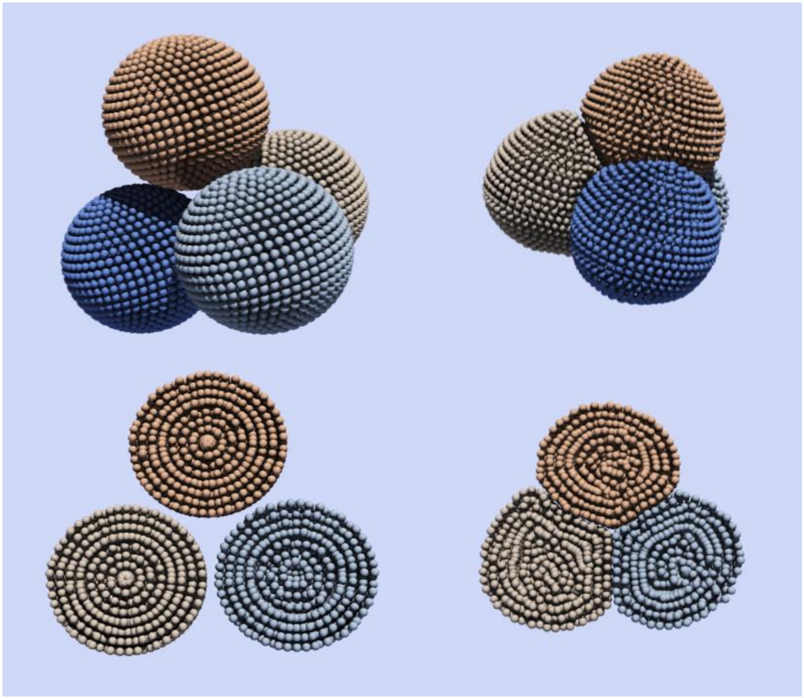


Separate two halves of a body.
The work on the interface bonds
is the surface energy.
Eulerian interactions.

VIDEO



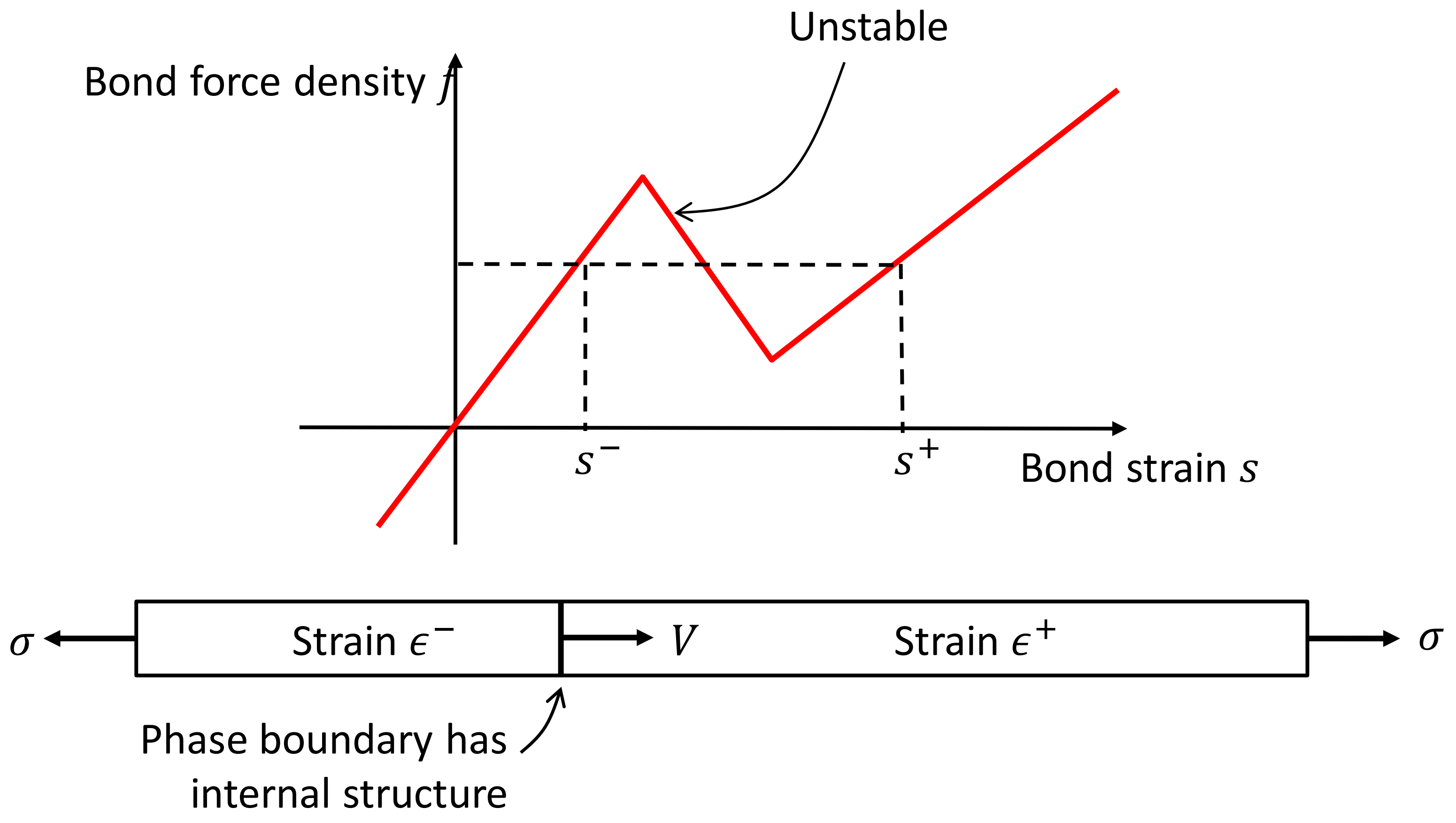
Droplet motion driven by surface energy



Sintering of 4 copper grains

Microstructure evolution is often driven by surface energy

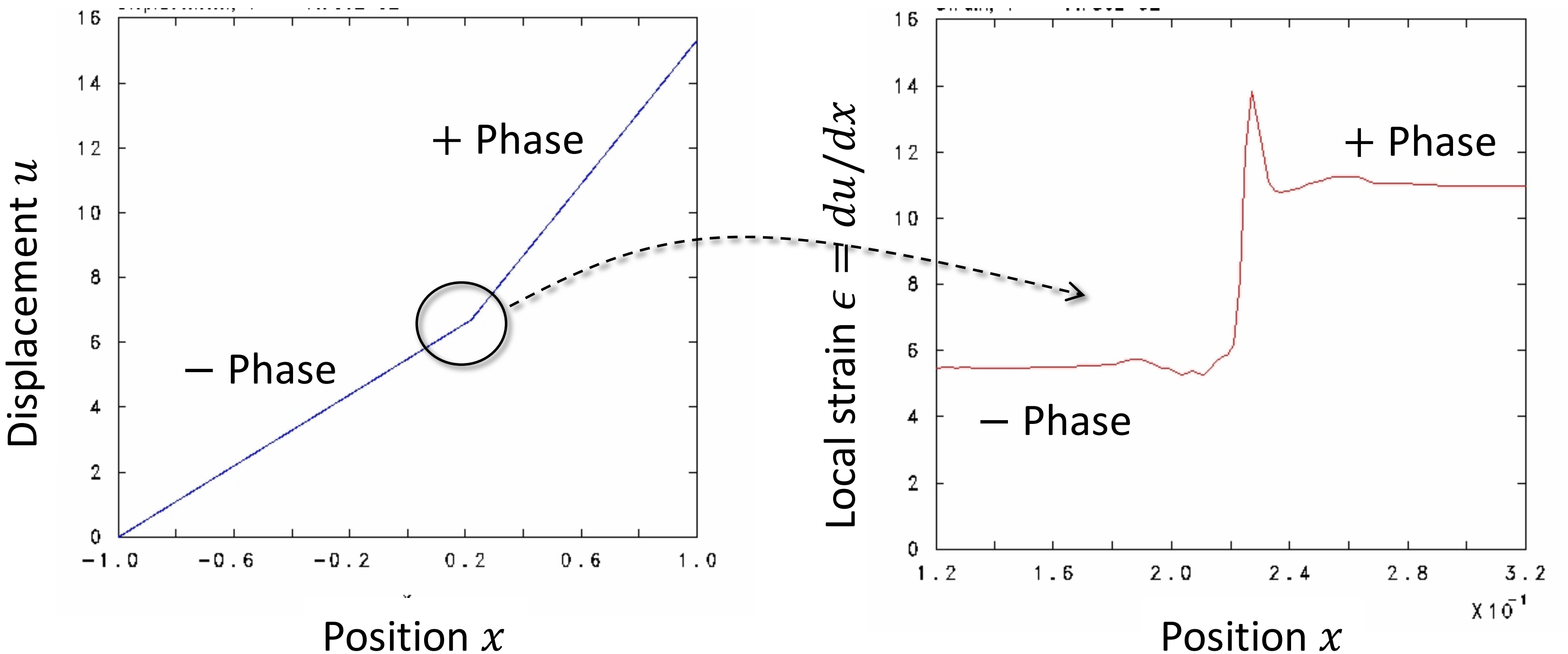
- Nonlocality can introduce interface energy between phases (grains).



- K. Dayal & K. Bhattacharya, *Journal of the Mechanics and Physics of Solids* (2006).

Structure of the phase boundary

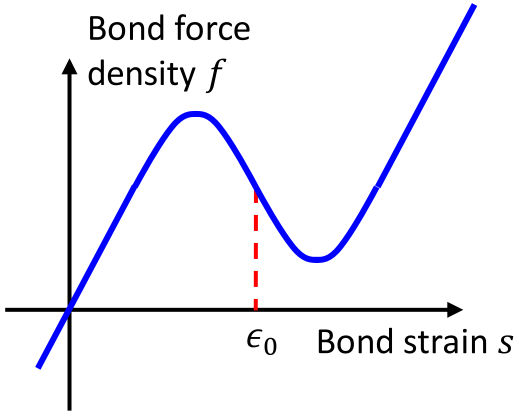
- Bonds that connect the phases don't quite fit into one branch of the material model or the other.
- These bonds have extra energy, resulting in interfacial energy.

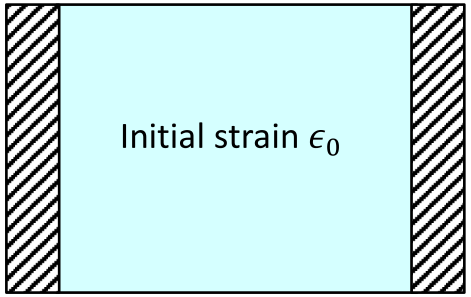


- K. Dayal & K. Bhattacharya, *Journal of the Mechanics and Physics of Solids* (2006).

2D microstructure evolution with a nonlocal model

- Plate with ends fixed. Global strain ϵ_0 is in the unstable part of the material model.
- Complex microstructure appears at first, then simplifies.
- Driving force is the energy stuck in a phase boundary.





VIDEO

Colors show bond strain

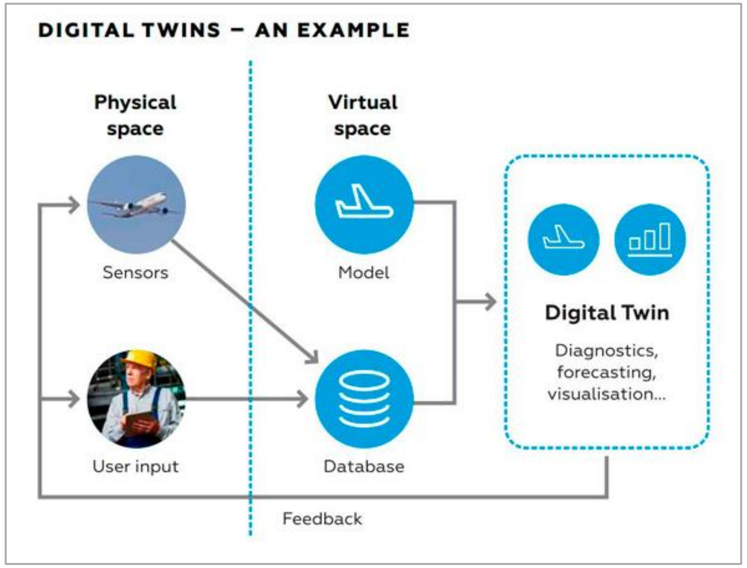
How can peridynamics contribute to research trends?

- Research directions come in waves.
- Catch a wave!
- PD can describe a broad range of phenomena in mechanics or beyond mechanics .

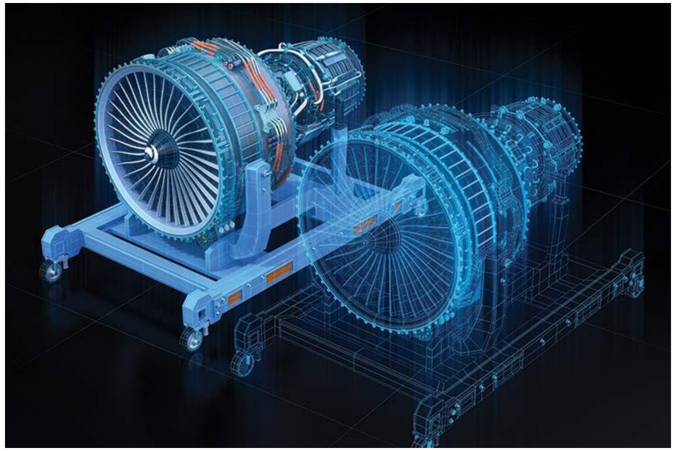
www.gosurfperth.com

Digital twins

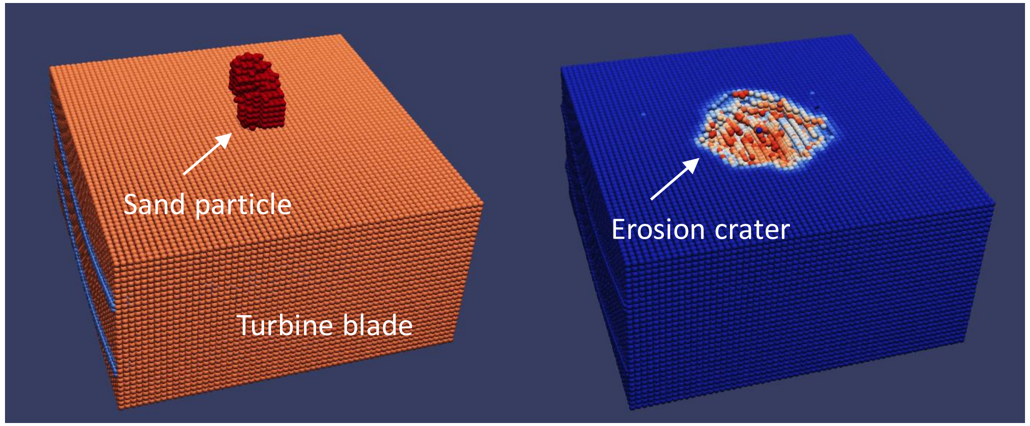
- Idea: A physical system has a virtual model.
- The physical system may have sensors.
  - Could include sensors for loading, usage, temperature, structural health.
- A PD module in the virtual twin of (say) a jet engine could help associate sensed variables with the condition of the turbine blades after flights through adverse environments.



www.anylogic.com



www.ptc.com



PD simulation of erosion particle impact (~300m/s)

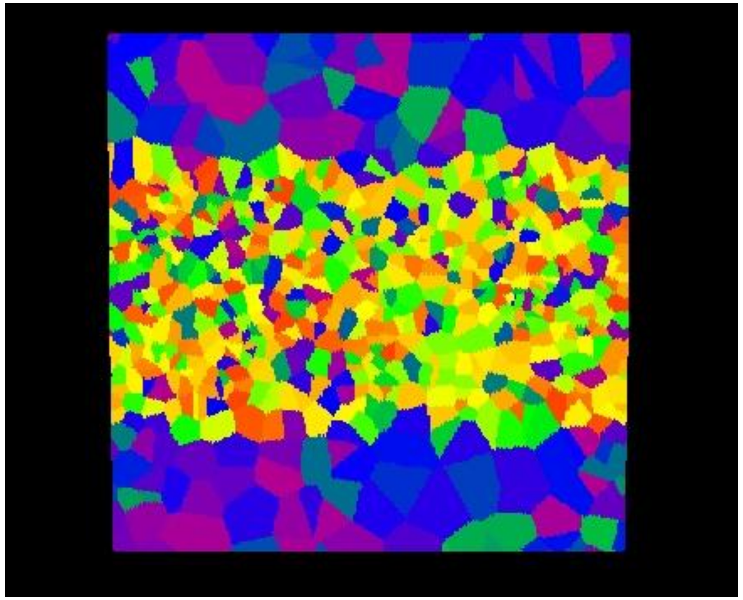
Reduced order modeling

- A large-scale 3D simulation is not what most engineers need.
- They often need a model that runs fast and can be used to examine alternatives in design.
- Can we somehow reduce the number of DOFs?
- Many systems can be modeled through interactions between DOFs separated by some finite distance. This is PD!

- Y.K. Galadima, E. Oterkus, &S. Oterkus, Model order reduction of linear peridynamic systems using static condensation. Mathematics and Mechanics of Solids. (2021).
- H. Dong et al.. An adaptive partitioned reduced order model of peridynamics for efficient static fracture simulation. Engineering Analysis with Boundary Elements. (2023)

Additive manufacturing

- PD can account for the multiple length scales in AM materials in determining bulk mechanical response and failure.
- Through coarse graining, we can study the effect of highly variable and random microstructure, impurities, defects, and thermal stresses.
- Creates opportunities to combine with synthetic microstructures, UQ for material variability, and optimization of fabrication processes and structural design.



Representative AM microstructure showing multiple length scales

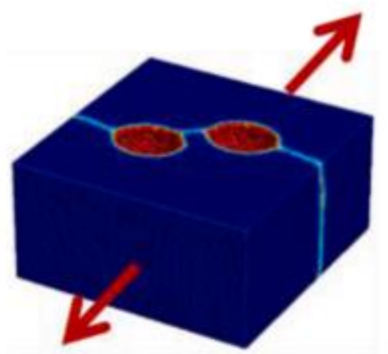
- S.S, S. Jafarzadeh, & Y. Yu, Peridynamic Models for Random Media Found by Coarse Graining. *Journal of Peridynamics and Nonlocal Modeling*, (2024) https://doi.org/10.1007/s42102-024-00118-y

Digital engineering

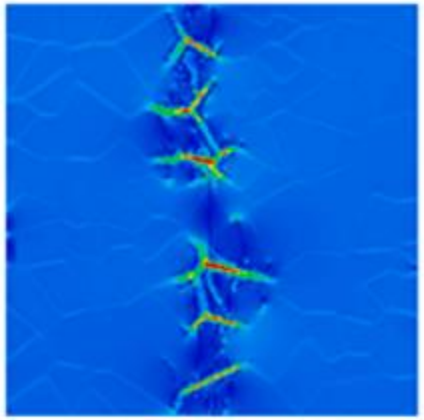
- Large organizations choose a set of software tools for different aspects of a project.
  - Everybody is supposed to use these tools.
  - A high-capacity network to allow people to work on the same dataset simultaneously.
- CAD/CAM is often the main focus.
- Can include real-time data from manufacturing, testing, end users.
- PD needs to be integrated into CAD/CAM tools to participate in digital engineering.
  - IGA
  - Optimization
  - Local-nonlocal coupling
  - Multiphysics

Multiphysics

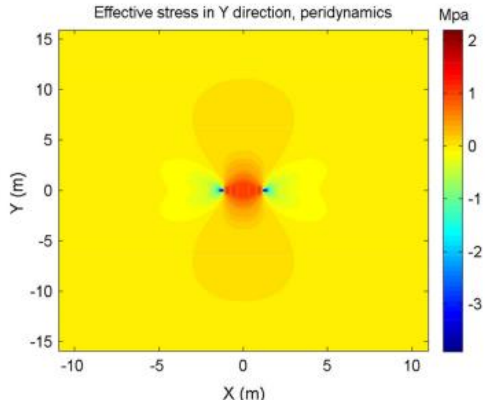
- Different physical fields can be treated either as point values or characteristics of a bond.
  - Thermal expansion.
  - Chemical reaction & diffusion of species leading to corrosion.
  - Combined fluid transport and solid response (including poroelasticity).
- Some physical fields can be coupled to PD with a separate PDE solver.
  - Electromagnetic.
  - Steady-state electrical condition can be treated as diffusive transport through bonds.



Coupled corrosion and fracture simulation**



Current density in a damaged composite*



Stress near a pressurized crack in a porous solid***

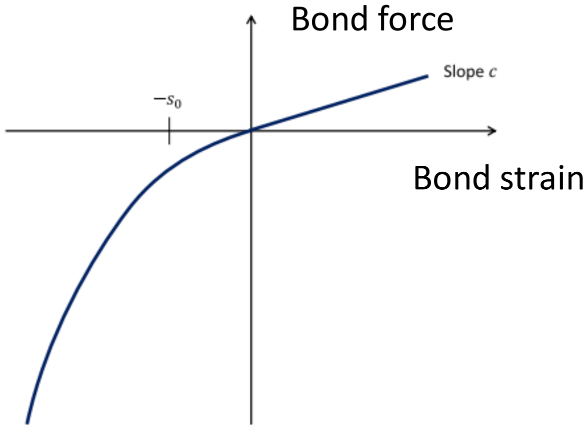
*P. Wu & Z. Chen, Peridynamic electromechanical modeling of damaging and cracking in conductive composites: A stochastically homogenized approach. Composite Structures (2023).
**Z. Chen et al., A coupled mechano-chemical peridynamic model for pit-to-crack transition in stress-corrosion cracking. JMPS (2021).
- S. Rokkam et al., A nonlocal peridynamics modeling approach for corrosion damage and crack propagation. Theoretical and Applied Fracture Mechanics. (2019).

*** H. Ouchi et al, A fully coupled porous flow and geomechanics model for fluid driven cracks: a peridynamics approach. Computational Mechanics. (2015).

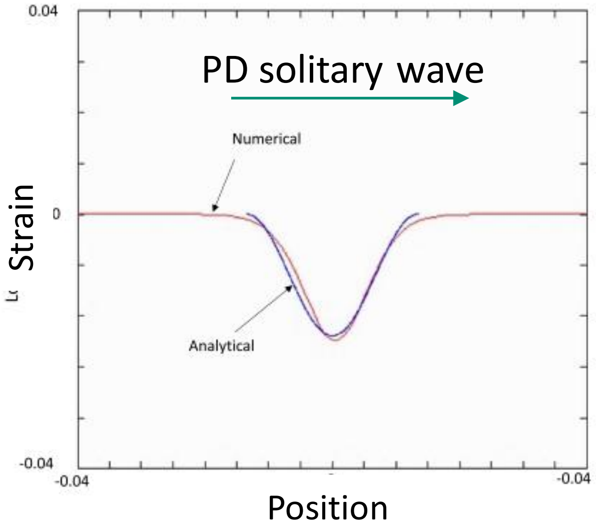
Discovery of models

- Suppose we're given a set of data, say from full field measurements.
- What equations describe the system?
- One approach is to discover a PDE.
  - Often a PD kernel can take the place of a PDE avoiding the need to define an order.

Solitary wave: PD acts similarly to a complicated nonlinear ODE



Nonlinear bond-based PD material



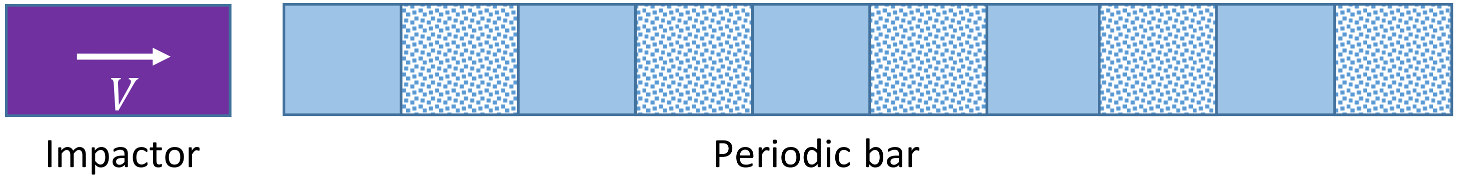
$$\left(\frac{\rho V^2}{E}-1\right)\epsilon' + \frac{2}{s_0}\epsilon\epsilon' + \left[-\frac{\epsilon'''}{24}+\frac{\epsilon'\epsilon''}{6s_0}+\frac{\epsilon\epsilon'''}{12s_0}\right]\delta^2 = 0.$$

ODE that approximates the PD wave (similar to KdV equation)

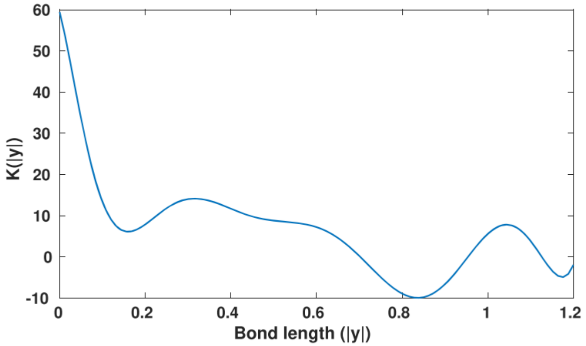
*SS, Solitary waves in a peridynamic elastic solid. *JMPS*. (2016)

Discovery of models example: Periodic elastic media*

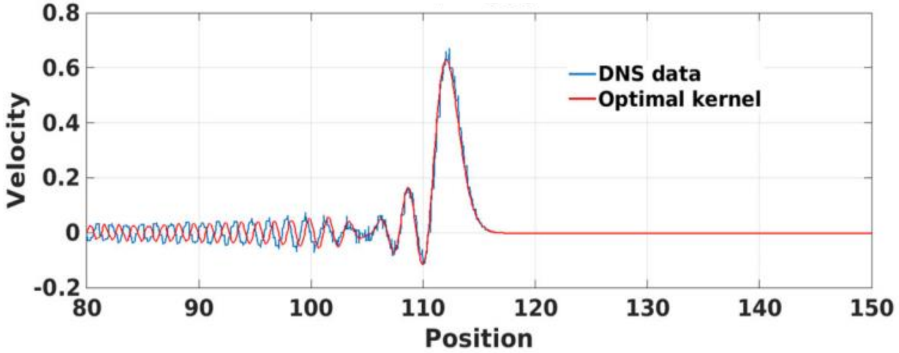
- Suppose we have a Direct Numerical Solution (DNS) method that can generate as much training data as we want.
    - Training data consists of wave dynamics under transient distributed loading.
- Learn an optimal peridynamic kernel.
- Local theory cannot predict the most prominent feature of the problem, which is wave dispersion.



Optimal kernel



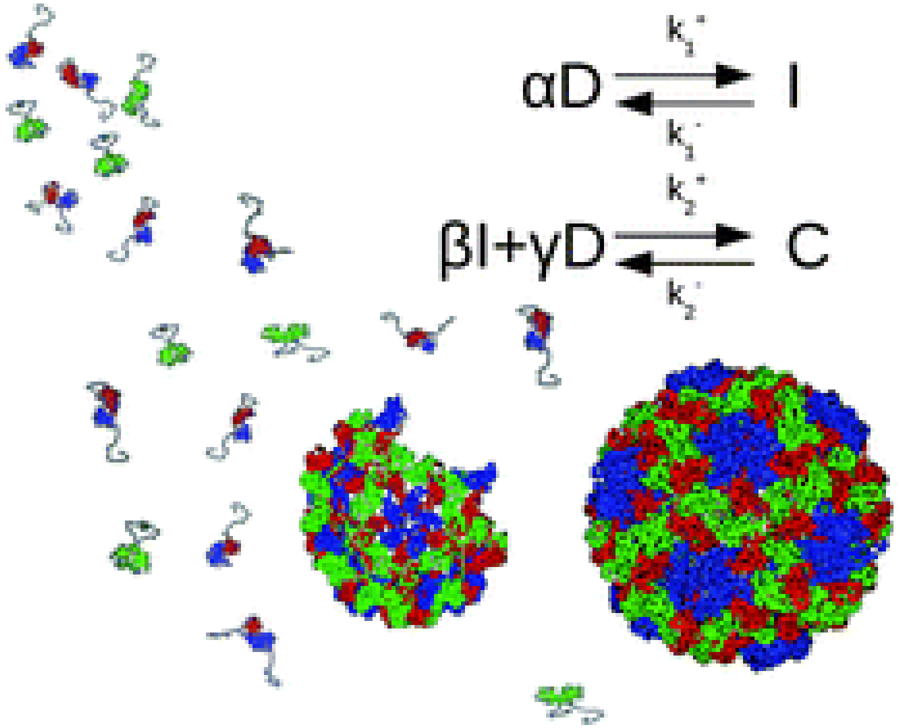
Validation: Impact problem



* H. You et al., Nonlocal Operator Learning for Homogenized Models: From High-fidelity Simulations to Constitutive Laws, *Journal of Peridynamics and Nonlocal Modeling*, https://doi.org/10.1007/s42102-024-00119-x (2024).

Nanoscale and biological materials

- Many phenomena in real materials and biological systems are nonlocal at small length scales.
  - Interatomic potentials.
  - Hydrogen bonding.
  - Electrostatic fields.
  - Forces between particles suspended in a liquid.
    - Van der Waals forces.

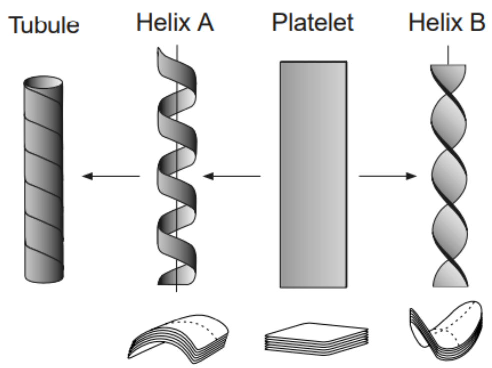


Self-assembly of a viral capsid (shell)*

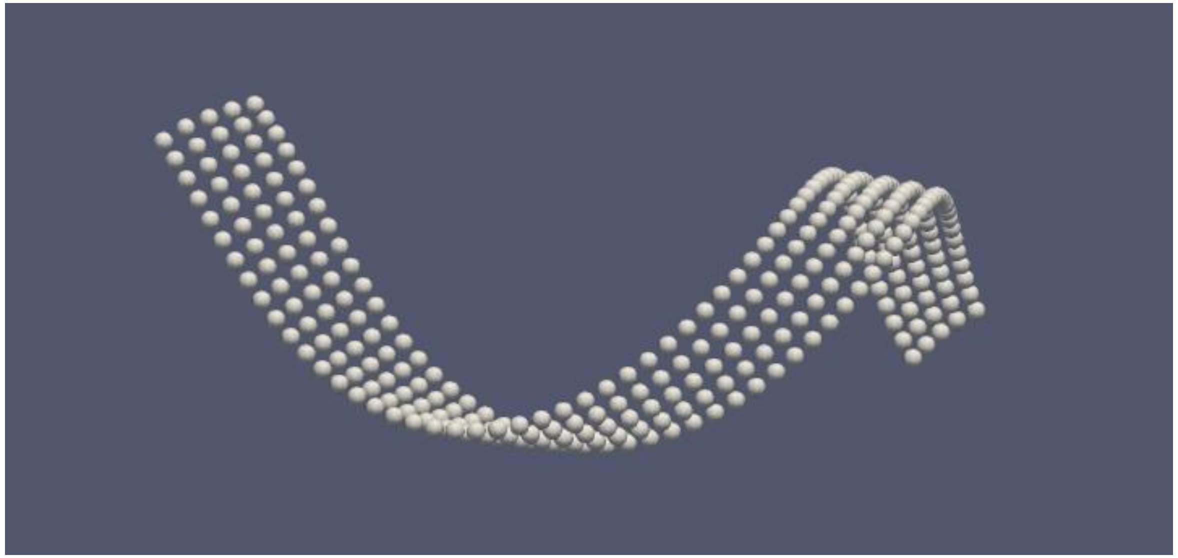
*D. Law-Hine, et al., *Soft Matter* (2016)

Nanoscale example: Self-shaping nanostructures

- Materials scientists can create 3D shapes from a flat layer using internal long-range forces.



Chemical composition of a ribbon induces internal forces*

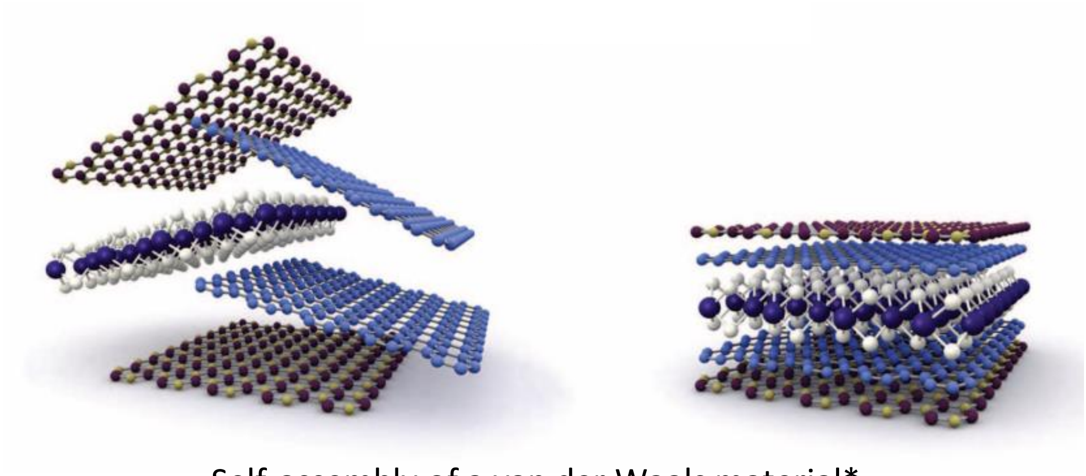


Peridynamic model with vdW forces that induce an elastic instability

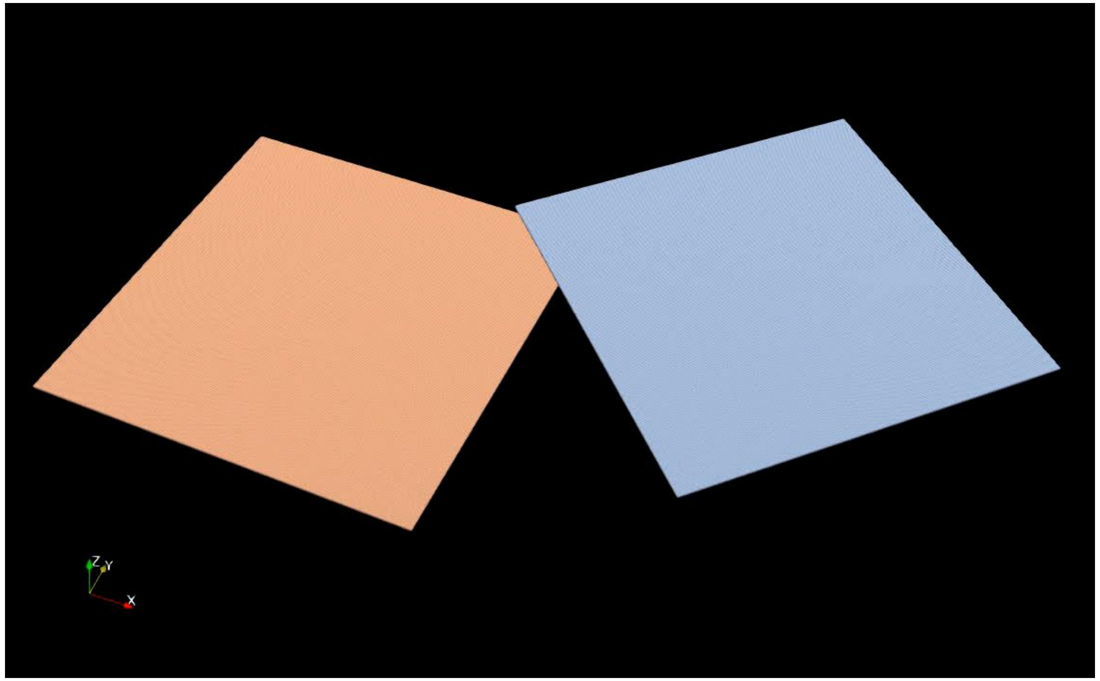
*R. Oda et al., *Nature* (1999)

Material design: Van der Waals materials

- Nanoscale materials can be “programmed” to assemble multiple parts in a desired way.


Self-assembly of a van der Waals material*

VIDEO



Peridynamic model of two sheets interacting through vdW forces

*K. S. Novoselov et al., *Science* (2016)

Social systems

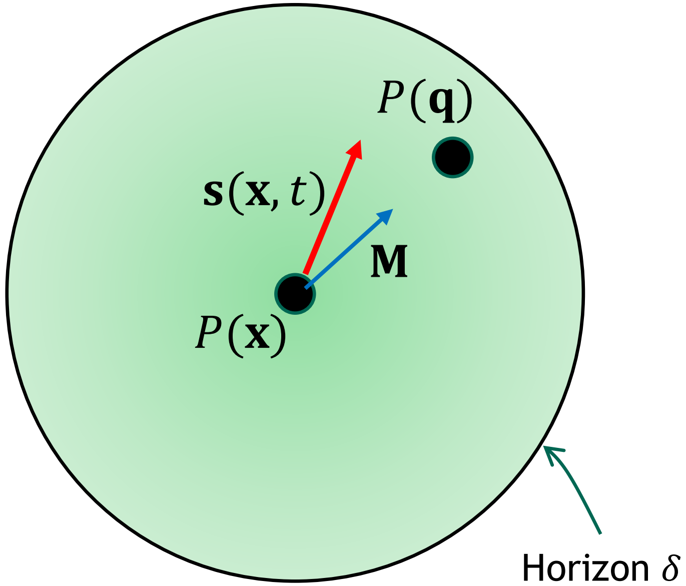
- Interactions in crowds are nonlocal – people account for others about 10m away.
- Dream up a nonlocal model (Eulerian configuration):

$$\dot{P}(\mathbf{x},t) = \int_{\mathcal{H}_{\mathbf{x}}} \{\underline{v}[\mathbf{x},t]\langle\mathbf{q}-\mathbf{x}\rangle - \underline{v}[\mathbf{q},t]\langle\mathbf{x}-\mathbf{q}\rangle\}\, d\mathbf{q}$$

$$\underline{v} = \alpha\underline{P} - \mathbf{s}\cdot\underline{\mathbf{M}}$$

where P=density (of people), $\mathbf{s}$=motivating force vector, $\underline{\mathbf{M}}$=bond direction state, α=diffusion coefficient, $\underline{v}$=flux state (scalar).

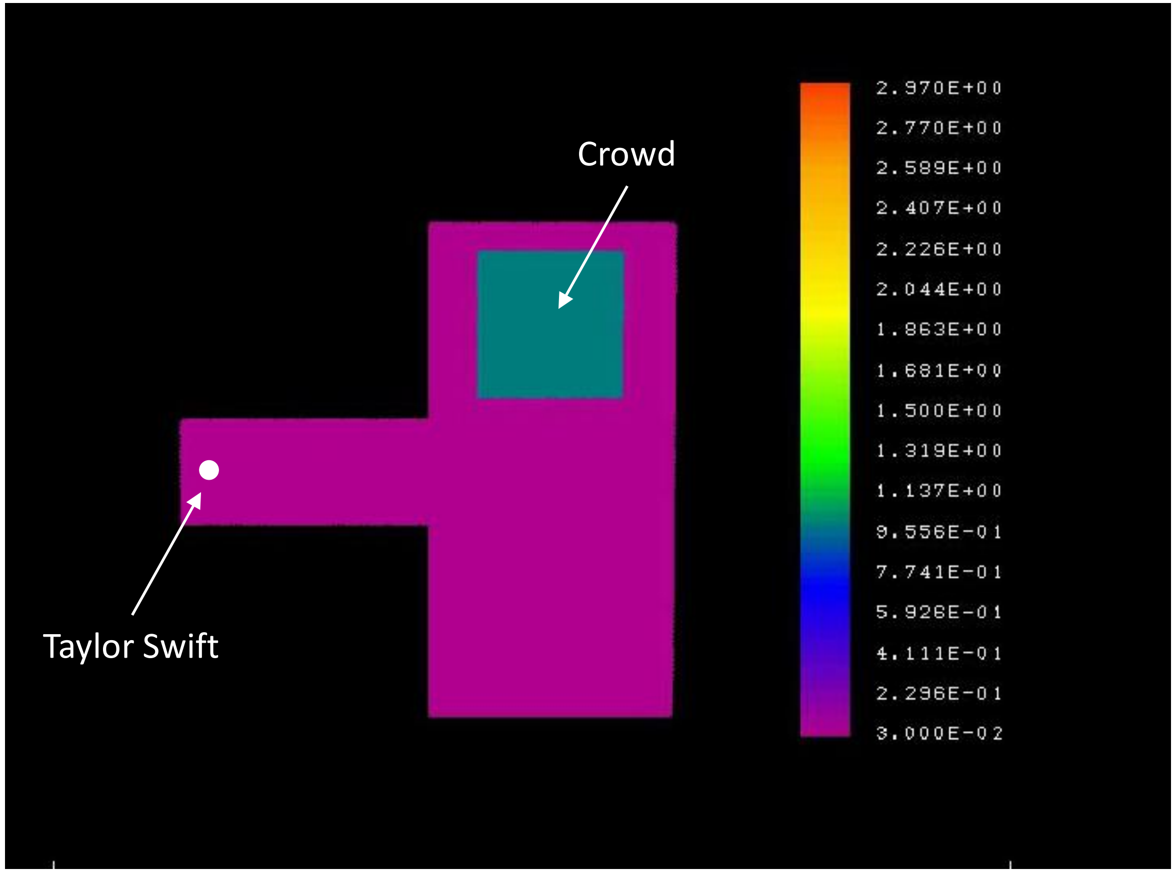
www.wabe.org



Social systems: PD crowd simulation

- Model of a large group of people who suddenly decide they need to be somewhere else.
- Example: Taylor Swift sighting in a busy airport.

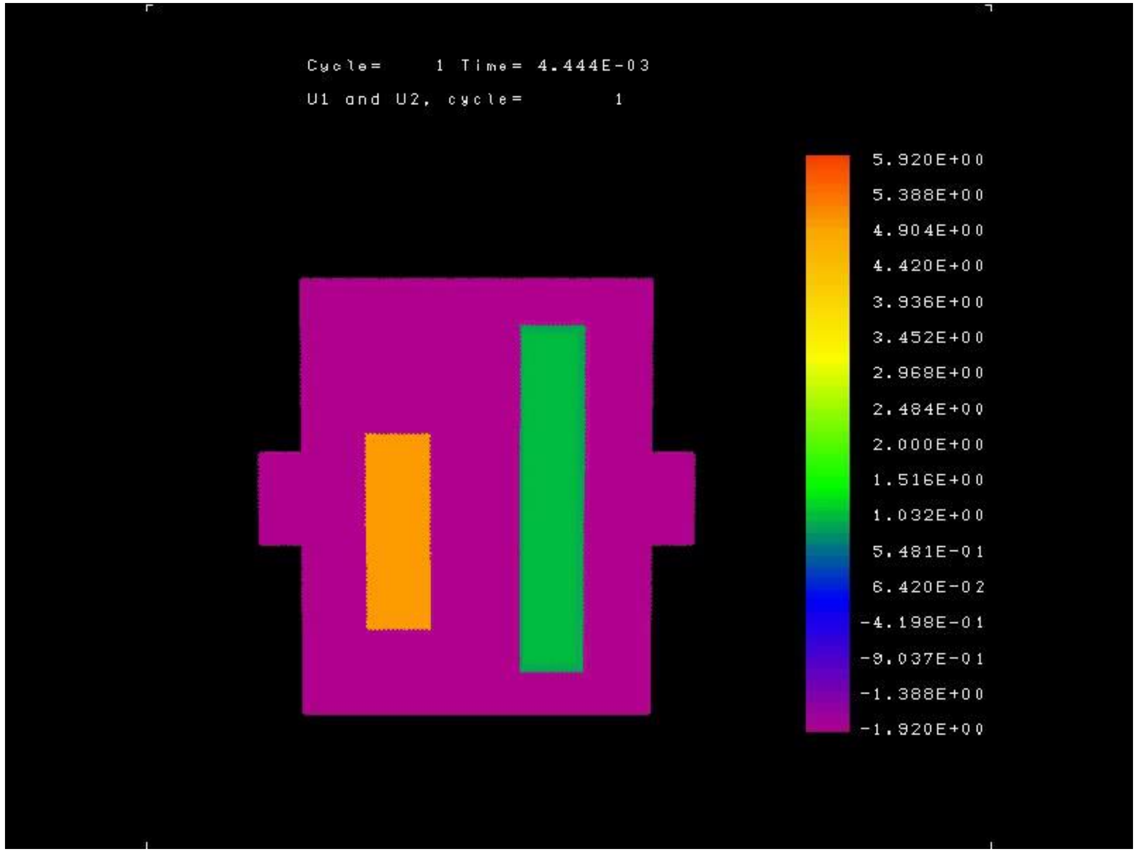
VIDEO



Colors show density (of people)

PD crowd simulation: Extension to 2 populations

VIDEO



- Could we coarse grain an agent-based model into PD?
- Similar considerations for contagious disease spread, social media phenomena, vehicle traffic.

Peridynamics and artificial intelligence

Can PD help AI work better?

- Once again consider crowd modeling.
- Cameras (in airports) record every person's movements everywhere at all times.
- This data could be used to train a neural network (like the ones in self-driving vehicles).
  - NN would predict, for example, unsafe conditions.
- Some AI/ML applications can made much easier using a deterministic model (like PD) embedded within the NN strategy.
  - Enforce conservation laws.
  - Reduce the number of unknowns by incorporating prior knowledge.

Example: Peridynamic Neural Operator* uses NNs as components in a state-based material model

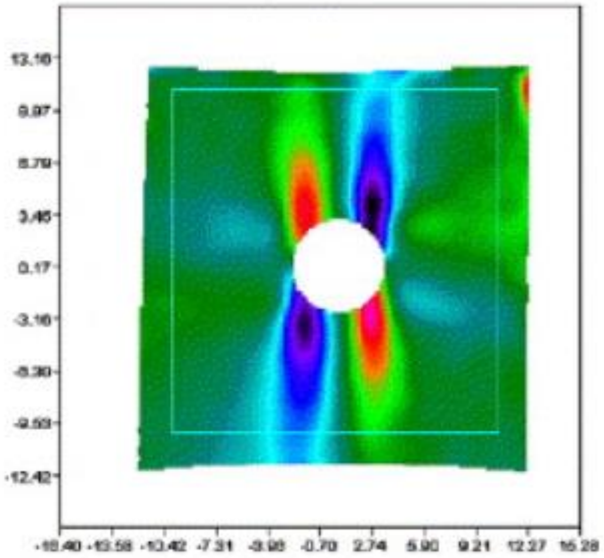
$$\underline{t}[\boldsymbol{x}, t]\langle\boldsymbol{\xi}\rangle := \sigma^{NN}(\omega(\boldsymbol{\xi}), \vartheta(\boldsymbol{x}, t), e(\boldsymbol{\xi}, \boldsymbol{\eta}), |\boldsymbol{\xi}|; \boldsymbol{v})$$

$$\omega(\boldsymbol{\xi}) := \omega^{NN}(\boldsymbol{\xi}; \boldsymbol{w})$$

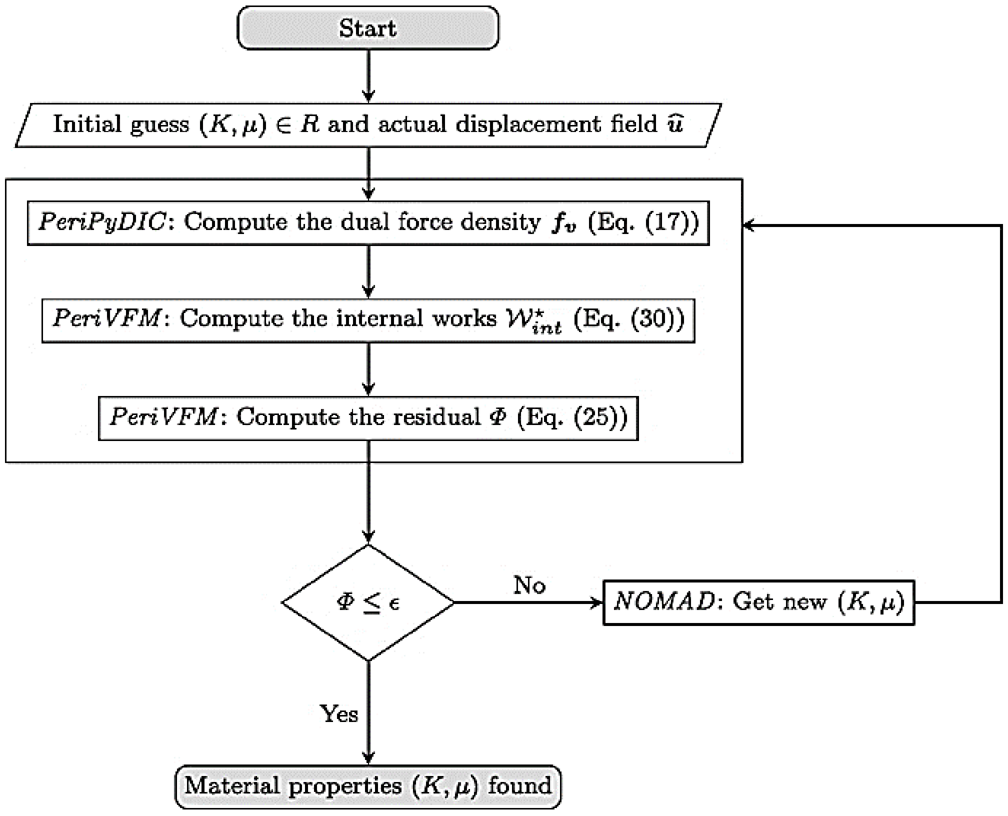
- S. Jafarzadeh et al., Peridynamic Neural Operators: A Data-Driven Nonlocal Constitutive Model for Complex Material Responses. arXiv preprint arXiv:2401.06070. (2024).

Data science: Nonlocal kernels can be derived from full-field data

- Digital image correlation (DIC).
- Virtual field method (VFM).
- Electronic speckle pattern interferometry (ESPI).



Strain concentration in a composite*

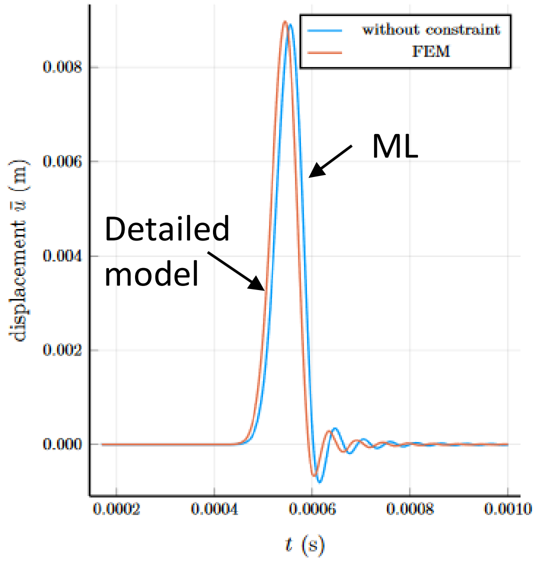


Flow chart for obtaining PD parameters by VFM**.

- *L. Toubal, M. Karama, & B. Lorrain, *Composite structures*, (2005).
- D. Turner, B.Van Bloemen Waanders, & M. Parks *J. Mechanics of Materials and Structures* (2015).
- D. Turner, *J. Engineering Mechanics* (2015).
- **Delorme, R., Diehl, P., Tabiai, I. et al., *J Peridyn Nonlocal Model* (2020)

AI can help to create nonlocal material models from data

- Machine learning can be used to help obtain nonlocal material models, based on data from
  - Small-scale simulation (including MD)
  - Experimental data (e.g. digital image correlation)



Dispersion of a wave pulse*

- You, H., Yu, Y., Silling, S. and D'Elia, M., 2020. Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws. arXiv preprint arXiv:2012.04157.
- *Xu, X., D'Elia, M. and Foster, J.T., 2021. A machine-learning framework for peridynamic material models with physical constraints. arXiv preprint arXiv:2101.01095.
- Nguyen, C.T., Oterkus, S. and Oterkus, E., 2020. A physics-guided machine learning model for two-dimensional structures based on ordinary state-based peridynamics. *Theoretical and Applied Fracture Mechanics*, p.102872.
- Haghighat, E., Bekar, A.C., Madenci, E. and Juanes, R., 2020. A nonlocal physics-informed deep learning framework using the peridynamic differential operator. arXiv preprint arXiv:2006.00446.
- Delorme, R., Diehl, P., Tabiai, I., Lebel, L. L., & Lévesque, M. (2020). Extracting Constitutive Mechanical Parameters in Linear Elasticity Using the Virtual Fields Method Within the Ordinary State-Based Peridynamic Framework. *Journal of Peridynamics and Nonlocal Modeling*, 1-25.
- Ebrahimi S. Mechanical Behavior of Materials at Multiscale Peridynamic Theory and Learning-based Approaches (Doctoral dissertation, UC Berkeley).
- Longzhen Wang, Jiangming Zhao, Florin Bobaru, Using Neural Networks to Obtain the Kernel for Peridynamic Thermal Diffusion Models, IMECE2020-25247

2001: A Space Odyssey (1968)
Astronaut disables higher-level AI functions of HAL9000

Quantum computing

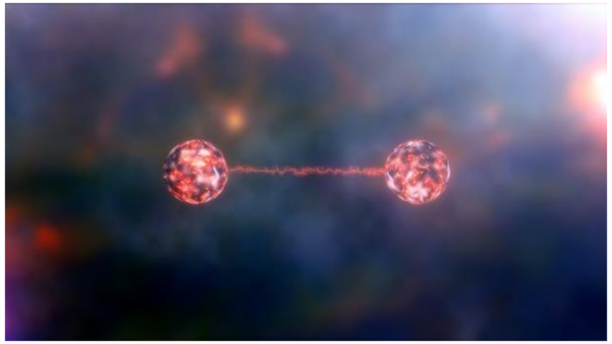
- **There doesn't seem to be a model to help design real devices taking into account quantum entanglement.**

$\uparrow\downarrow$ 2 particles in a quantum state $|\psi>$ with 0 total angular momentum

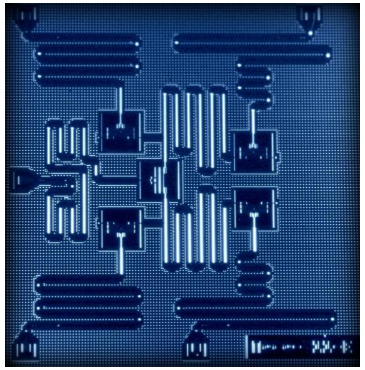
A ← 1 km → B Divide into 2 samples

- Measurement of spin in a given sample is random (coin flip).
- However:
  - If A is measured $\uparrow$ then B is always found to be $\downarrow$.
  - If A is measured $\downarrow$ then B is always found to be $\uparrow$.

- It seems plausible that a nonlocal model could reproduce this for engineering purposes.
  - …without dealing with the time-dependent Schrodinger equation and other difficult subjects.



caltech.edu



quanscient.com

Conclusions

- There is still work to be done on:
  - Fundamentals of fracture in PD
  - Earning and building trust
- We should continue to look for instances where nonlocality provides a fresh perspective.
- We should work to apply the natural advantages of PD to currently trending areas of research opportunity.