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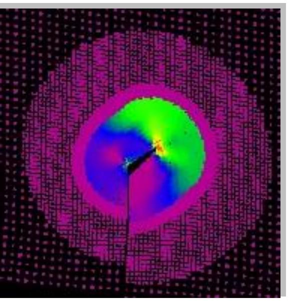

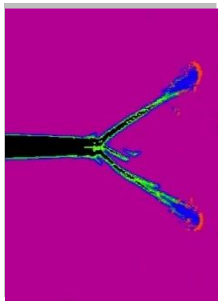

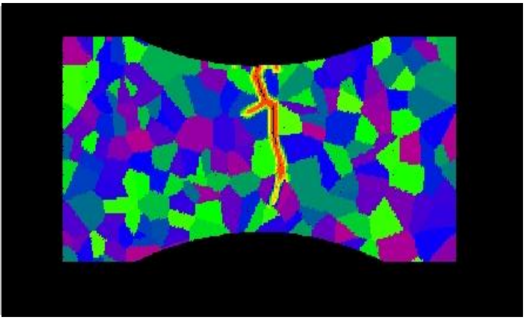

Defects and Interfaces in Peridynamics: A Multiscale Approach

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Albuquerque, New Mexico

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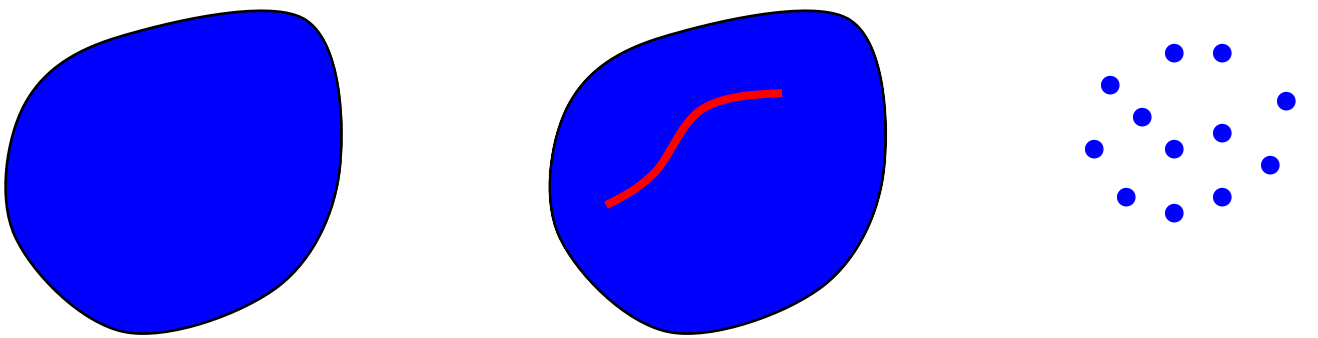
Outline

- Peridynamics background and examples
- Concurrent hierarchical multiscale method
- Calibrating a bond damage model using MD
- Coarse graining

Purpose of peridynamics*

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



Continuous body

Continuous body with a defect

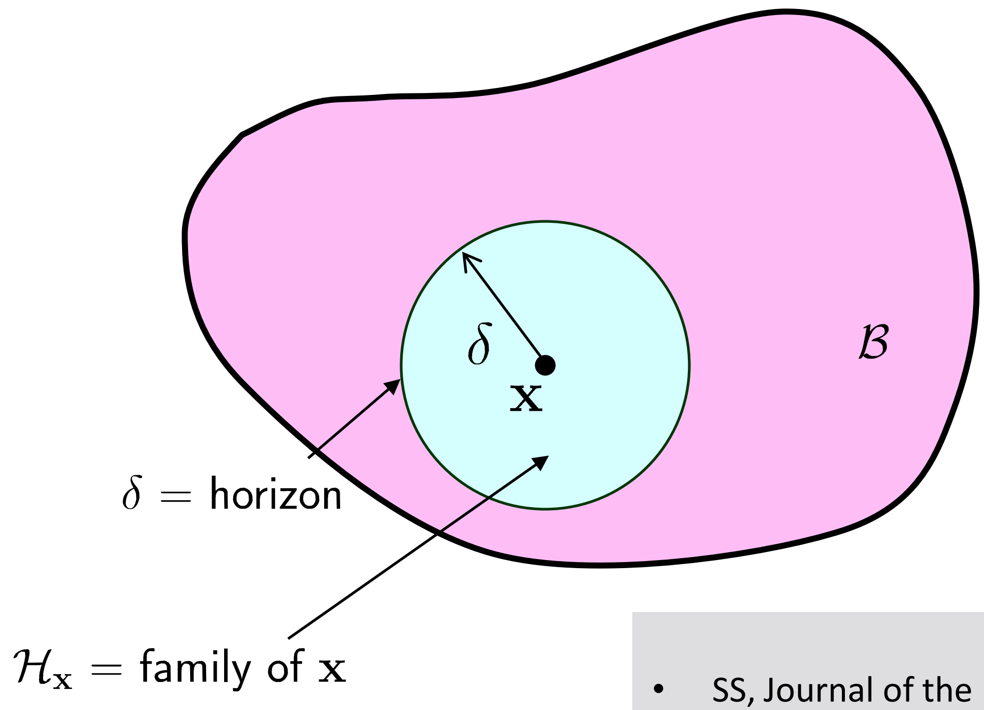
Discrete particles

- Why do this?
  - Avoid coupling dissimilar mathematical systems (A to C).
  - Model complex fracture patterns.
  - Communicate across length scales.

* Peri (near) + dyn (force)

Peridynamics basics: Horizon and family

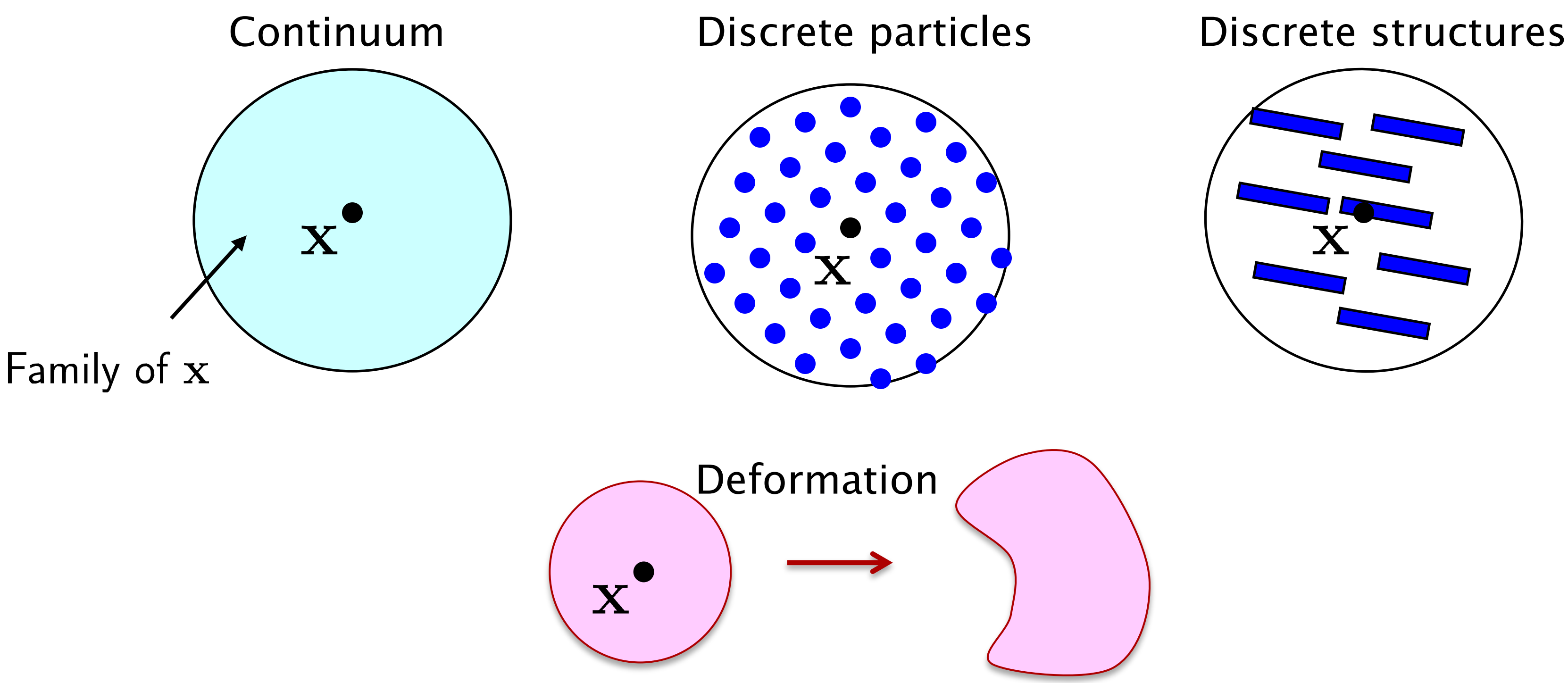
- Any point $\mathbf{x}$ interacts directly with other points within a distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}_{\mathbf{x}}$.



General references

- SS, Journal of the Mechanics and Physics of Solids (2000)
- SS and R. Lehoucq, Advances in Applied Mechanics (2010)
- Madenci & Oterkus , *Peridynamic Theory & Its Applications* (2014)

Point of departure:
Strain energy at a point



- Key assumption: the strain energy density at $\mathbf{x}$ is determined by the deformation of its family.

Potential energy minimization yields the peridynamic equilibrium equation

- Potential energy:

$$\Phi = \int_{\mathcal{B}} (W - \mathbf{b} \cdot \mathbf{y}) \, dV_{\mathbf{x}}$$

where W is the strain energy density, $\mathbf{y}$ is the deformation map, $\mathbf{b}$ is the applied external force density, and $\mathcal{B}$ is the body.

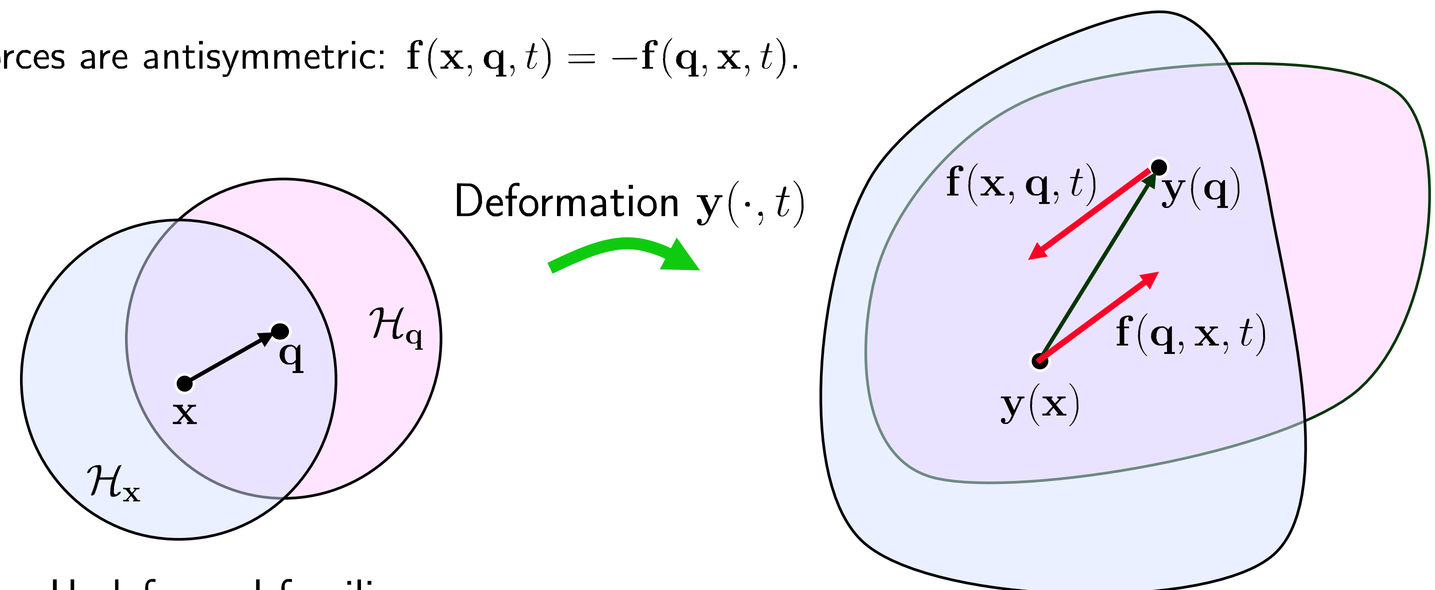
- Euler-Lagrange equation is the equilibrium equation:

$$\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q}, \mathbf{x}) \, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}) = 0$$

for all $\mathbf{x}$. $\mathbf{f}$ is the *pairwise bond force density*.

Peridynamics basics:
Material model determines bond forces

- Each pairwise bond force vector $\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$ is determined jointly by:
- the *collective* deformation of $\mathcal{H}_{\mathbf{x}}$, and
- the *collective* deformation of $\mathcal{H}_{\mathbf{q}}$.
- Bond forces are antisymmetric: $\mathbf{f}(\mathbf{x}, \mathbf{q}, t) = -\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$.



Undeformed families

Deformed families and bond forces

Peridynamic vs. local equations

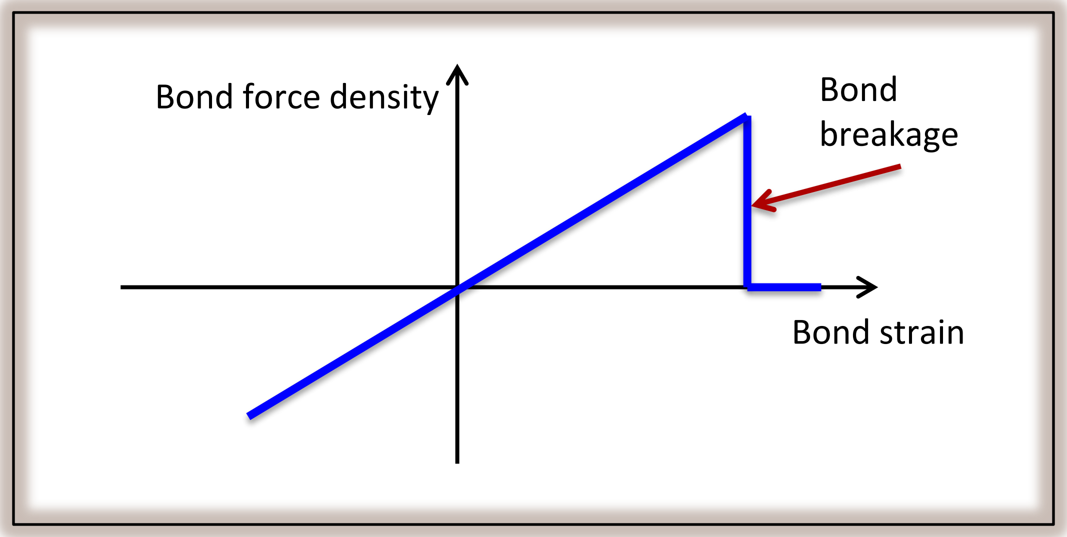
- The structures of the theories are similar, but peridynamics uses nonlocal operators.

Relation	*Peridynamic theory*	*Standard theory*
Kinematics	$\underline{\mathbf{Y}}\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q}) - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \dfrac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \int_{\mathcal{H}} \Big(\mathbf{t}(\mathbf{q},\mathbf{x}) - \mathbf{t}(\mathbf{x},\mathbf{q})\Big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\mathbf{t}(\mathbf{q},\mathbf{x}) = \underline{\mathbf{T}}\langle\mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular momentum balance	$\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle\mathbf{q}-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle\mathbf{q}-\mathbf{x}\rangle\, dV_{\mathbf{q}} = \mathbf{0}$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{\mathbf{Y}}}$ (Fréchet derivative)	$\boldsymbol{\sigma} = W_{\mathbf{F}}$ (tensor gradient)
First law	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + q + r$	$\dot{\varepsilon} = \boldsymbol{\sigma}\cdot\dot{\mathbf{F}} + q + r$

$$\underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} := \int_{\mathcal{H}} \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \cdot \dot{\underline{\mathbf{Y}}}\langle\boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}$$

Bond based material models

- If each bond response is independent of the others, the resulting material model is called bond-based.
- The material model is then simply a graph of bond force density vs. bond strain.
- Damage can be modeled through bond breakage.
- Bond response is calibrated to:
  - Bulk elastic properties.
  - Critical energy release rate.



Linearized theory

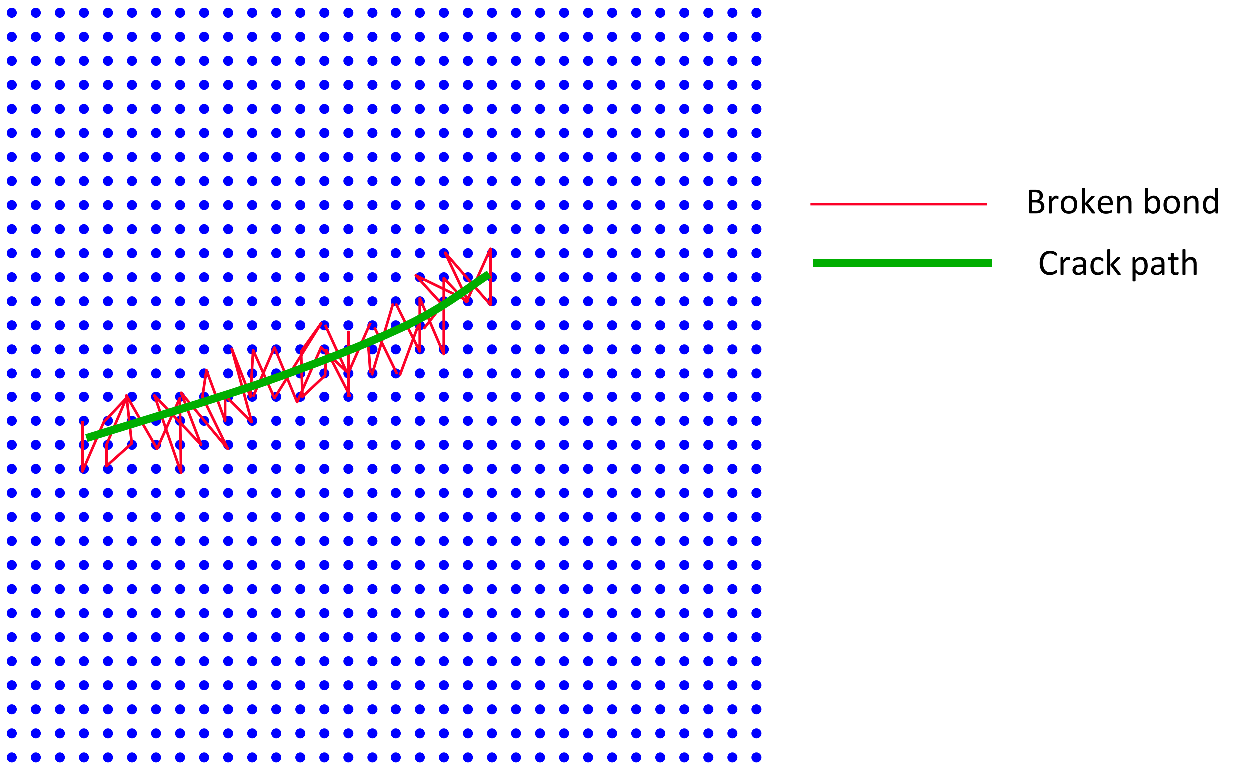
- For small displacements (possibly superposed on a large deformation):

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t)=\int_{\mathcal{H}}\mathbf{C}(\mathbf{x},\mathbf{q})(\mathbf{u}(\mathbf{q},t)-\mathbf{u}(\mathbf{x},t))\,dV_{\mathbf{q}}+\mathbf{b}(\mathbf{x},t)$$

  where $\mathbf{C}$ is the tensor-valued *micromodulus* field.

- Equation is formally the same as in Kunin's nonlocal theory.
- Can still have bond breakage.
- Most of the following discussion uses the linearized theory.
- Will see how to get $\mathbf{C}$ by multiscale methods.

Autonomous crack growth



- When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.

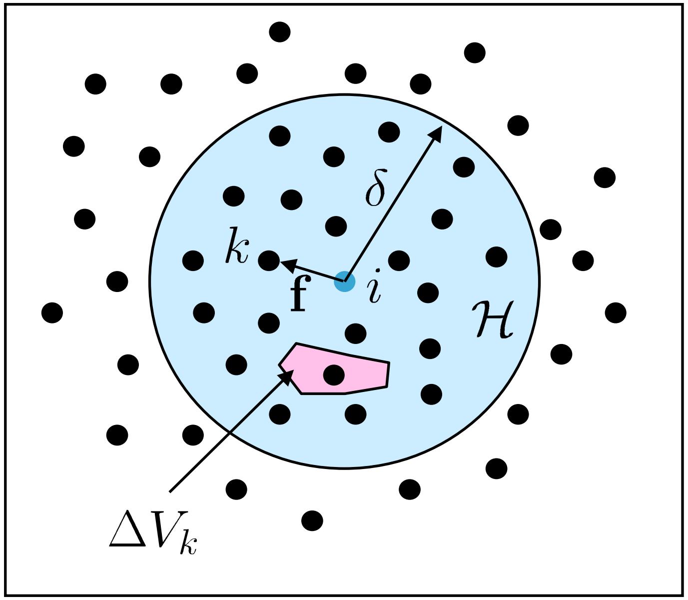
EMU numerical method

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

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

- Linearized model:

$$\rho\ddot{\mathbf{u}}_i = \sum_{k\in\mathcal{H}_i} \mathbf{C}_{ik}(\mathbf{u}_k - \mathbf{u}_i)\Delta V_k + \mathbf{b}_i$$



Peridynamics fun facts

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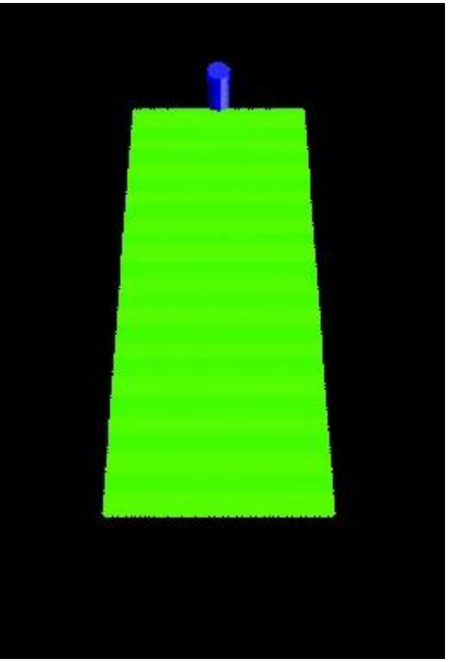
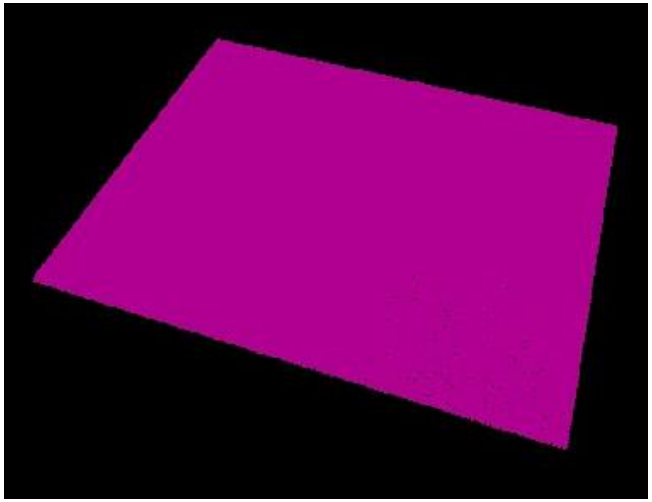
- Molecular dynamics is a special case of peridynamics
  - Any multibody potential can be made into a peridynamic material model (Seleson & Parks, 2014).
- Classical (local) PDEs are a limiting case of peridynamics as $\delta \to 0$ (SS & Lehoucq, 2008).
- Any material model from the classical theory can be included.
  - e.g., Strain-hardening viscoplastic (Foster & Chen, 2010.)
  - Classical material models with the Emu discretization are similar to
    - RKPM (Bessa, Foster, Belytschko, & Liu, 2014).
    - SPH (Ganzenmüller, Hiermaier, & May, 2014).
- Waves are dispersive
  - Material properties can be deduced from dispersion curves (Weckner & SS, 2011).
- It's possible to model crack nucleation and growth without damage (!).
  - Use nonconvex bond energy (Lipton, 2014).

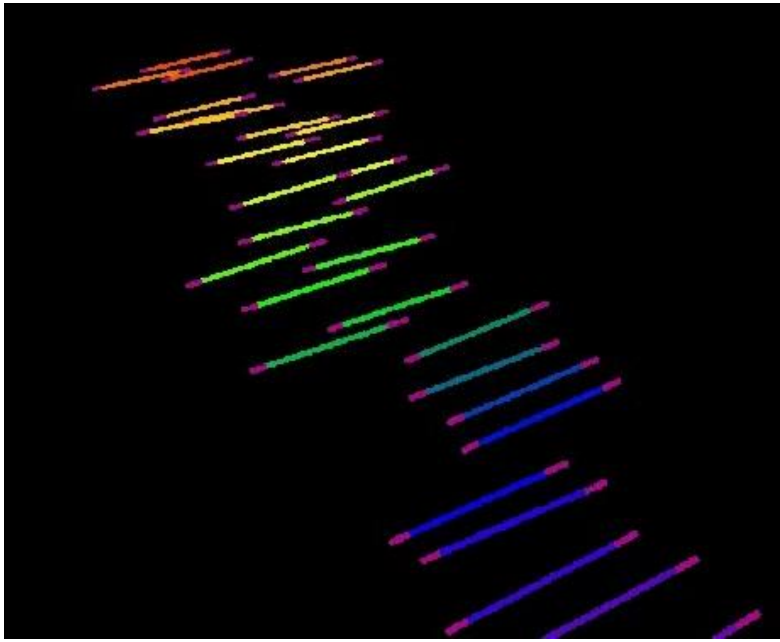
Examples: Membranes and thin structures (videos)



Oscillatory crack path



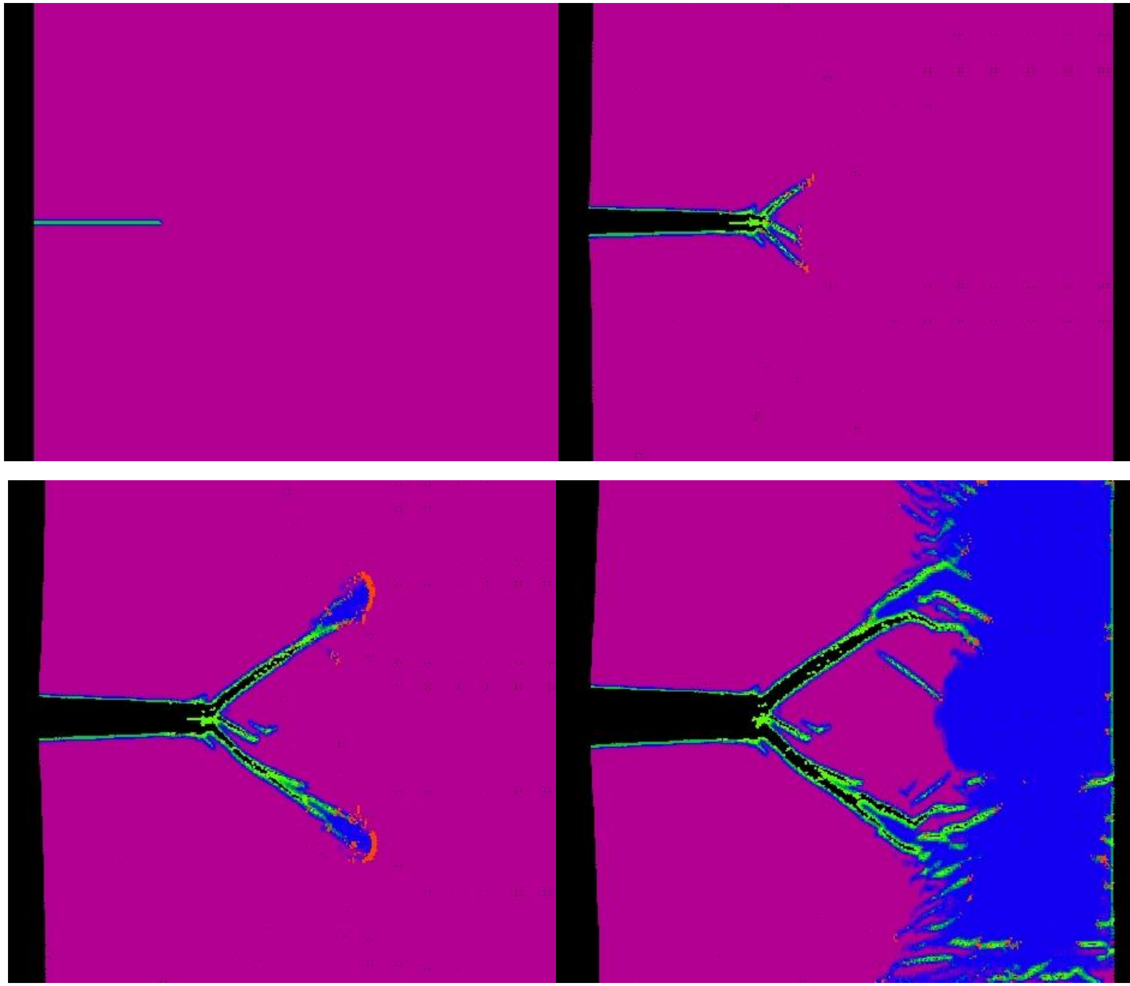
Crack interaction in a sheet



Self-assembly

Dynamic crack branching

- Similar to previous example but with higher strain rate applied at the boundaries.
- Red indicates bonds currently undergoing damage.
    - These appear ahead of the visible discontinuities.
- Blue/green indicate damage (broken bonds).
- More and more energy is being built up ahead of the crack – it can't keep up.
    - Leads to fragmentation.



More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Dynamic crack branching (video)

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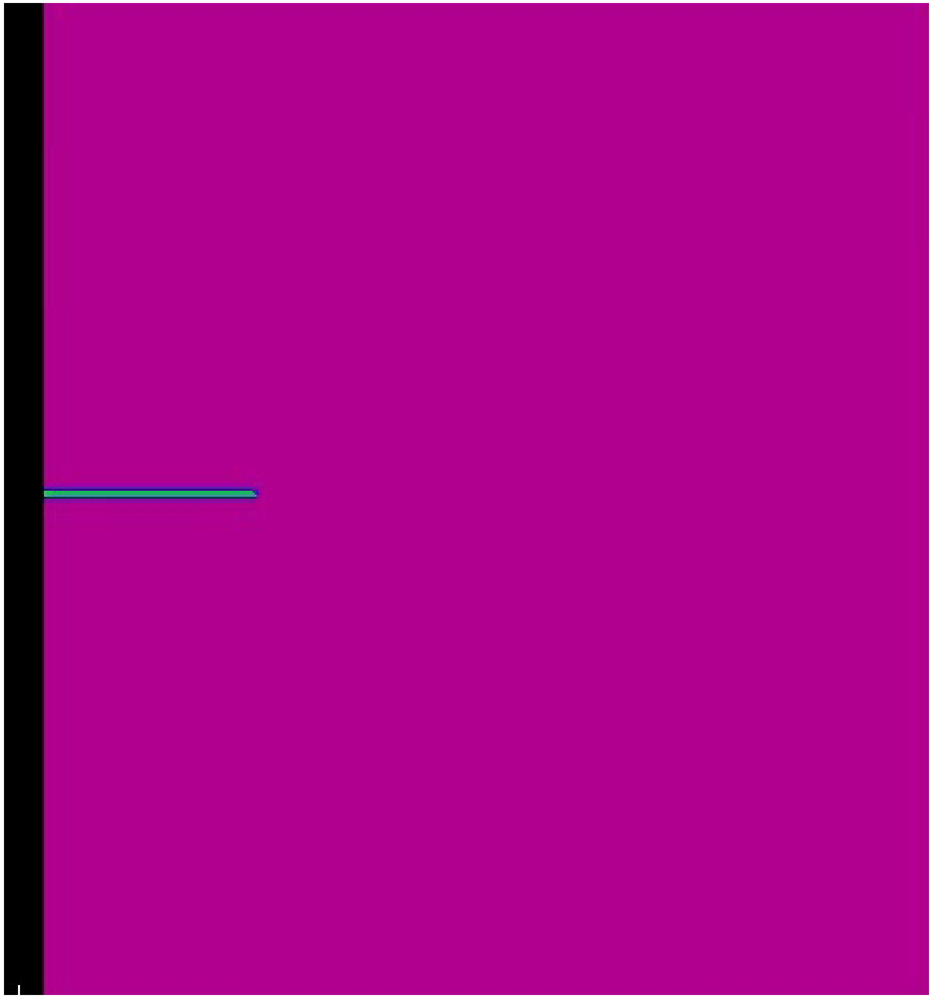


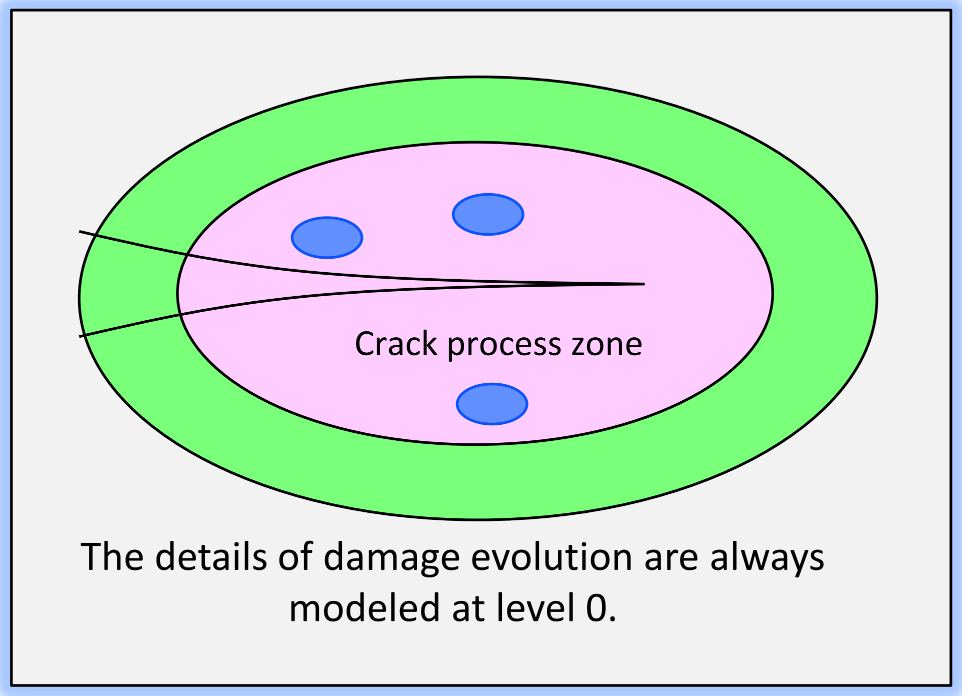
More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Some peridynamic multiscale methods and results

- Derivation of peridynamic equations from statistical mechanics (Lehoucq & Sears, 2011).
- Higher order gradients to connect MD to peridynamic (Seleson, Parks, Gunzburger, & Lehoucq, 2005).
- Adaptive mesh refinement (Bobaru & Hu, 2011).
- Coarse-graining (SS, 2011).
- Two-scale evolution equation for composites (Alali & Lipton, 2012).
- PFHMM method for atomistic-to-continuum coupling (Rahman, Foster, & Haque, 2014).

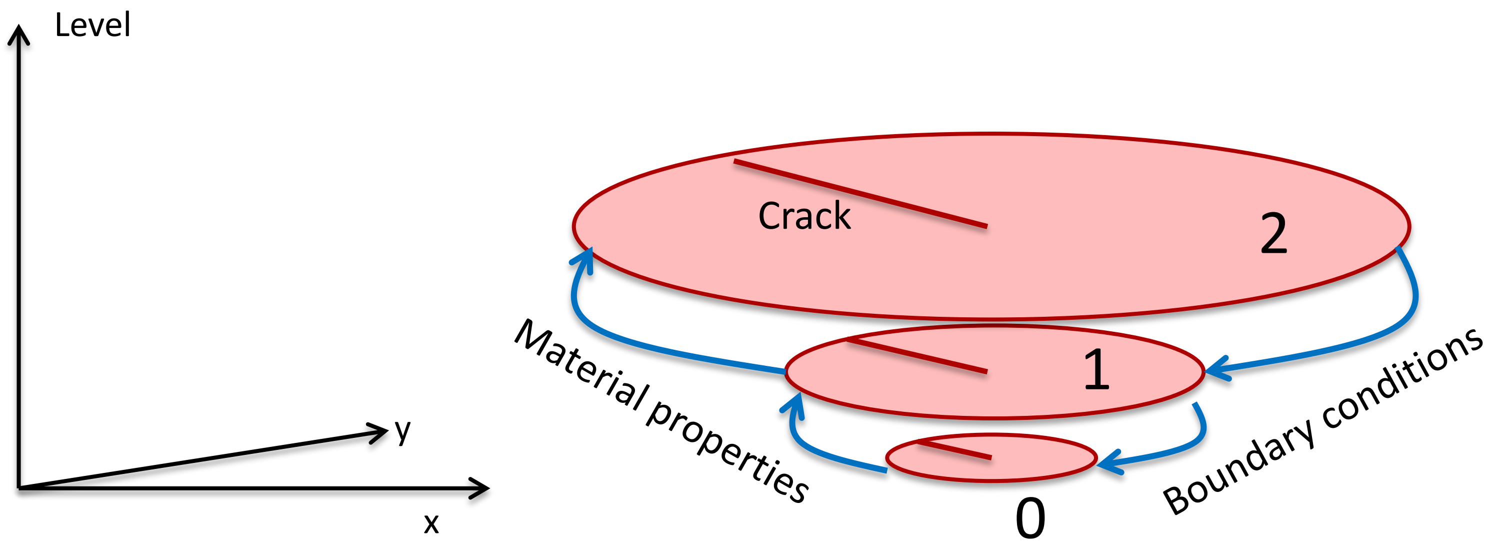
Concurrent multiscale method for defects

- Apply the best practical physics at the smallest length scale (near a crack tip).
- Scale up hierarchically to larger length scales.
- Each level is related to the one below it by the same equations.
  - Any number of levels can be used.
- Adaptively follow the crack tip.



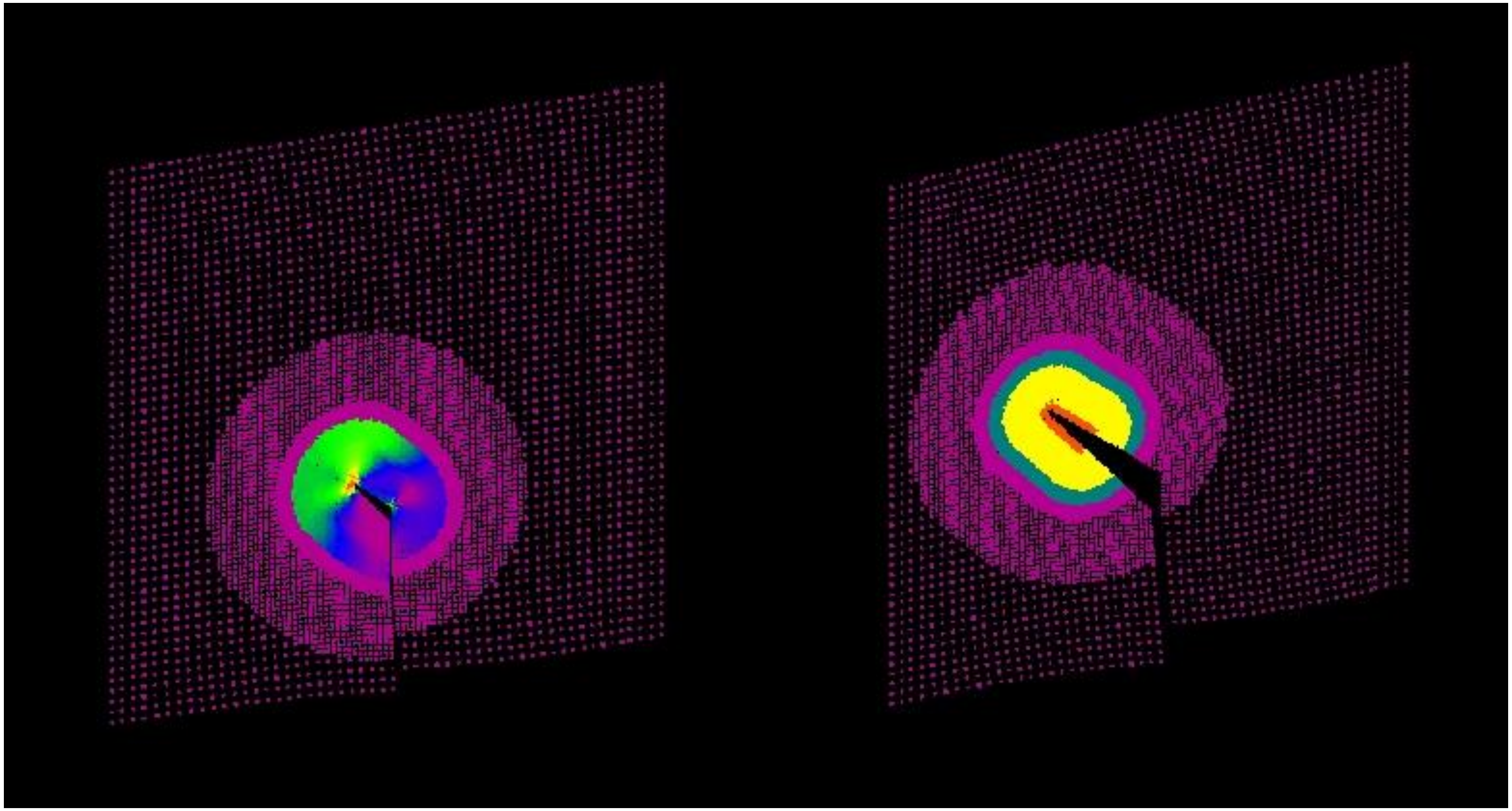
Concurrent solution strategy

- The equation of motion is applied only within each level.
- Higher levels provide boundary conditions on lower levels.
- Lower levels provide coarsened material properties (including damage) to higher levels.



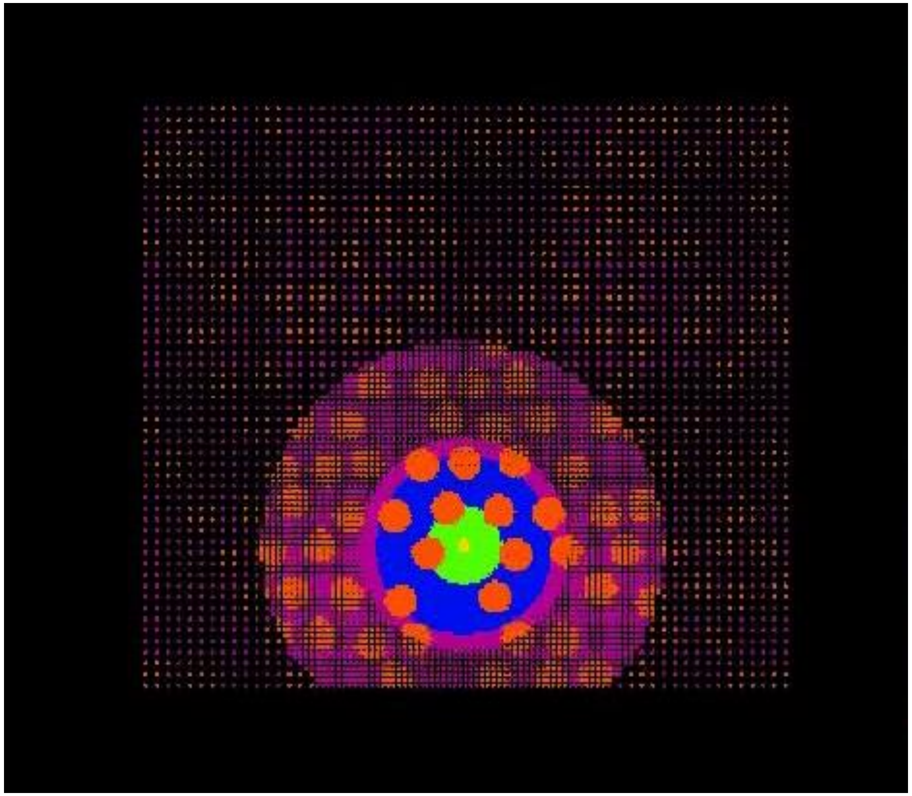
Schematic of communication between levels in a 2D body

Concurrent multiscale example: shear loading of a crack



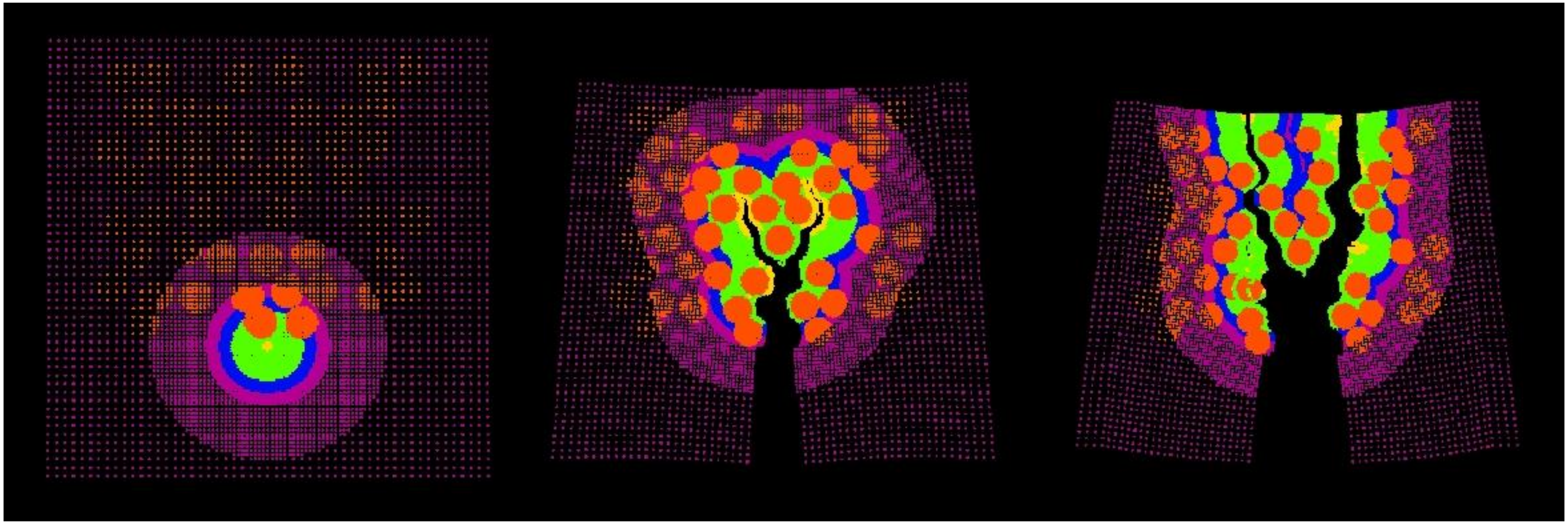
Bond strain | Damage process zone

Multiscale crack growth in a heterogeneous medium (video)



Branching in a heterogeneous medium

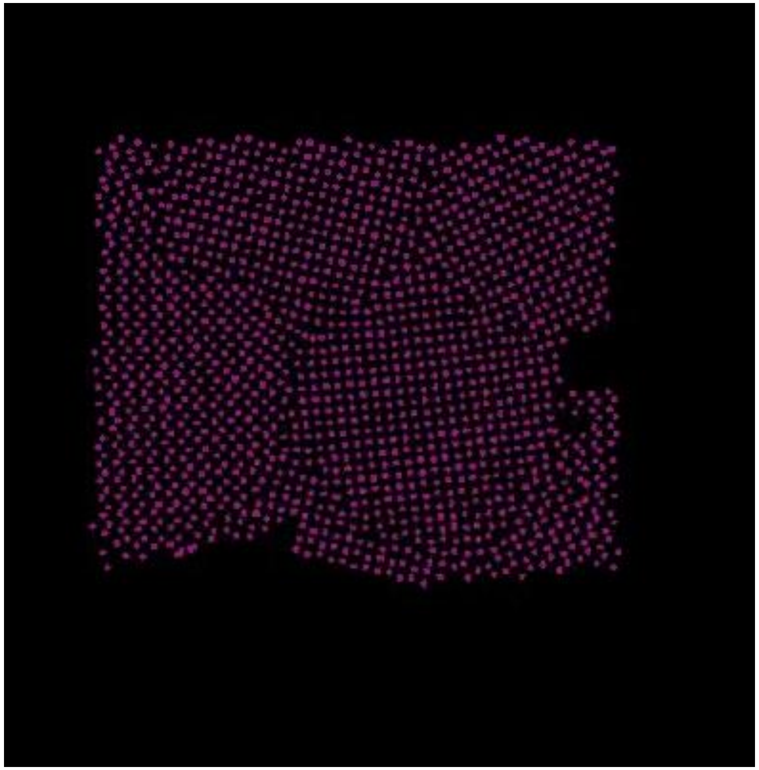
- Crack grows between randomly placed hard inclusions.



Level 0: calibrating a peridynamic model using molecular dynamics

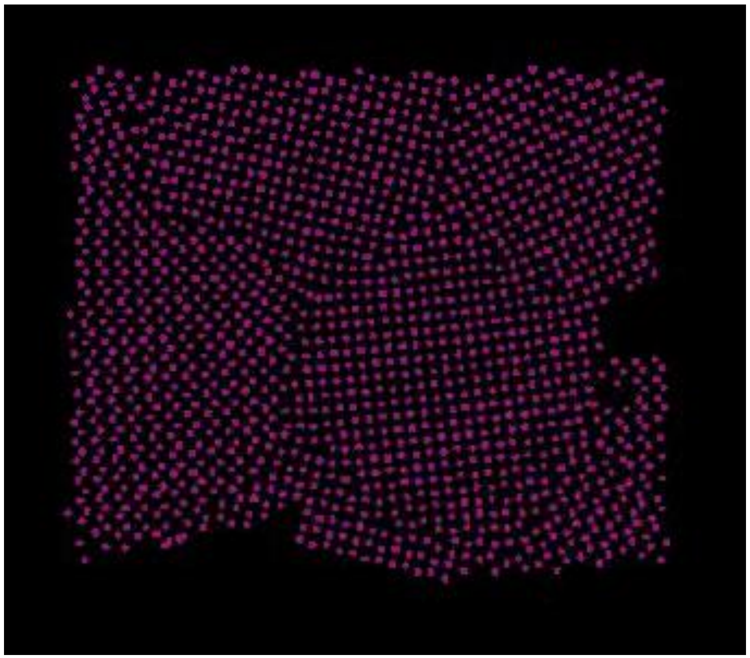
- The concurrent multiscale method, in spite of subcycling the lower levels, is still not efficient enough to use MD in level 0 for growing cracks.
- Instead: Use MD to calibrate a continuum model.

- Video show smoothed atomic positions in a LAMMPS model of Al polycrystal (courtesy David Newsome, CFD Research Corp.)
- Yellow-red: bond strains > 1.0.



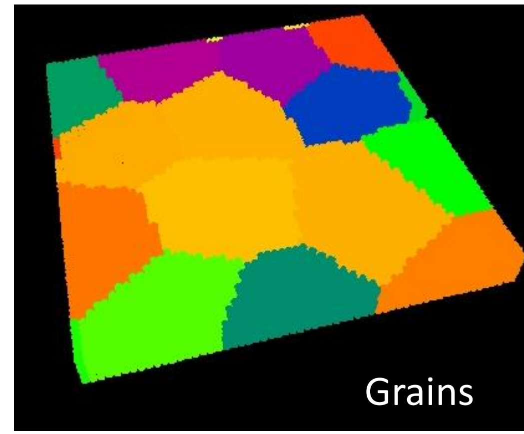
Peridynamic mesoscale simulations using properties determined from MD

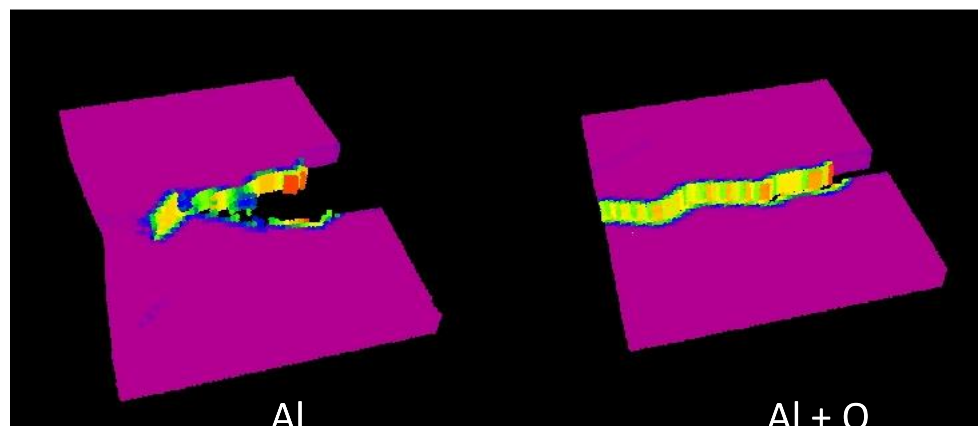
- Continuum model of a polycrystal shows the effect of embrittlement due to oxide.



Time-averaged atomic positions (LAMMPS).
Colors = peridynamic bond strain.

Calibrated peridynamic bond interactions →

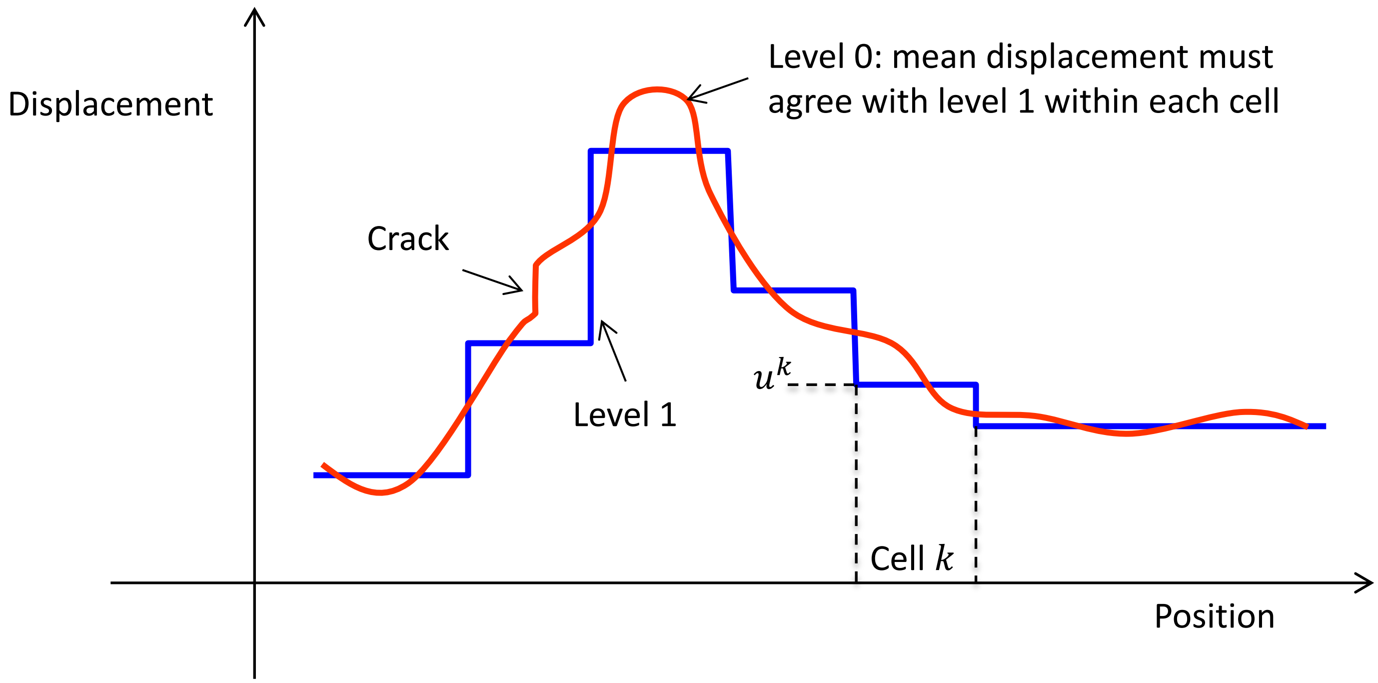




Colors indicate damage (broken bonds)

Coarse-graining to get higher-level material properties

- How can we rigorously derive higher-level material properties from lower levels?
- Divide the level 0 region into K "cells" $\mathcal{B}^k$.
- The mean displacement in each cell is a coarse-grained DOF u^k.



Coarse-graining, ctd.

- Define a functional of u and K Lagrange multipliers λ_k by

$$J = \int_{\mathcal{B}} (W - bu)\, dx - \sum_{k=1}^{K} \lambda^k \left(\int_{\mathcal{B}} (\phi^k u \, dx - u^k \right)$$

  where $\phi^k(x) = 1/\mathrm{vol}\, \mathcal{B}^k$ in cell k, 0 elsewhere.

- The Euler-Lagrange equation is

$$\int_{\mathcal{H}_{\mathbf{x}}} f(q,x)\, dq + b + \lambda^k \phi^k = 0$$

  where k is the cell that contains x.

- So, λ^k is the force density required to constrain the mean displacements.

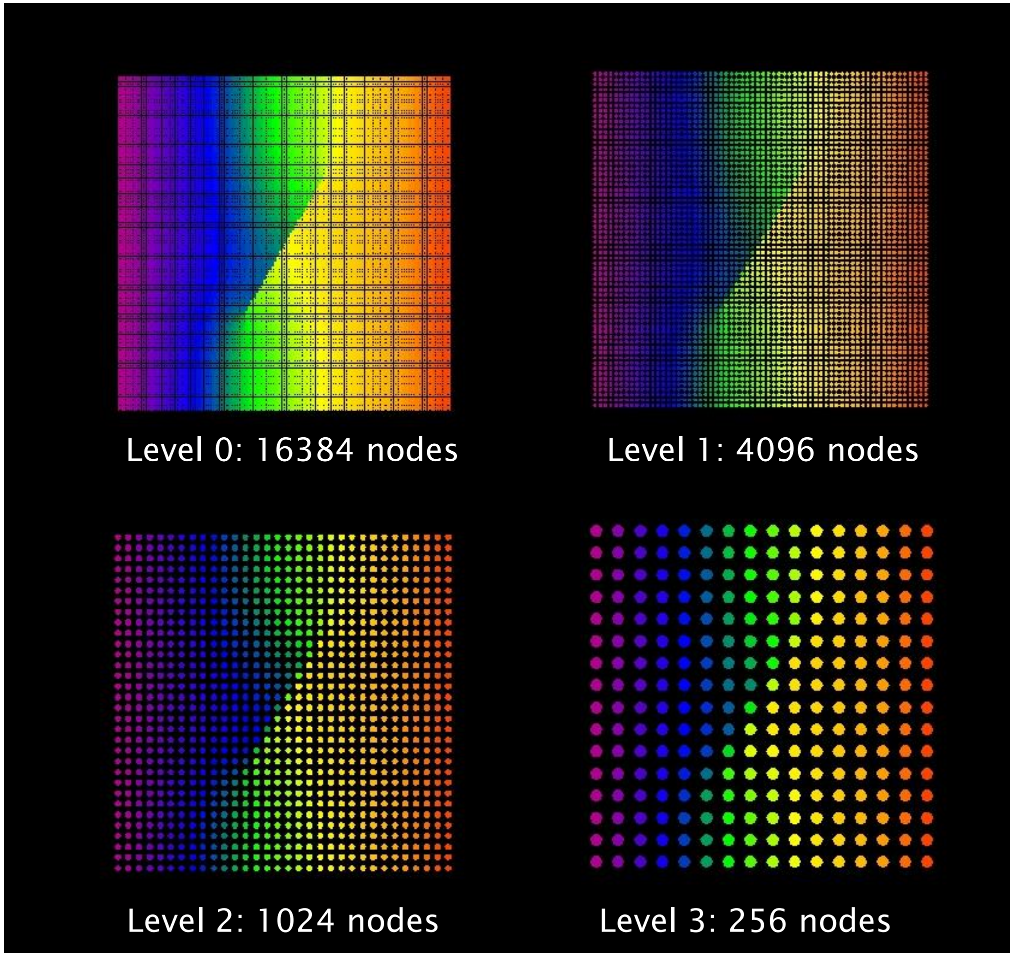
- The coarse-grained micromodulus is

$$C_{ki} = \lambda^k / u^i$$

  if we set $0 < u^i << 1$, all other cell displacements 0.

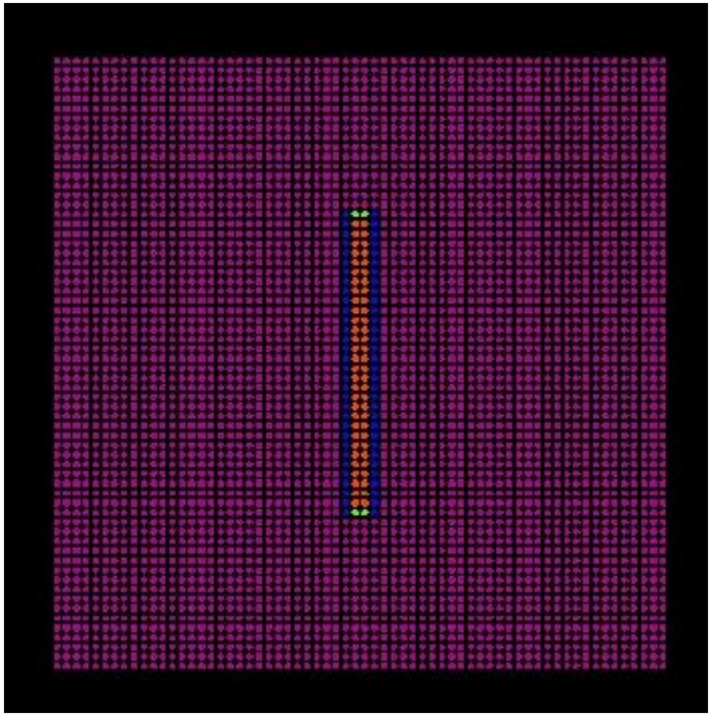
Coarse graining verification: crack in a plate

- Example: Solve the same problem in four different levels – results are the same.



Defining damage from coarse-grained material properties

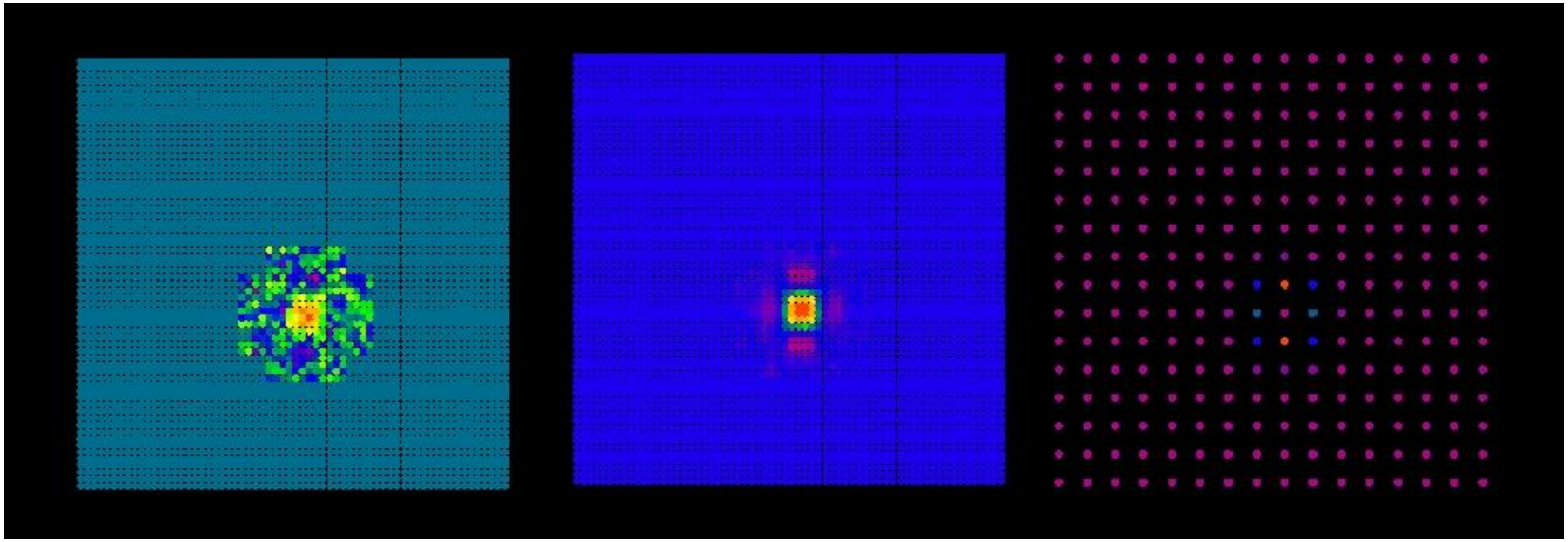
- Define bonds to be damaged if their coarse-grained micromodulus is less than a tolerance.
- This allows damage to be determined without deforming the MD grid.



Level 1 damage contours deduced from coarse-grained properties

Coarse graining MD directly into peridynamics

- The level 0 physics can be anything: PD, standard continuum, MD, MC(?), DFT(?)



Level 0: MD showing thermal oscillations

MD time-averaged displacements

Level 1: Coarse grained micromodulus

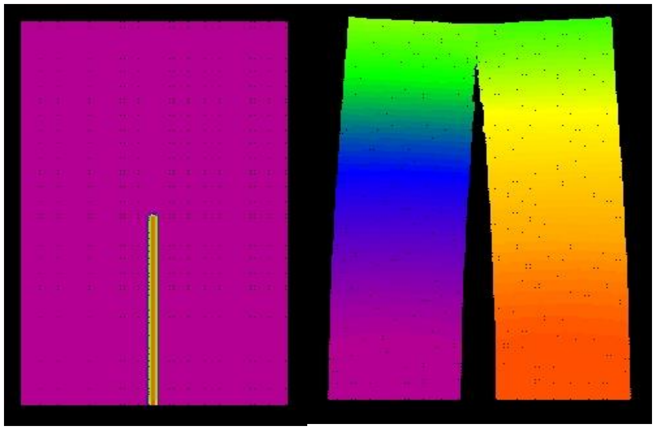
Summary

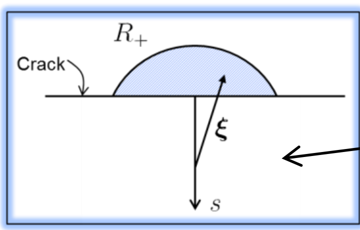
- Concurrent multiscale:
  - Adaptively follow crack tips.
  - Apply the best practical physics in level 0.
  - MD time step is impractical. Instead…
- Calibrate a peridynamic damage model from an MD simulation.
  - Derives continuum damage parameters ("parameter passing").
- Coarse-graining:
  - Derives incremental elastic properties at higher levels.
  - Does not rely on a representative volume element (RVE).

- Methods are "scalable:" can be applied any number of times to obtain any desired increase in length scale.

Extra slides

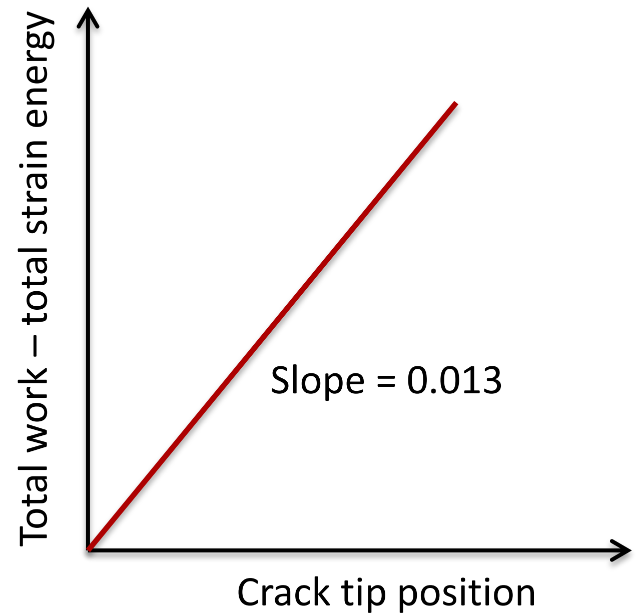
Constant bond failure strain reproduces the Griffith crack growth criterion





From bond properties, energy release rate should be

G = 0.013



- This confirms that the energy consumed per unit crack growth area equals the expected value from bond breakage properties.

Rescaling a material model

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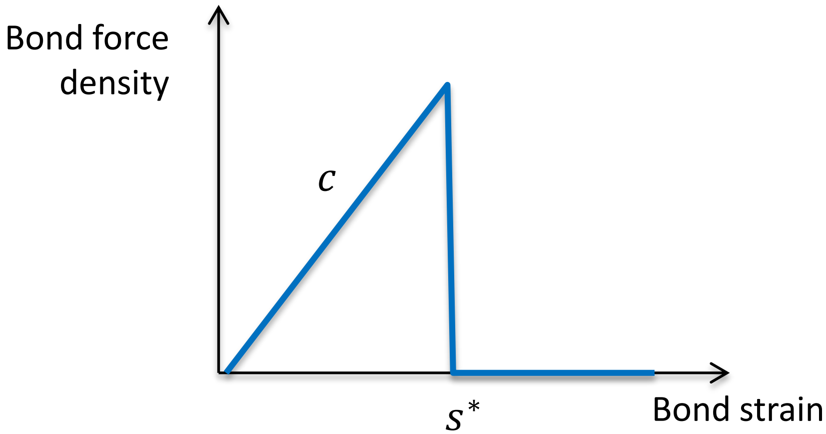
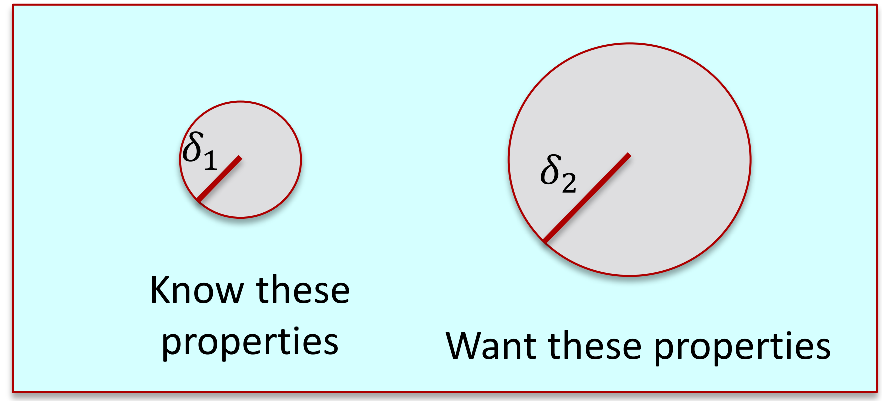




For bond based models, can show (SS & Askari, 2005):

- Bulk elastic properties are invariant if we set

$$\frac{c_2}{c_1} = \left(\frac{\delta_2}{\delta_1}\right)^{-4}$$

- Critical energy release rate is invariant if we set

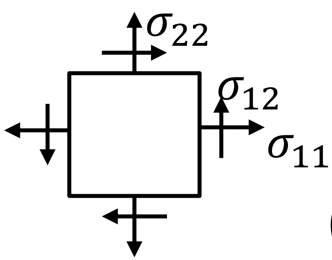
$$\frac{{s^*}_2}{{s^*}_1} = \left(\frac{\delta_2}{\delta_1}\right)^{-1/2}$$

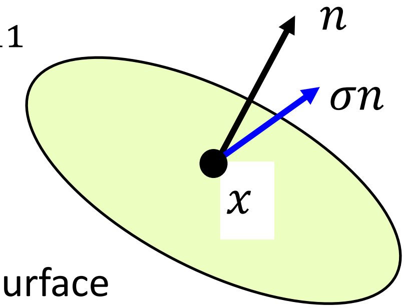
- There are similar relations for other classes of material models.
- Not a good method for heterogeneous materials.

Peridynamics basics: The nature of internal forces

Standard theory

Stress tensor field
(assumes continuity of forces)





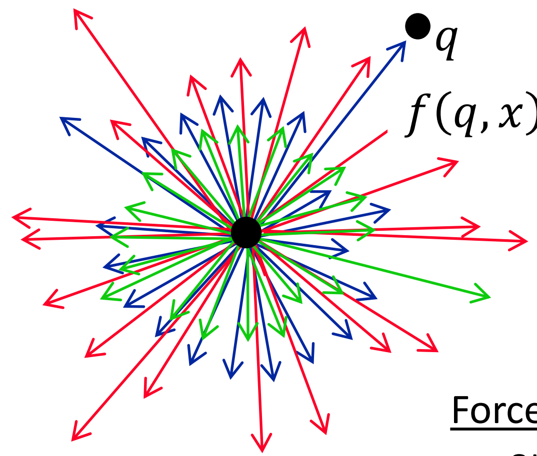
Stress tensor maps surface normal vectors onto surface forces

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

Differentiation of surface forces

Peridynamics

Bond forces between neighboring points
(allowing discontinuity)



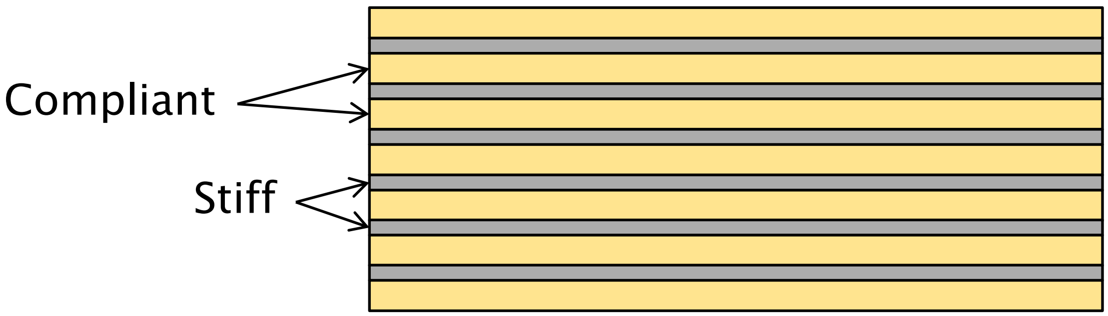
Force state maps bonds onto bond forces

$$\rho\ddot{u}(x,t) = \int_{H_x} f(q,x)dV_q + b(x,t)$$

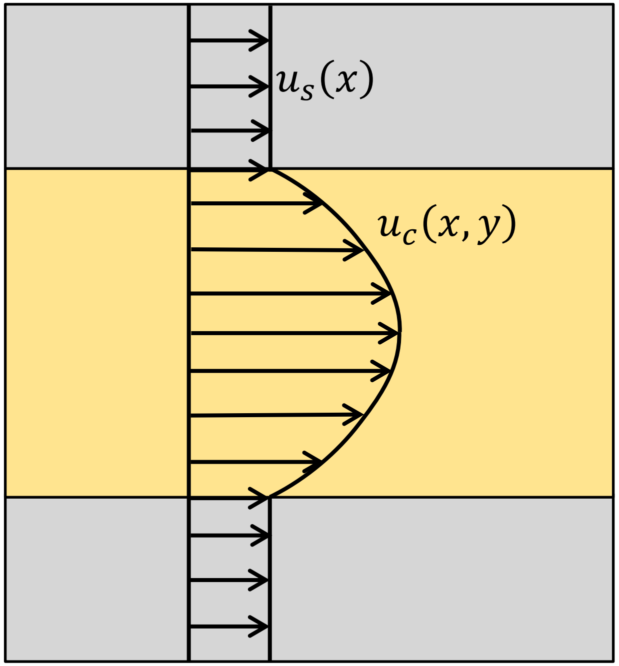
Summation over bond forces

Nonlocality – is it real?

- It is commonly assumed that the local model (PDE-based) is an excellent approximation for continuous media, due to the small size of interatomic distances.
- This is true if we model the system in sufficient detail.
- When we use a “smoothed out” displacement field, nonlocality appears in the equations. Example…

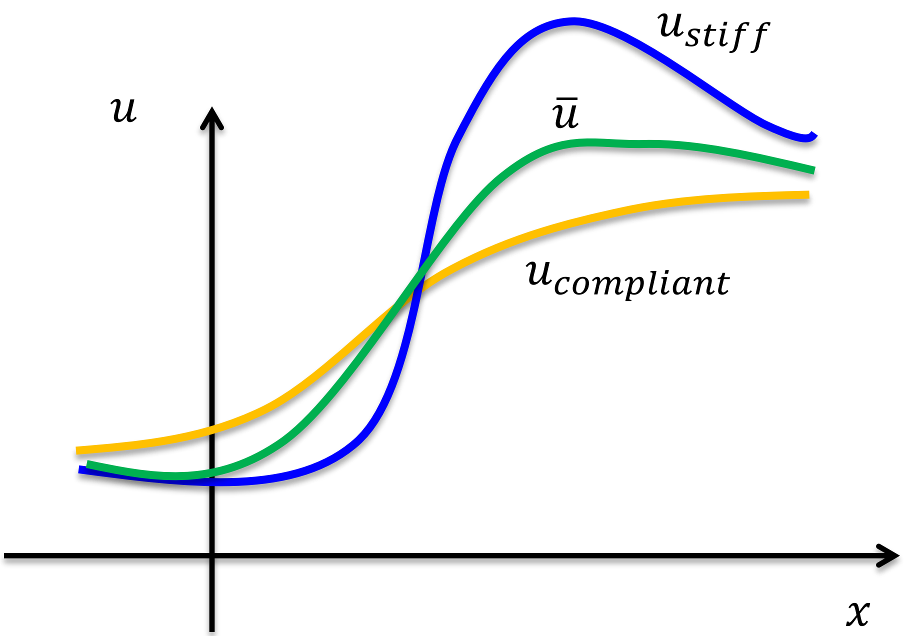


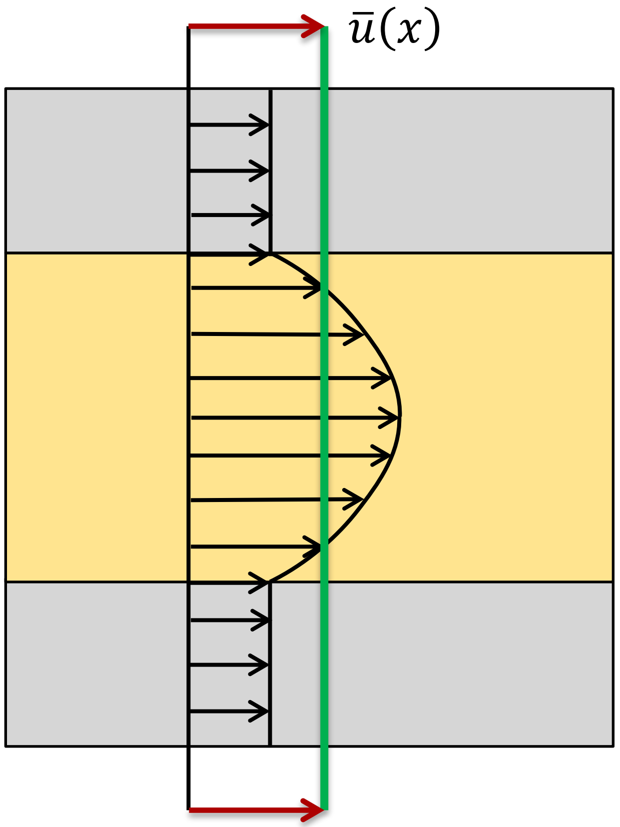
Layered composite (1D)



Nonlocality in a homogenized model

- Choose to model the composite as a single mass-weighted average displacement field $\bar{u}(x)$.





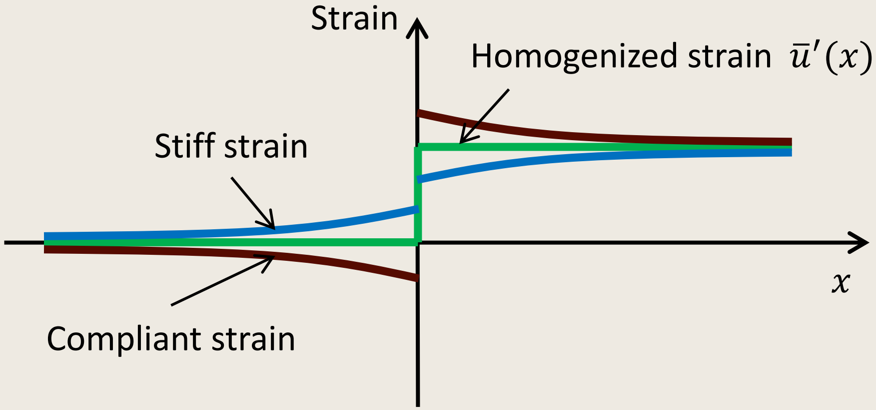
Nonlocality in a homogenized model

- After computing the force transfer between the phases, the equation of motion turns out to be

$$\rho\ddot{\bar{u}}(x,t) = E_c\bar{u}''(x,t) + \gamma k\lambda^4 \int_{-\infty}^{\infty} (\bar{u}(p,t) - \bar{u}(x,t))e^{-\lambda|x-p|}\,dp + b(x,t),$$

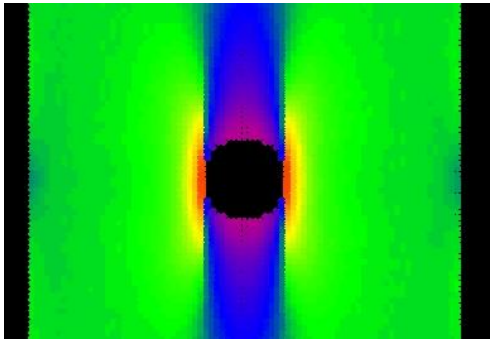
$$\frac{1}{\lambda} = \sqrt{\frac{E_s h_s h_c^2}{3\mu_c(h_s+h_c)}} = \text{length scale.}$$

Strain in each phase if the homogenized strain follows a step function

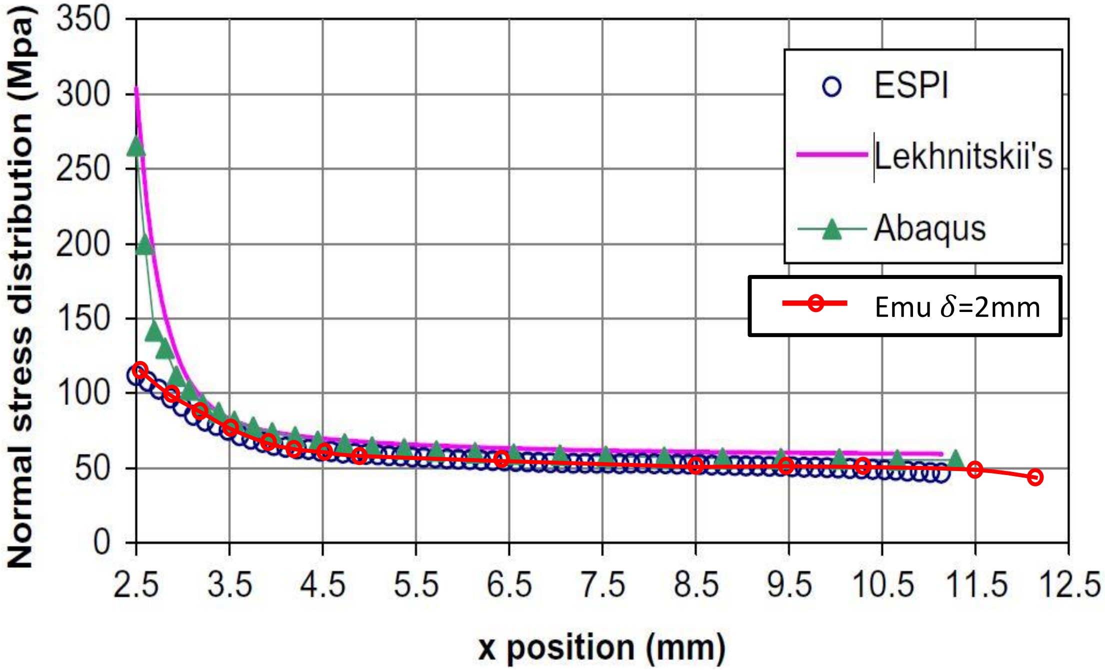


Are composites nonlocal?

- Peridynamic model is more accurate than the local model for predicting stress concentration in a laminate.
- $h_s = h_c$ =0.4mm, $E_s = 150$GPa, μ_c =4GPa.
- $\Rightarrow 1/\lambda = 1.41$mm.



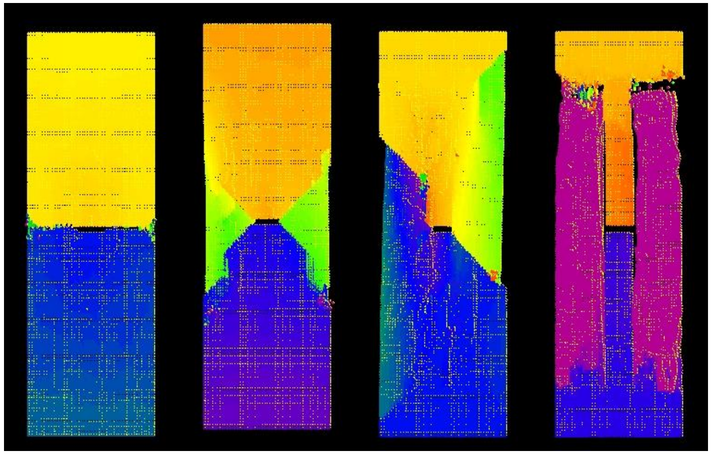
EMU: contours of longitudinal stress
Horizon = 2mm



Data of Toubal, Karama, and Lorrain, Composite Structures 68 (2005) 31-36

Splitting and fracture mode change in composites

- Distribution of fiber directions between plies strongly influences the way cracks grow.

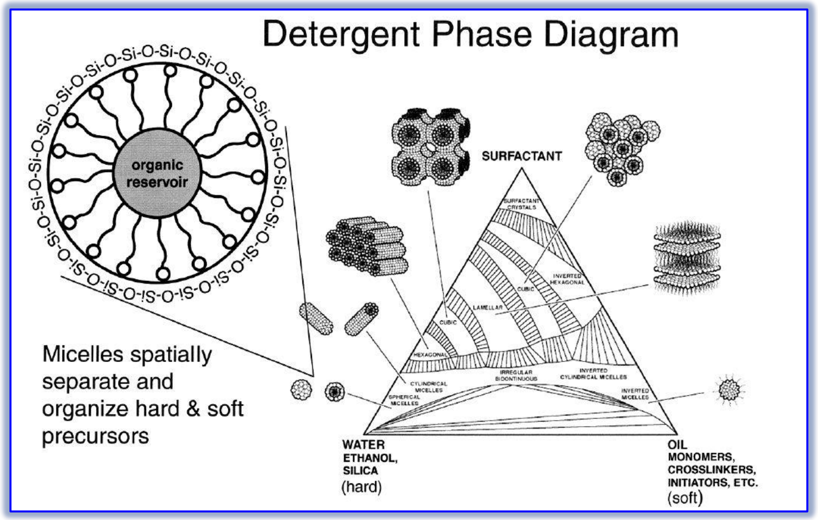


EMU simulations for different layups

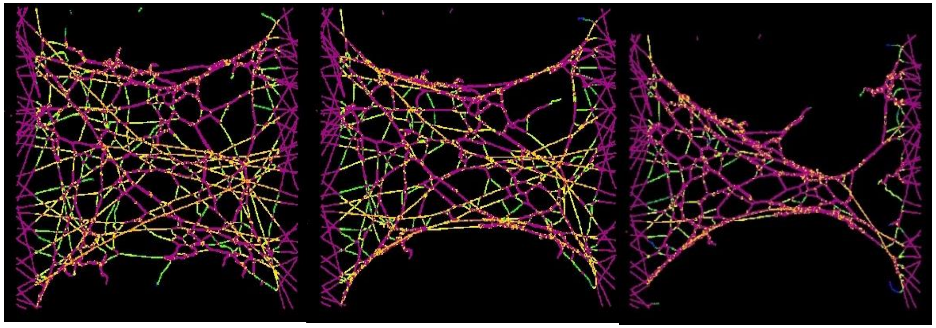
Typical crack growth in a notched laminate (photo courtesy Boeing)

Self-assembly and long-range forces

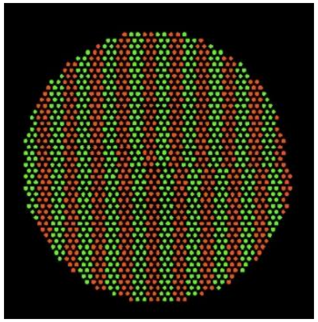
• Potential importance for self-assembled nanostructures.
• All forces are treated as long-range.



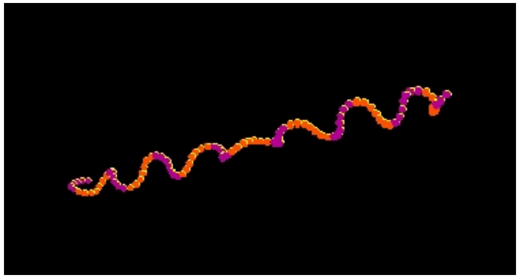
Self-assembly is driven by long-range forces
Image: Brinker, Lu, & Sellinger, Advanced Materials (1999)



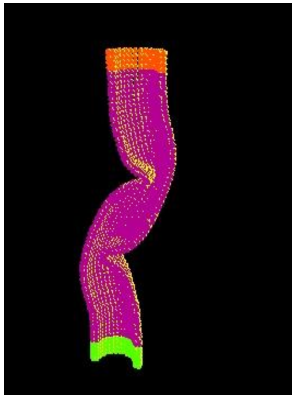
Failure in a nanofiber membrane
(F. Bobaru, Univ. of Nebraska)



Dislocation



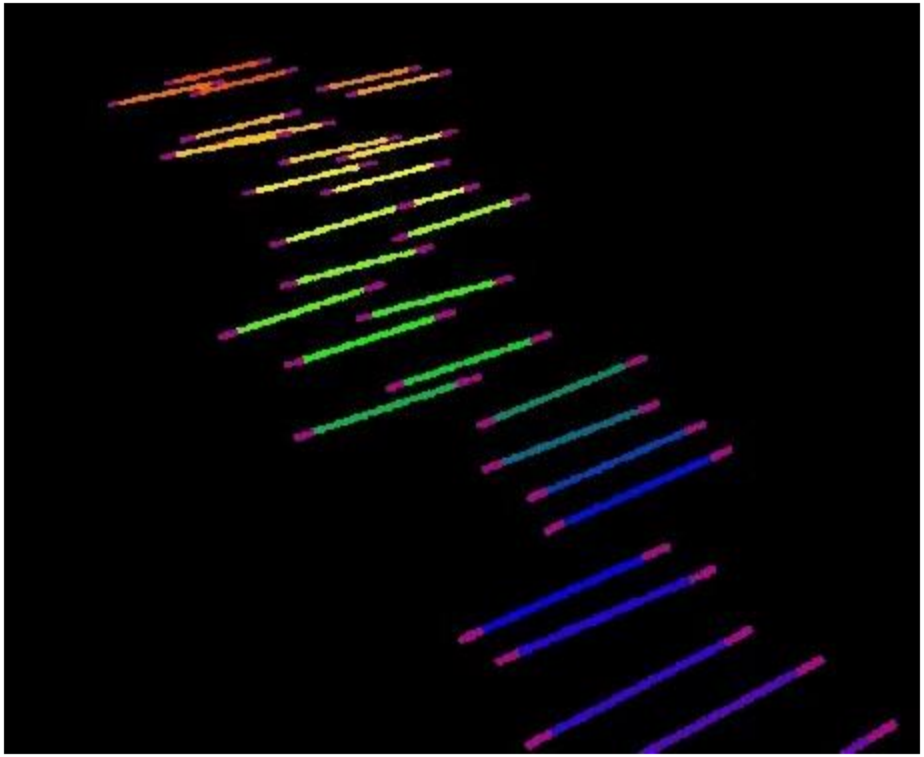
Nanofiber self-shaping



Carbon nanotube

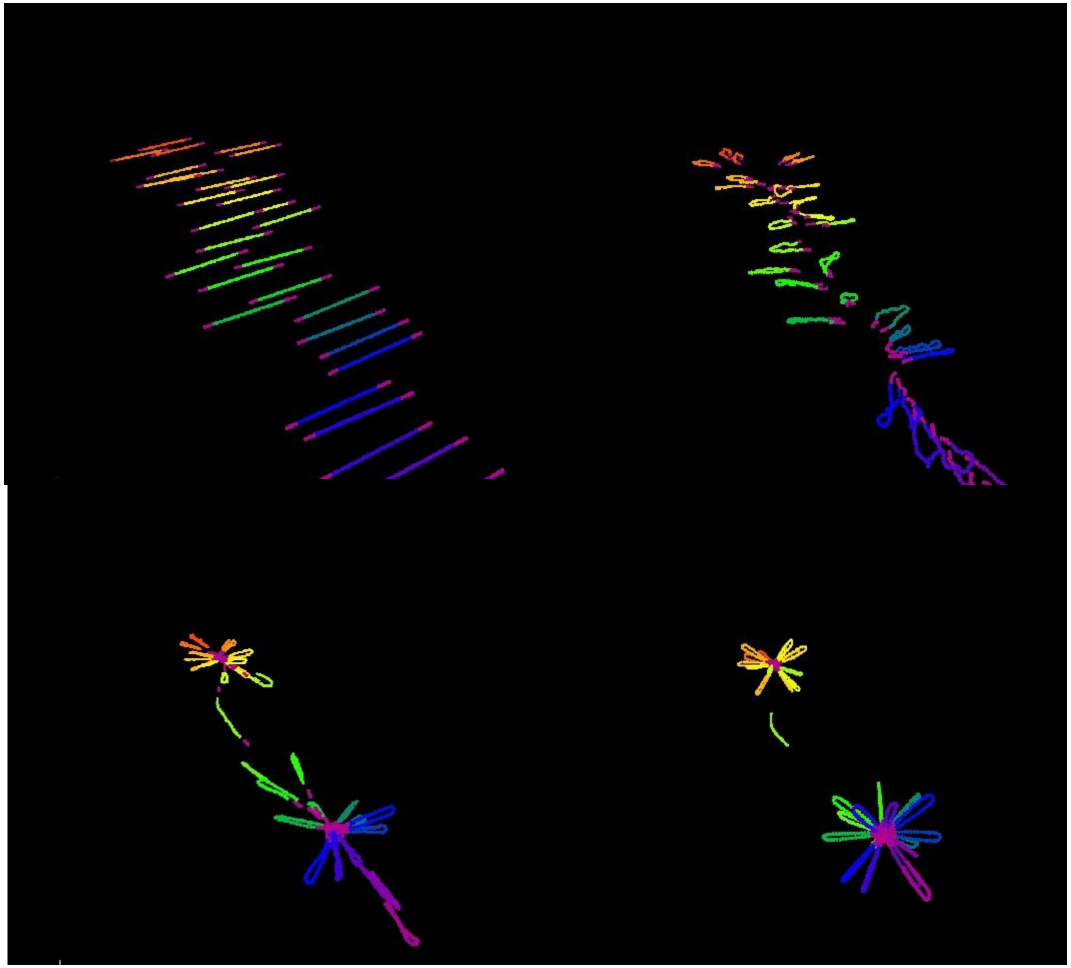
Self-assembly example

- Solution of long rods modeled as a peridynamic continuum:
  - Ends of the rods attract.
  - Inner parts of the rods repel.
  - Rods have a small resistance to bending.
- Rods are initially straight, then find a lower energy configuration.
- Peridynamics is useful because of the problem involves both continuum and long-range interactions.

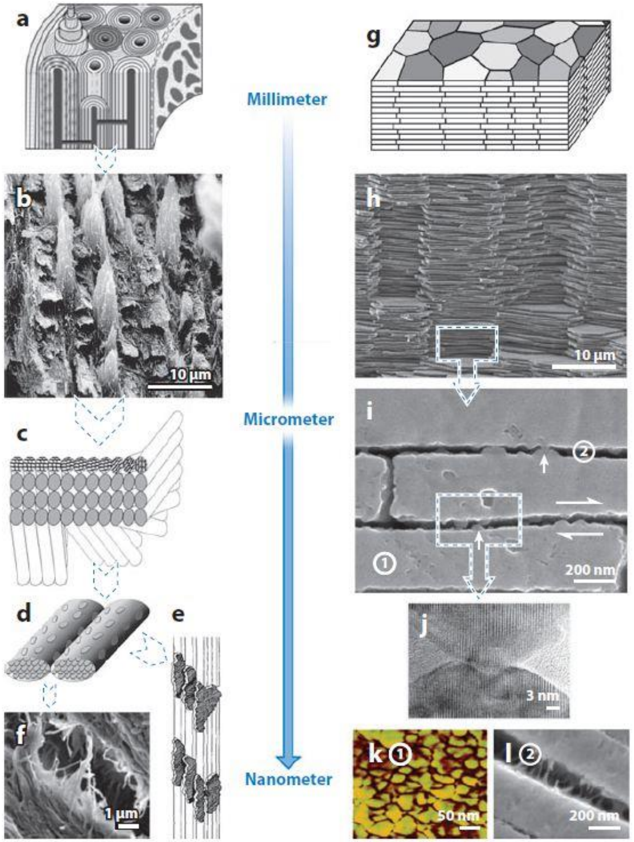


Video

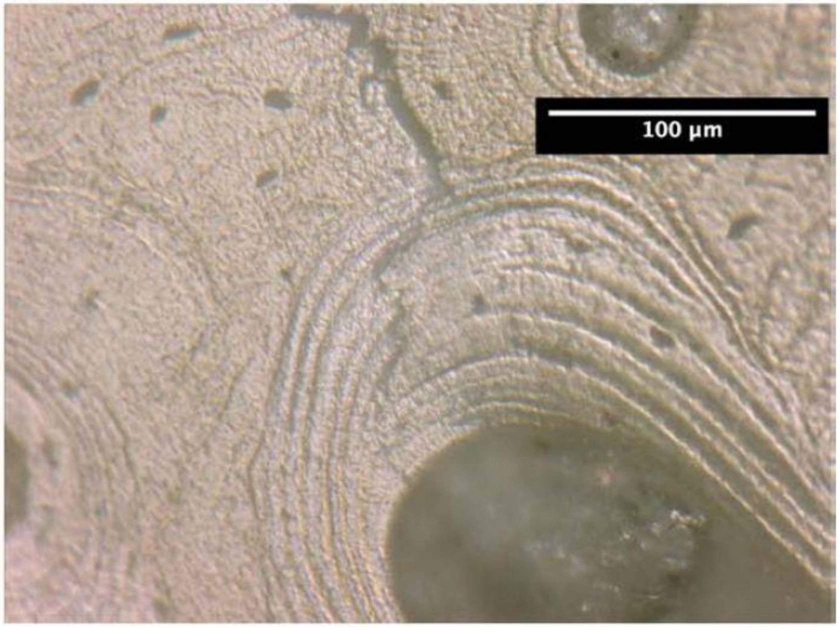
Self-assembly example



Bone: A composite material with many length scales



Bone contains a heirarchy of structures at many length scales. Image: Wang and Gupta, *Ann. Rev. Mat. Sci.* 41 (2011) 41-73



Bone structure helps delay, deflect crack growth. Image: Chan, Chan, and Nicolella, *Bone* 45 (2009) 427–434

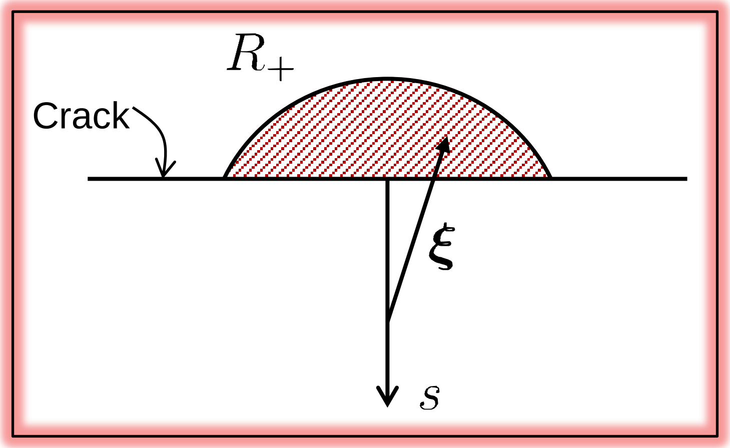
Discussion

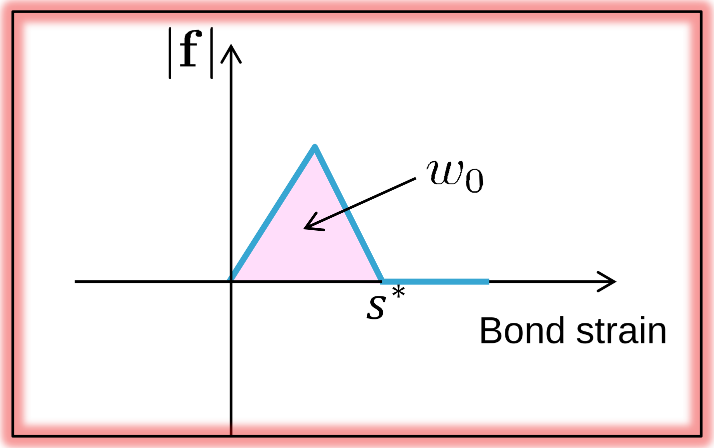
- All forces are treated as long-range forces.
- The basic equations allow discontinuities – compatible with cracks.
- Cracks do whatever they want – no need for supplemental equations.
- Some practical difficulties:
    - Slower than standard finite elements.
    - Boundary conditions are different than in the standard theory.

Critical bond strain: Relation to critical energy release rate

If the work required to break the bond $\boldsymbol{\xi}$ is $w_0(\boldsymbol{\xi})$, then the energy release rate is found by summing this work per unit crack area (J. Foster):

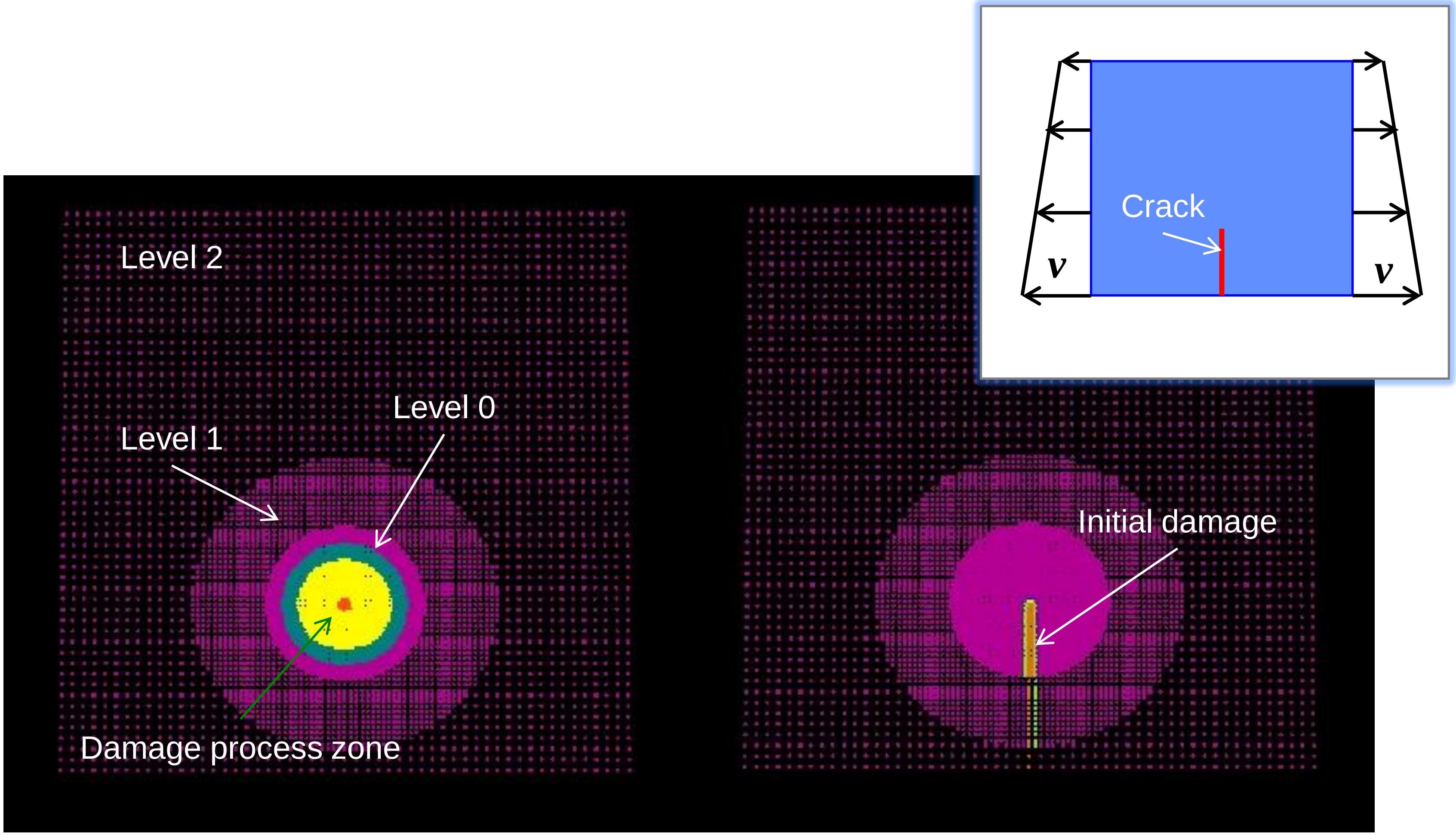
$$G = \int_0^{\delta} \int_{R_+} w_0(\boldsymbol{\xi}) \; dV_{\boldsymbol{\xi}} \; ds$$



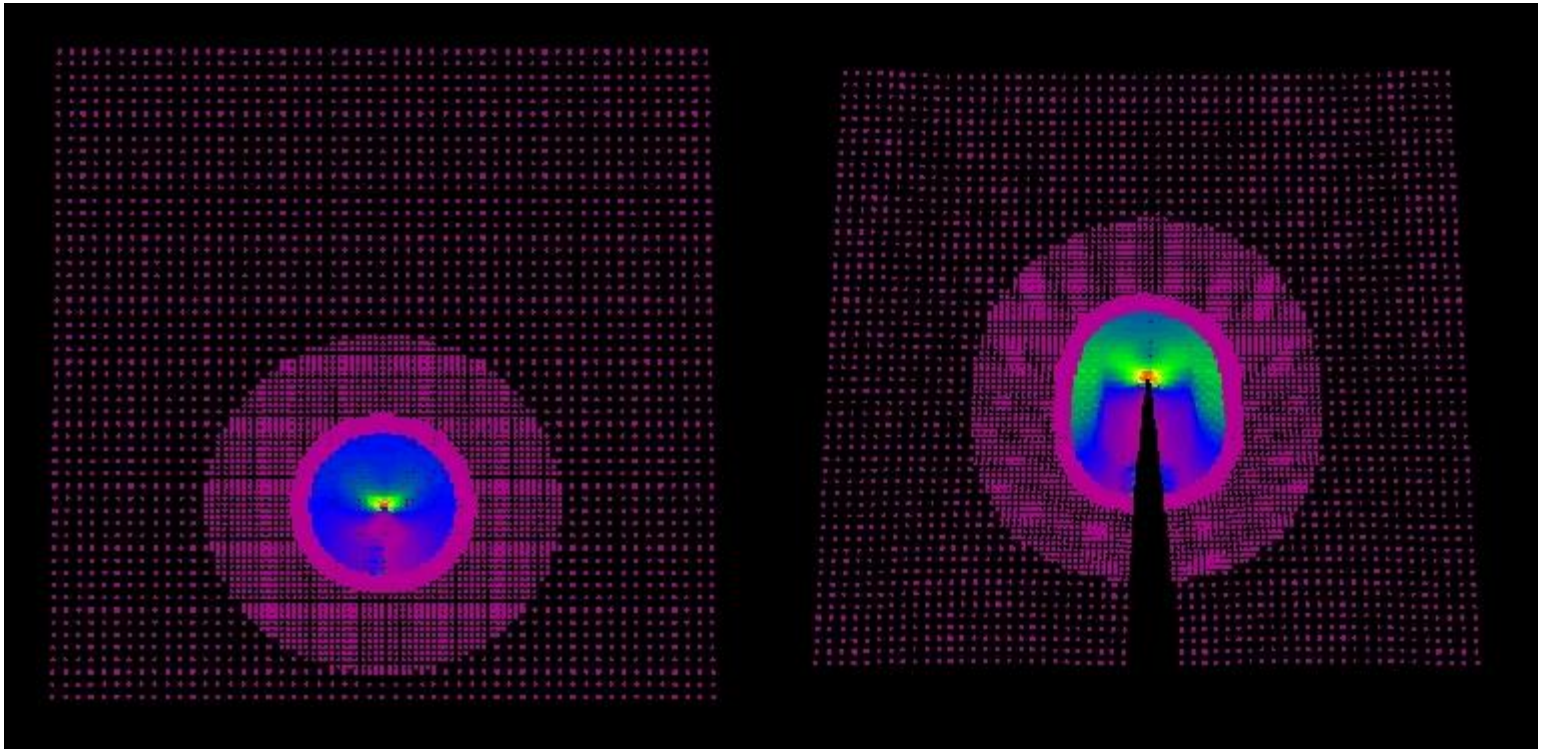


- Can then get the critical strain for bond breakage s^* in terms of G.
- Could also use the peridynamic J-integral as a bond breakage criterion.

Multiscale examples: Crack growth in a brittle plate

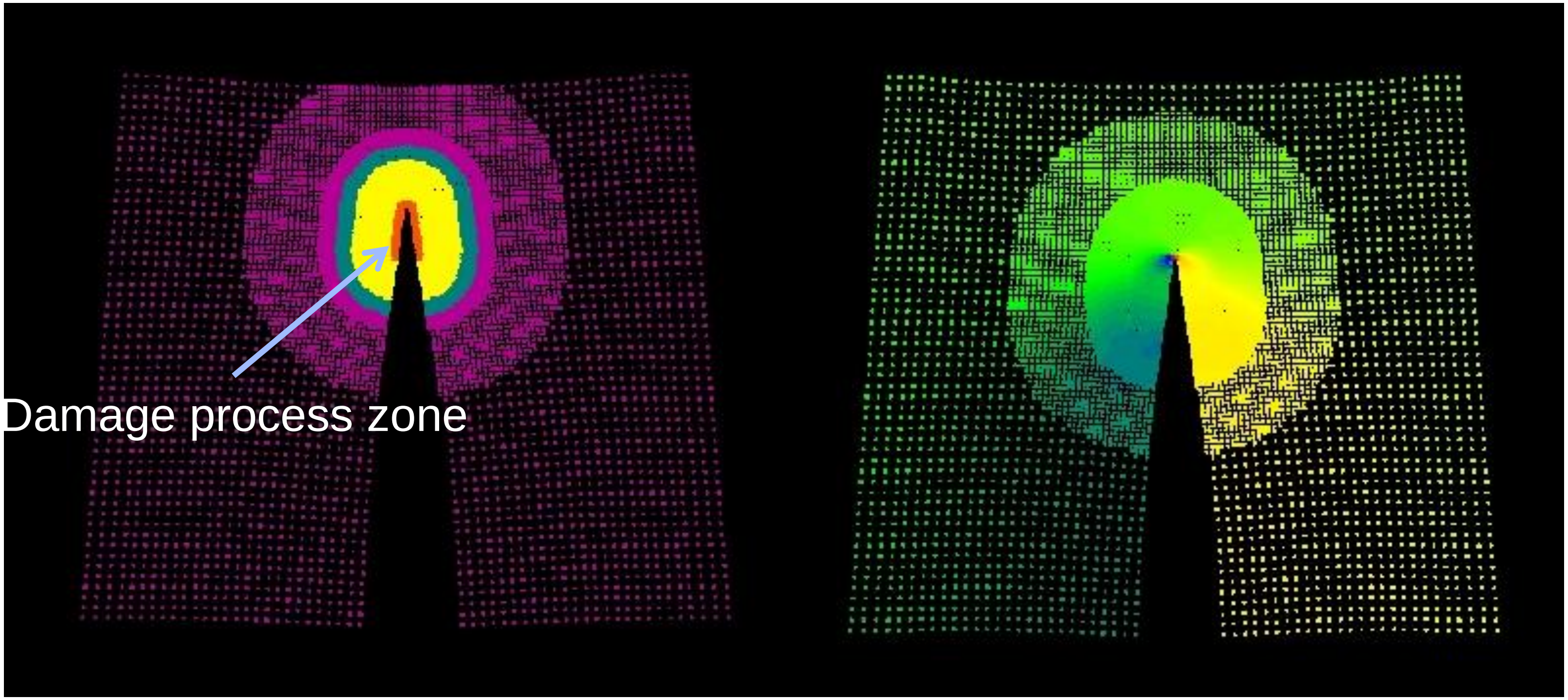


Crack growth in a brittle plate: Bond strains



Colors show the largest strain among all bonds connected to each node.

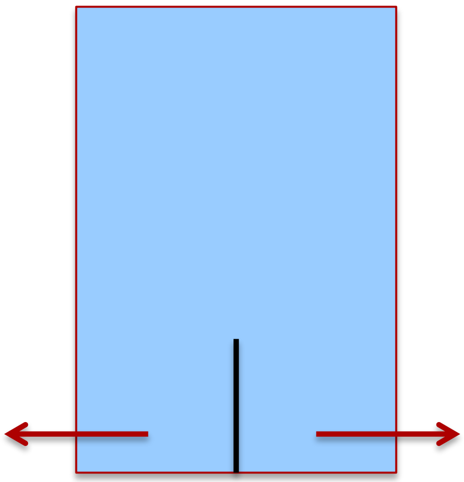
Levels move as the crack grows

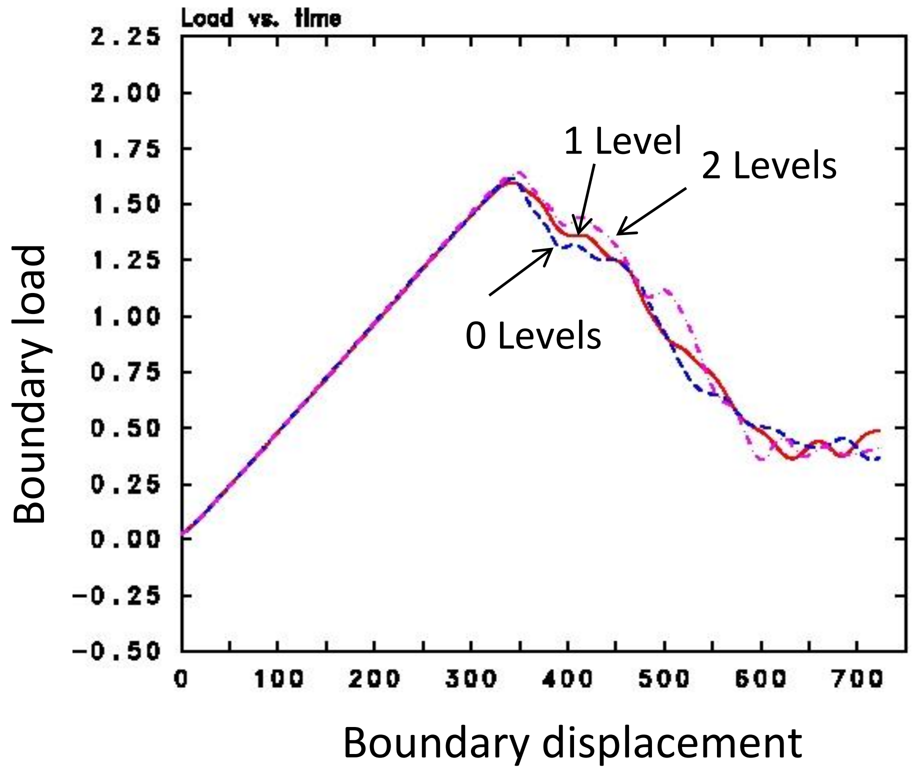


v_1 velocity

Results with and without multiscale

- All three levels give essentially the same answer.
- Higher levels substantially reduce the computational cost.



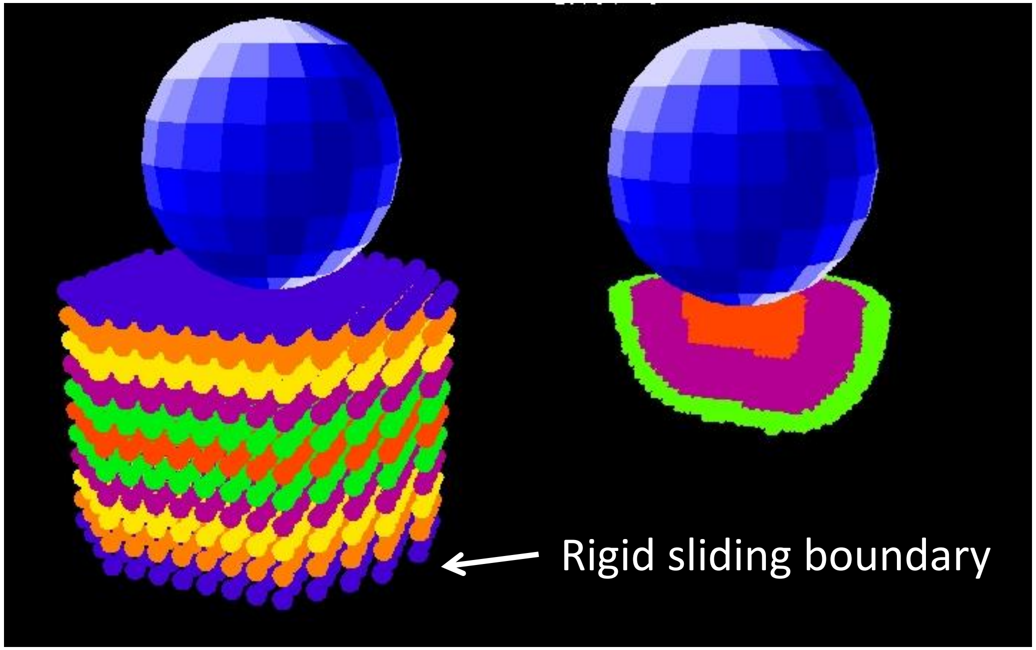


Level	Wall clock time (min) with 28K nodes in coarse grid	Wall clock time (min) with 110K nodes in coarse grid
0	30	168
2	8	16

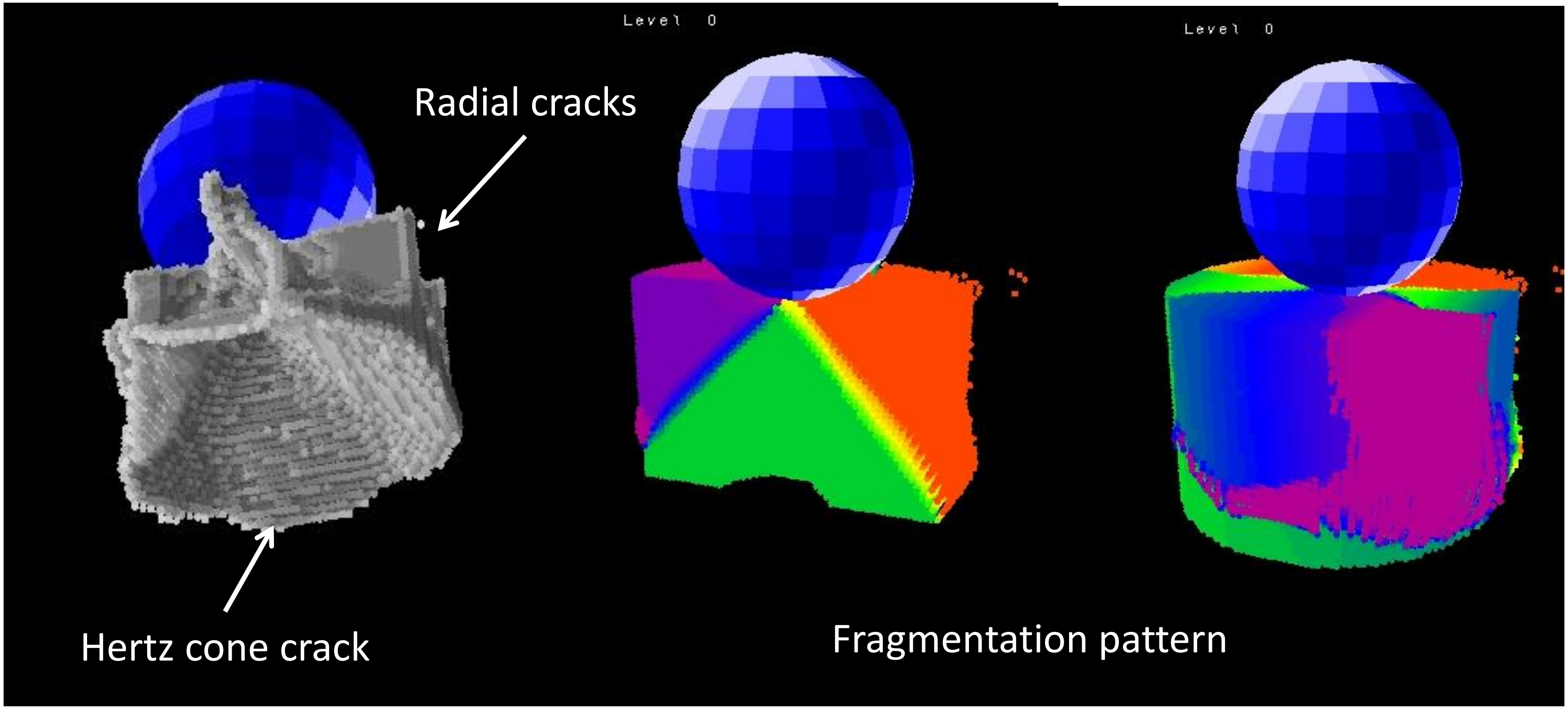
Contact mechanics: Rigid spherical indenter

Level 2

Level 0



Spherical indenter, ctd.



Multiscale method discussion

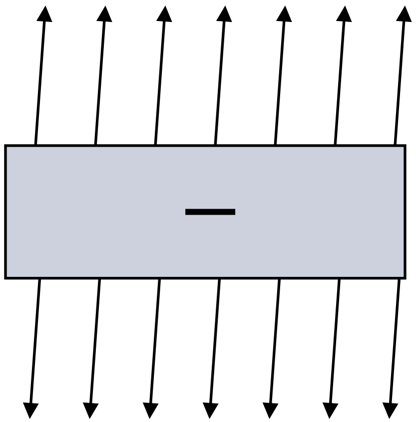
- Advantages
  - Avoids need for strong coupling (forces acting between different levels).
  - Combines multiscale with adaptive refinement.
  - Provides damaged material properties to higher levels.

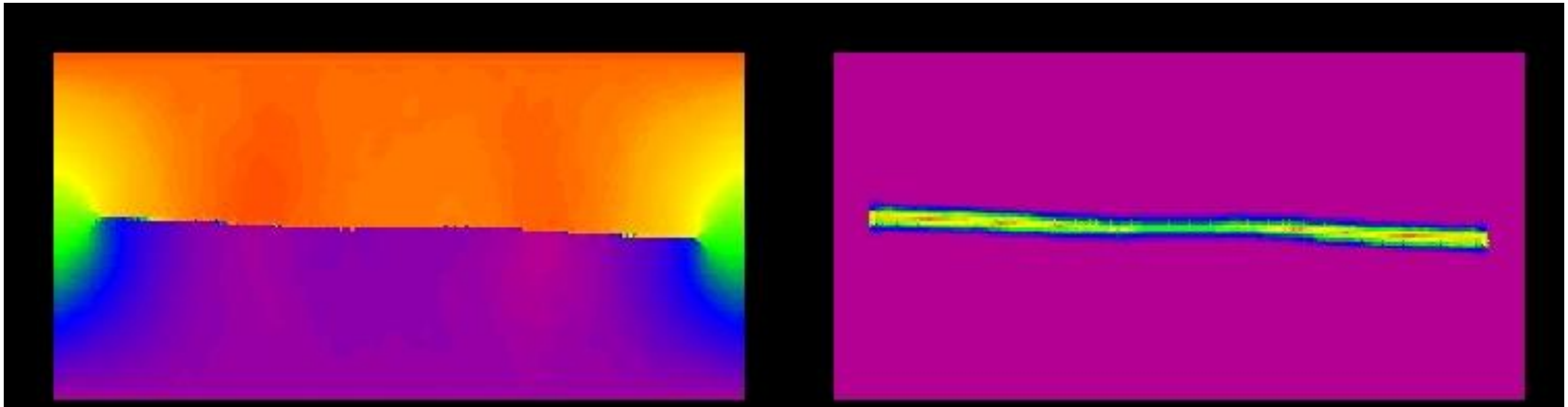
- Disadvantages
  - Difficult to know where to unrefine.
  - Pervasive fracture leads to a large number of level 0 DOFs.
  - Don’t yet have a general coarse graining method for heterogenous media.

Reduced mesh effects

- Plate with a pre-existing defect is subjected to prescribed boundary velocities.
- These BC correspond to mostly Mode-I loading with a little Mode-II.

$$\dot{\varepsilon} = (0.25\text{s}^{-1}) \begin{bmatrix} 0 & 0.1 \\ 0 & 1 \end{bmatrix}$$

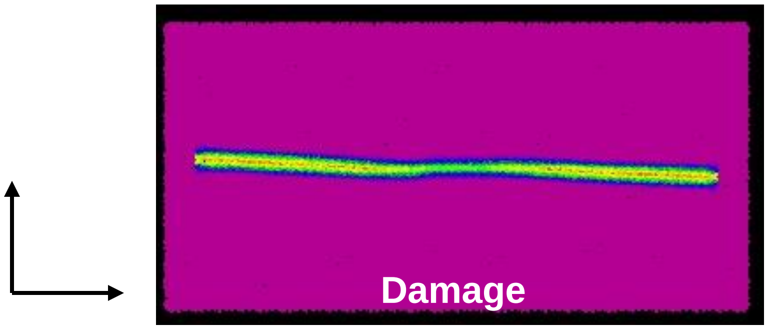




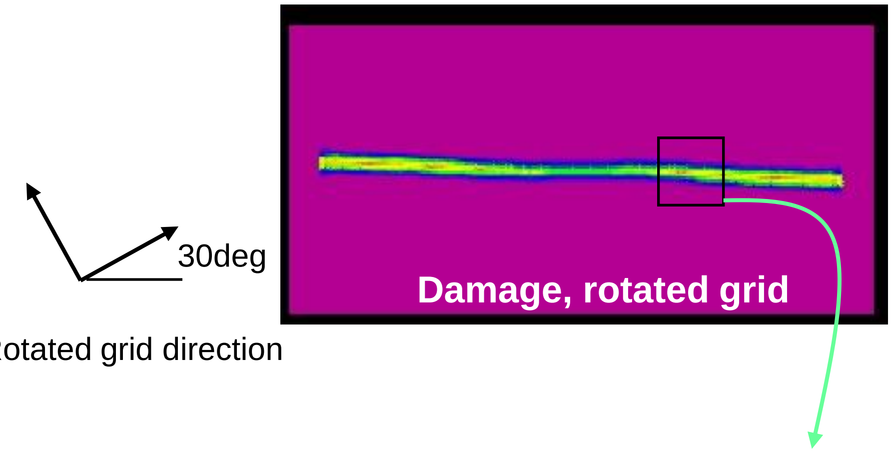
Contours of vertical displacement

Contours of damage

Effect of rotating the grid

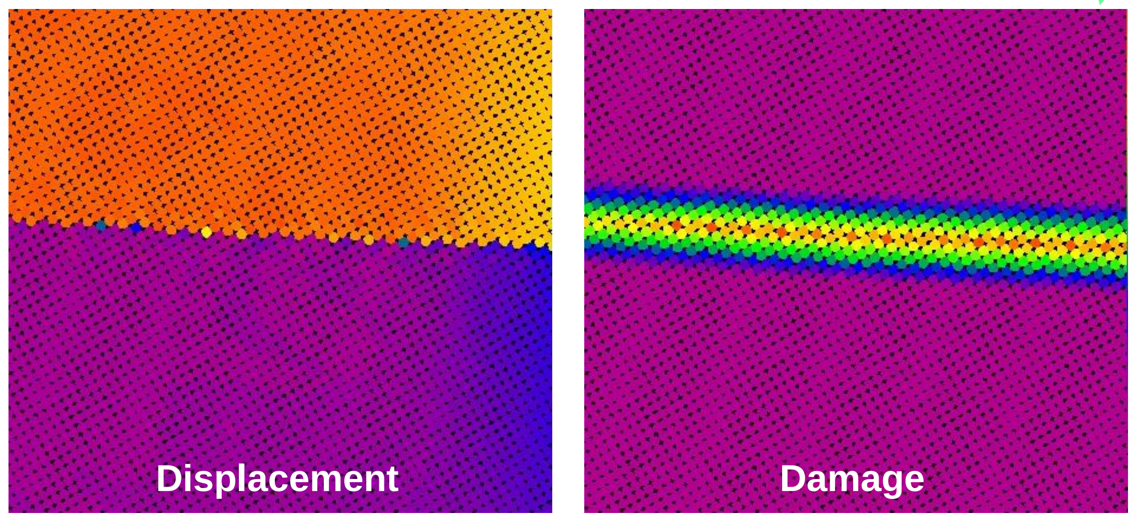


Original grid direction

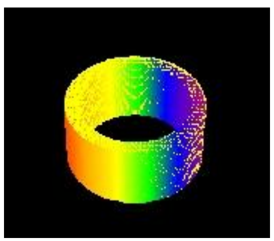


Rotated grid direction

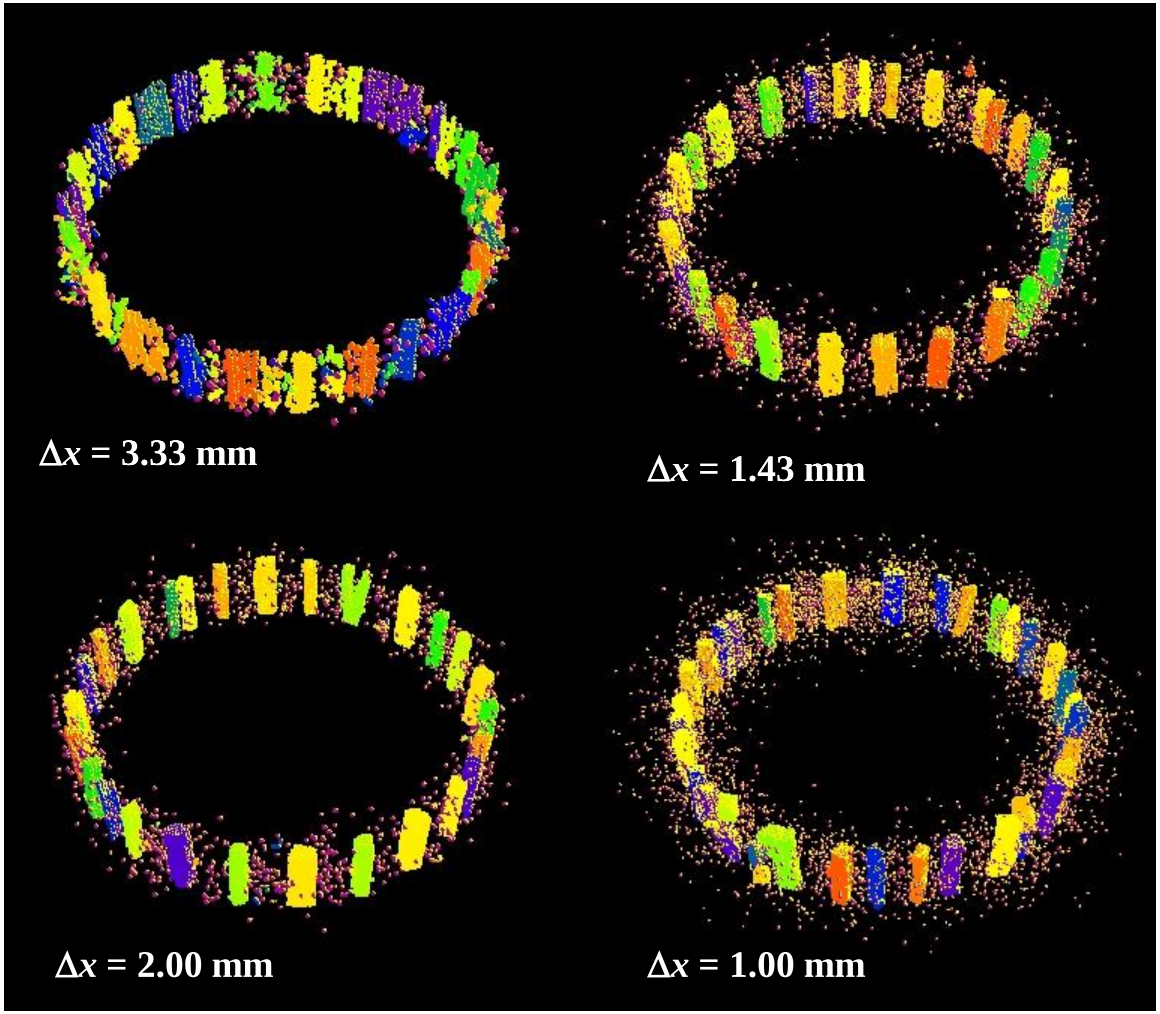
Network of identical bonds in many directions allows cracks to grow in any direction.



Convergence in a fragmentation problem



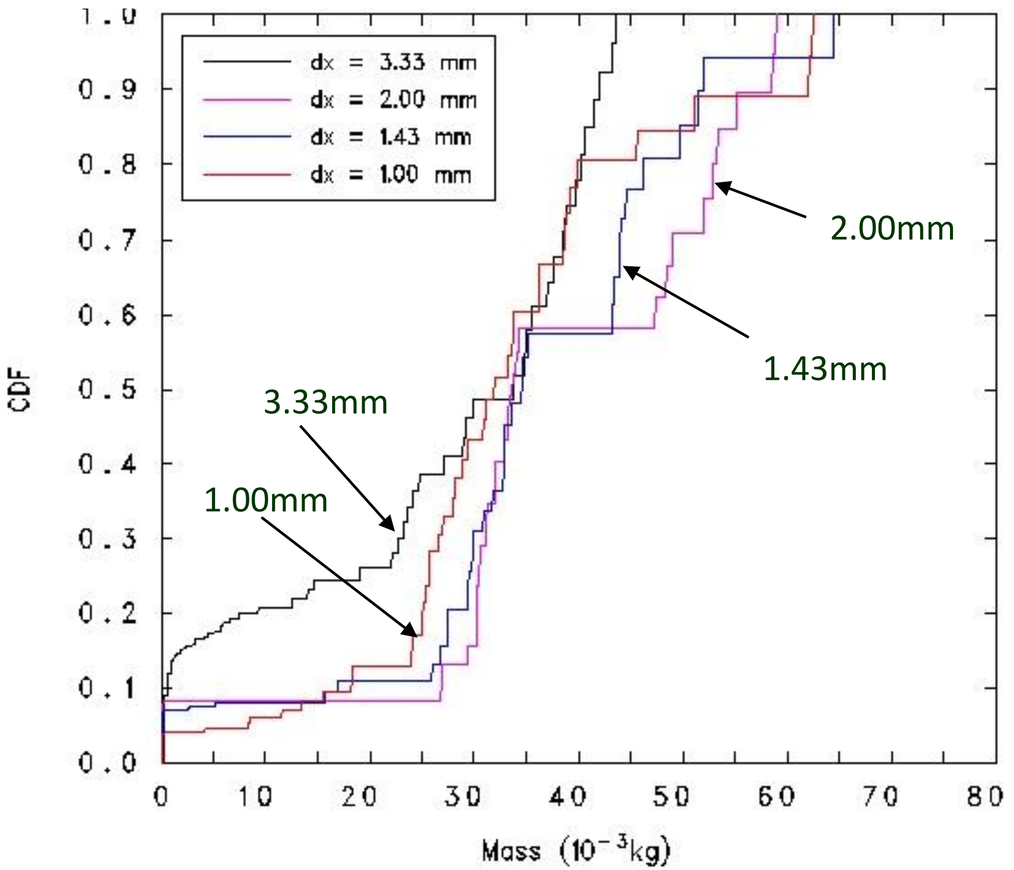
Brittle ring with initial radial velocity



$$\delta = 3\Delta x$$

Convergence in a fragmentation problem

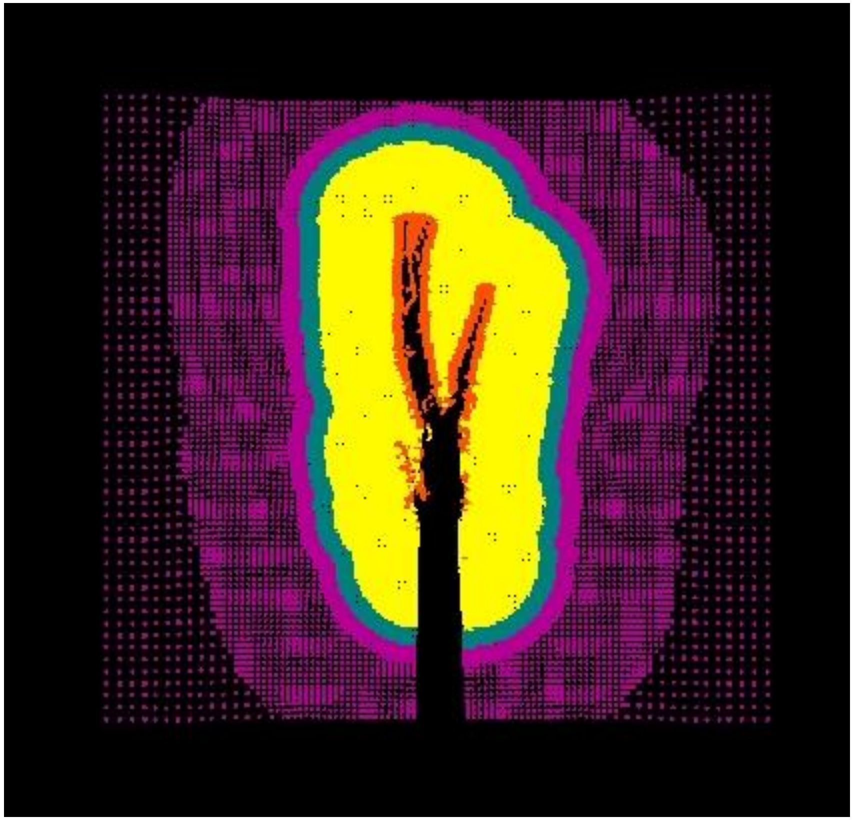
Cumulative distribution function for 4 grid spacings



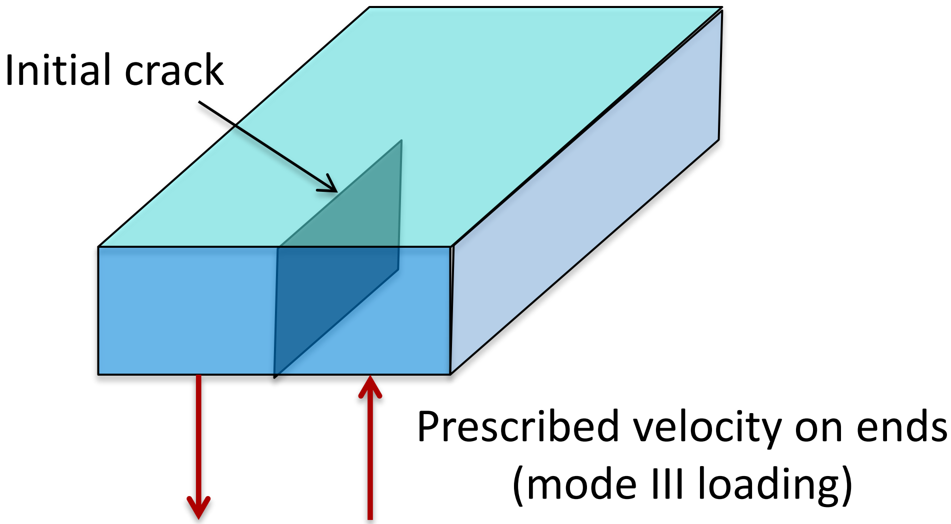
Δx (mm)	Mean fragment mass (g)
3.33	27.1
2.00	37.8
1.43	35.9
1.00	33.5

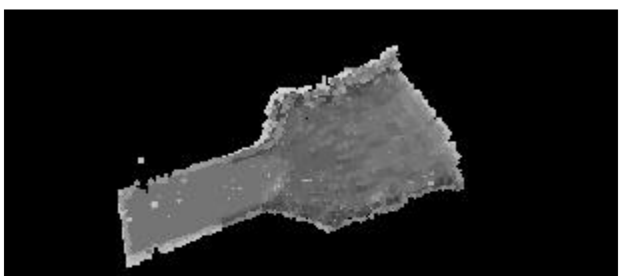
Solution appears essentially converged

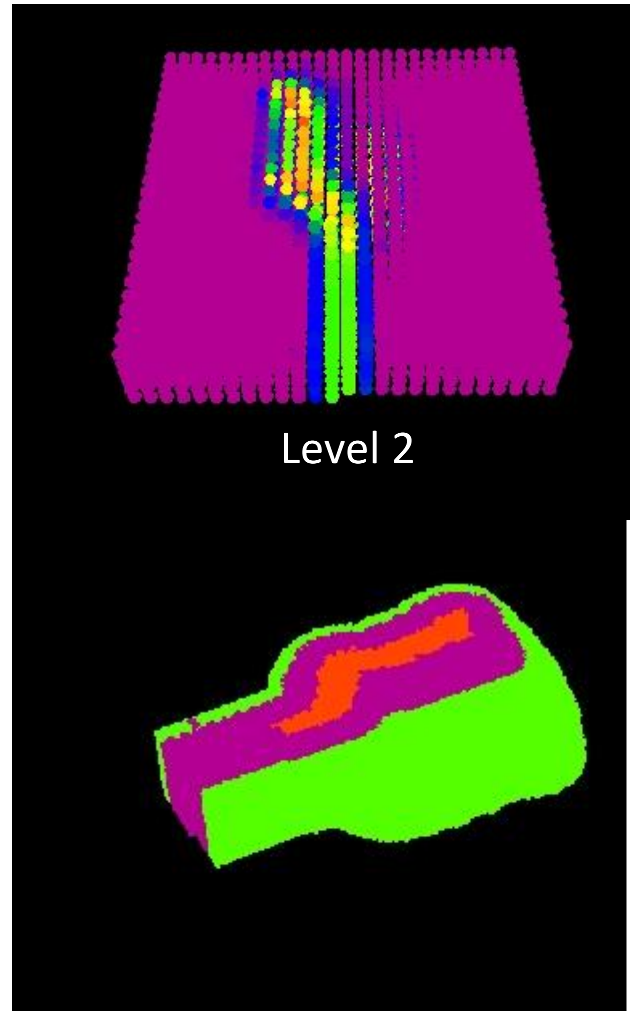
Dynamic fracture



Fracture mode transition

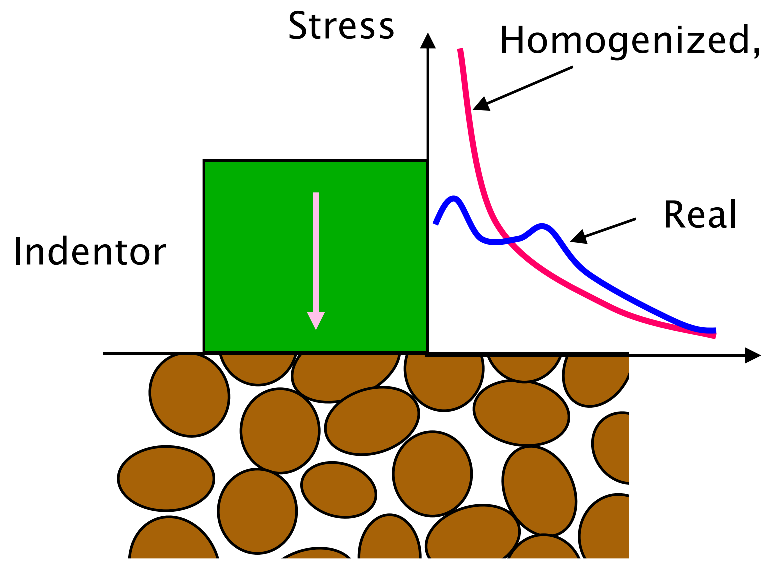



Crack plane rotates 45deg, continues as mode I



Nonlocality as a result of homogenization

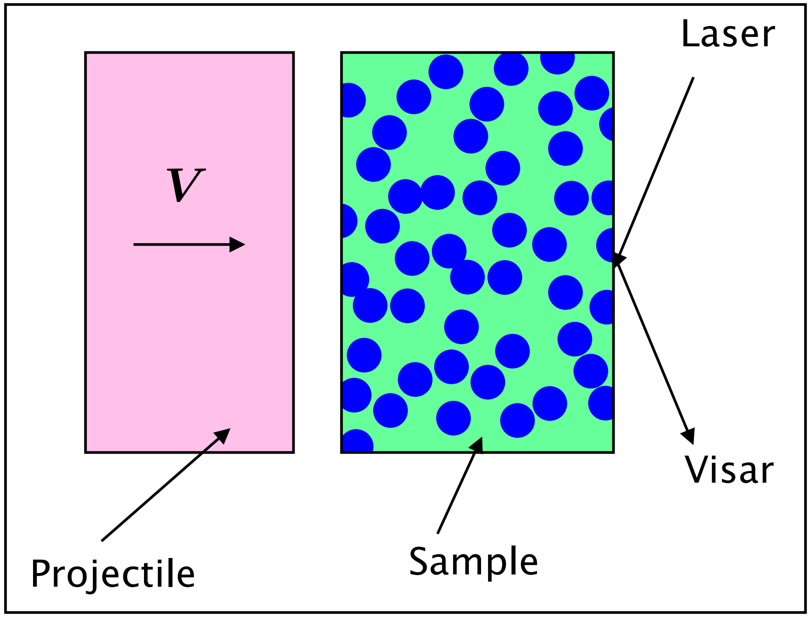
- Homogenization, neglecting the natural length scales of a system, often doesn't give good answers.

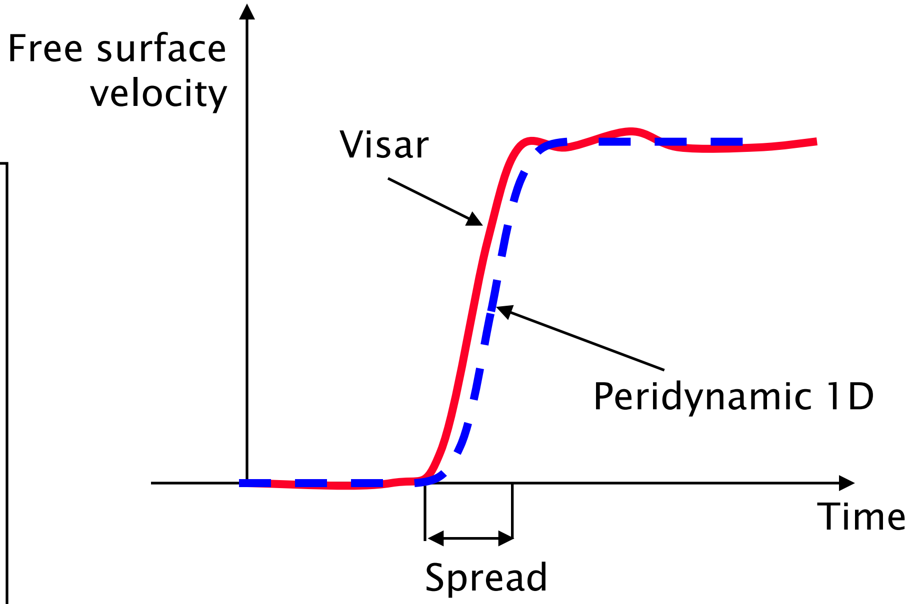


Claim: Nonlocality is an essential feature of a realistic homogenized model of a heterogeneous material.

Proposed experimental method for measuring the peridynamic horizon

- Measure how much a step wave spreads as it goes through a sample.
- Fit the horizon in a 1D peridynamic model to match the observed spread.



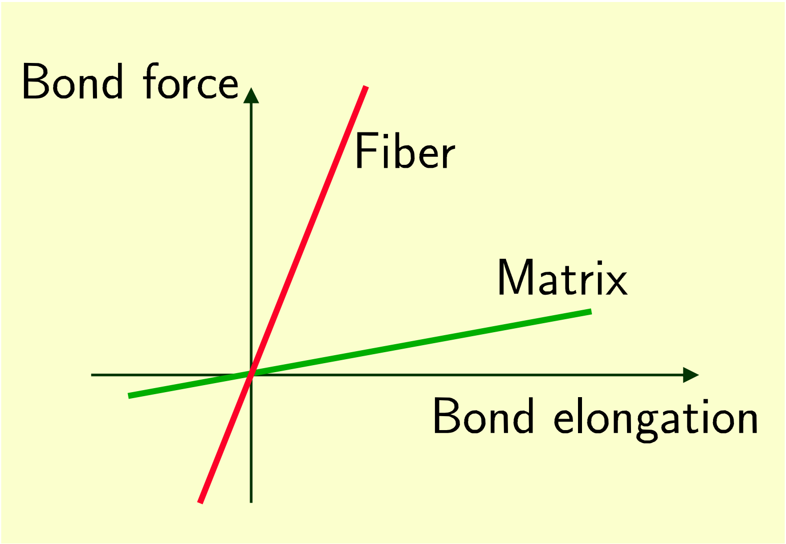


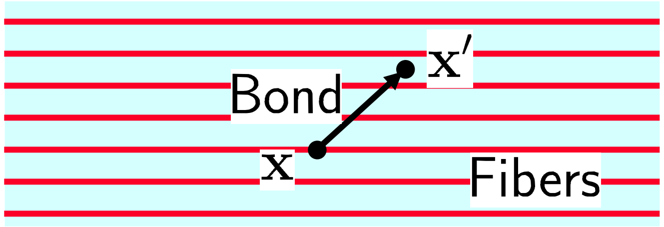
Local model would predict zero spread.

Sandia National Laboratories

Material modeling: Composites

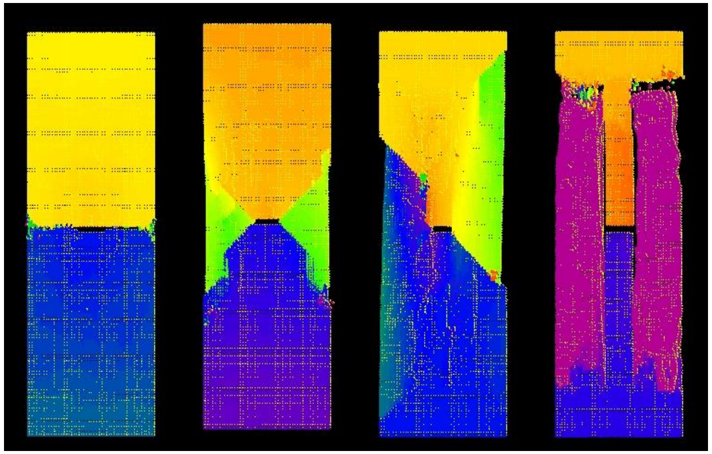
- Special case: fiber reinforced composite lamina.
- Bonds in the fiber direction are stiffer than the others.





Splitting and fracture mode change in composites

- Distribution of fiber directions between plies strongly influences the way cracks grow.

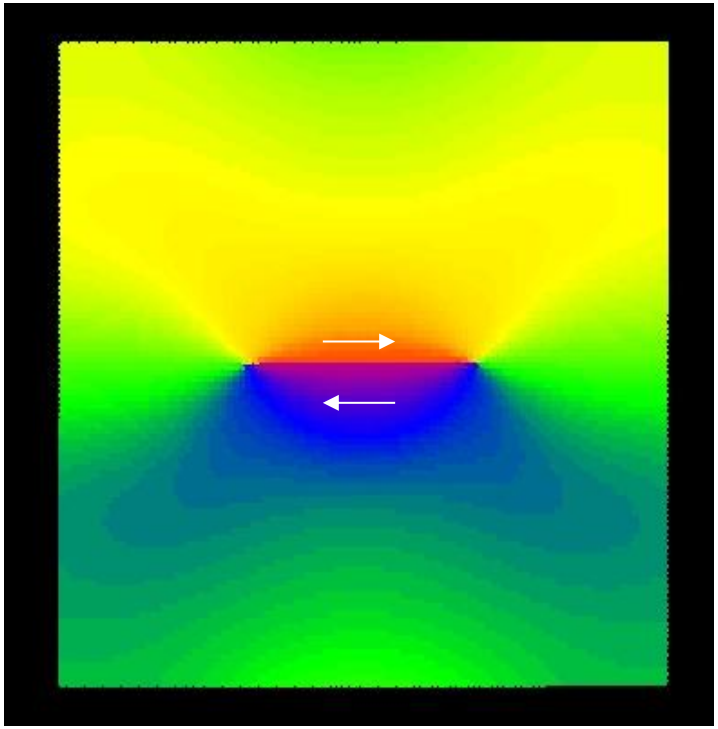


EMU simulations for different layups

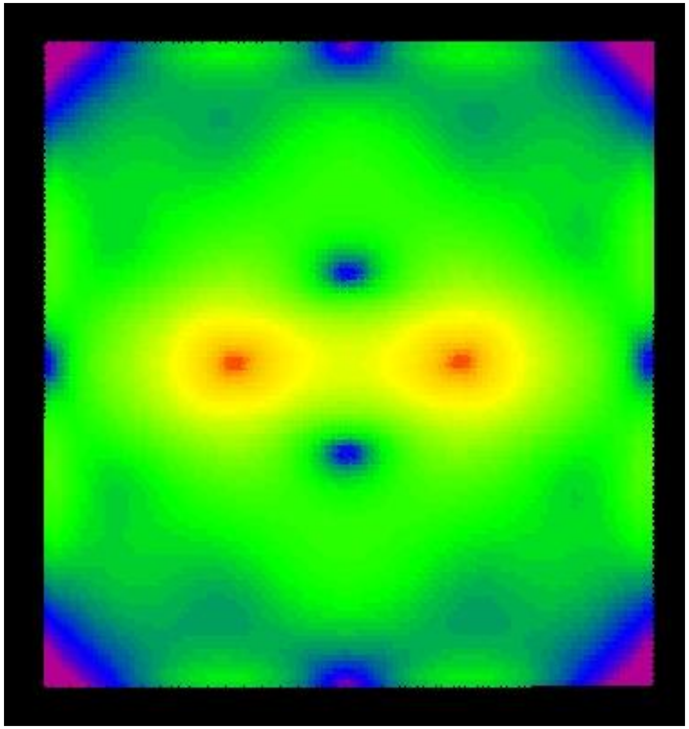
Typical crack growth in a notched laminate (photo courtesy Boeing)

Peridynamic dislocation model

Example: Dislocation segment in a square with free edges
100 x 100 EMU grid



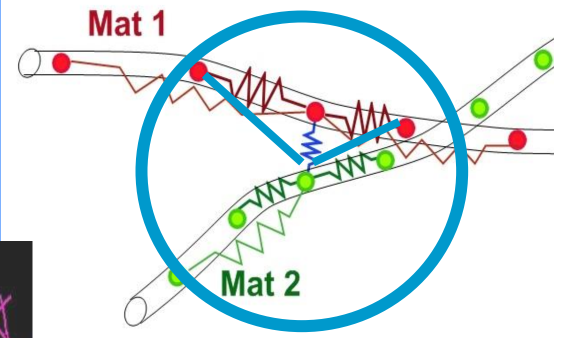
Contours of u_1



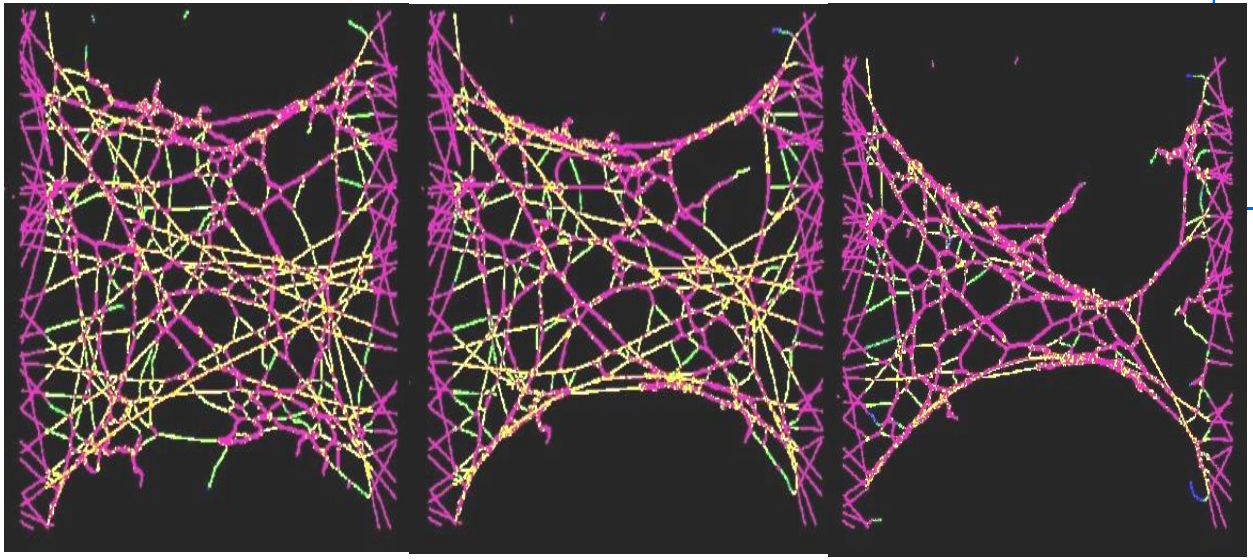
Contours of $\log W$
W=elastic energy density

Example of long-range forces: Nanofiber network

- Peridynamics treats all internal forces as long-range.
- This makes it a natural way to treat van der Waals and surface forces.



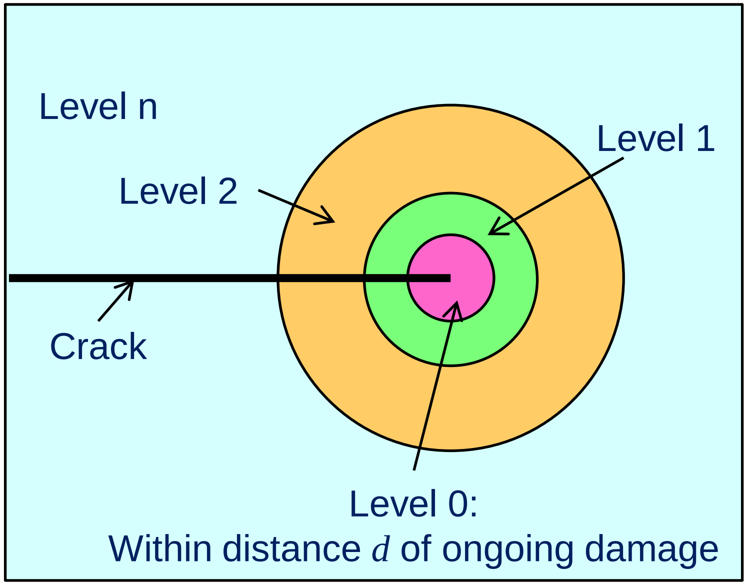
Nanofiber interactions due to van der Waals forces



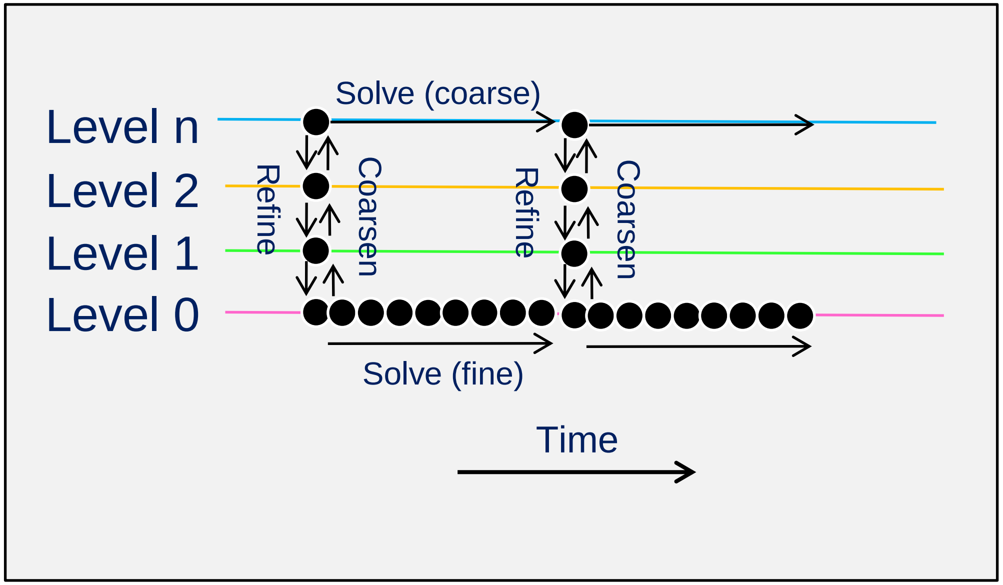
Nanofiber membrane (F. Bobaru, Univ. of Nebraska)

Concurrent solution strategy

Level 0 region follows the crack tip



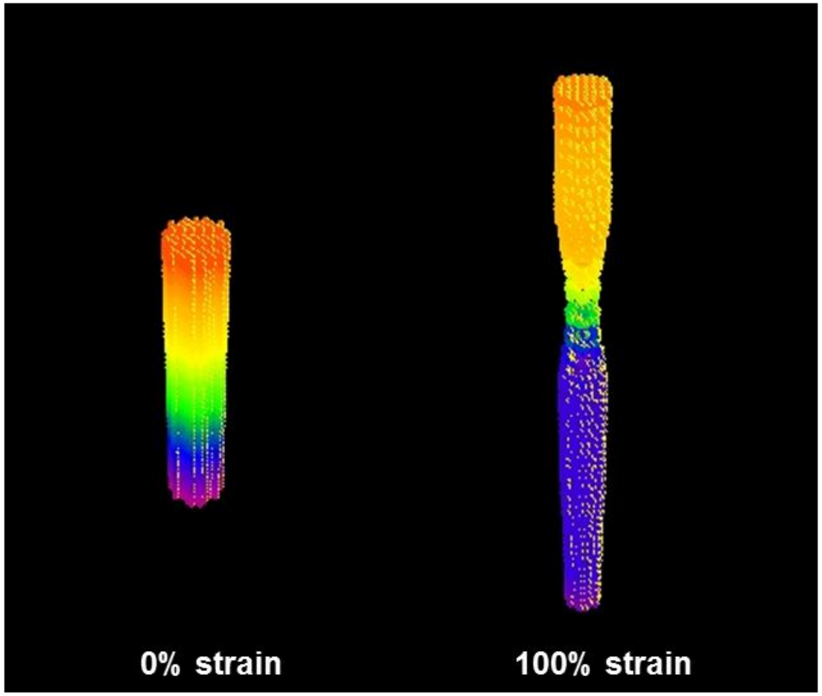
Concurrent solution strategy



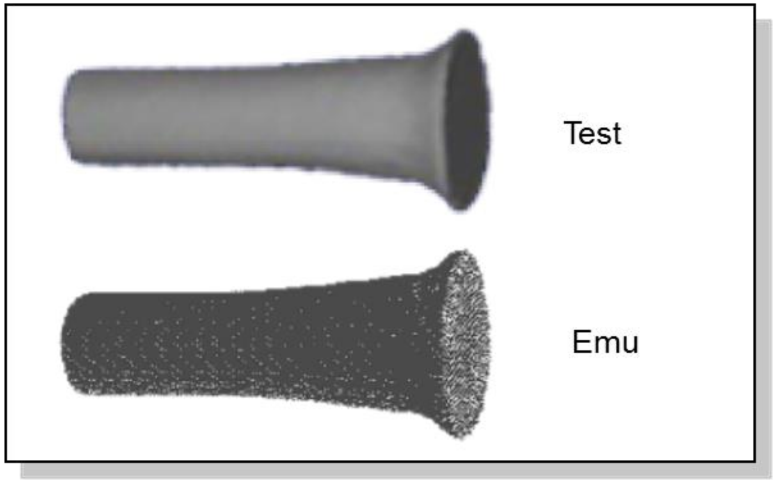
- Refinement:
  - Level 1 acts as a boundary condition on level 0.
- Coarsening:
  - Level 0 supplies material properties (e.g., damage) to higher levels.

Any standard material model can be used in peridynamics

- Example: Large-deformation, strain-hardening, rate-dependent material model.
  - Material model implementation by John Foster.



Necking of a bar under tension



Taylor impact test

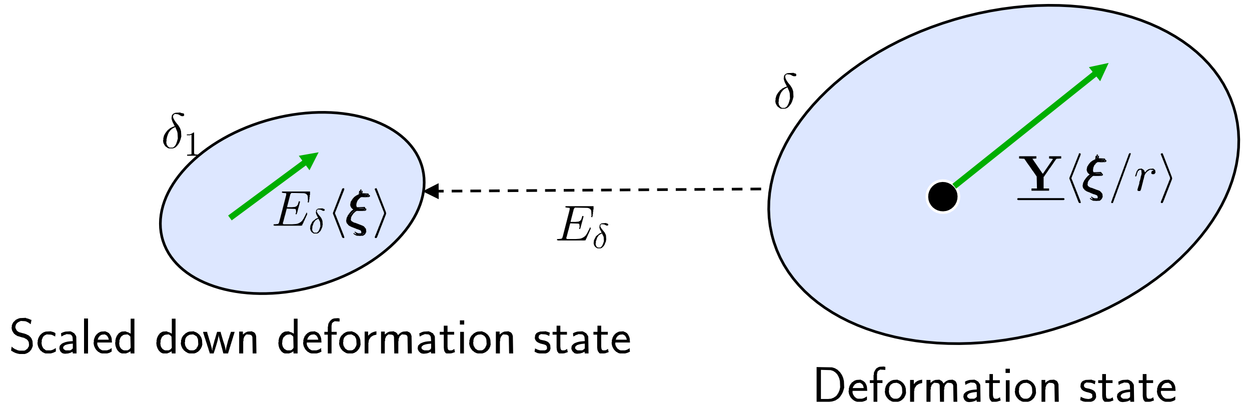
Rescaling an elastic material model

- Start with a material model W_1 which has some fixed horizon δ_1.
- Define a mapping that takes a new, larger horizon δ into the original:

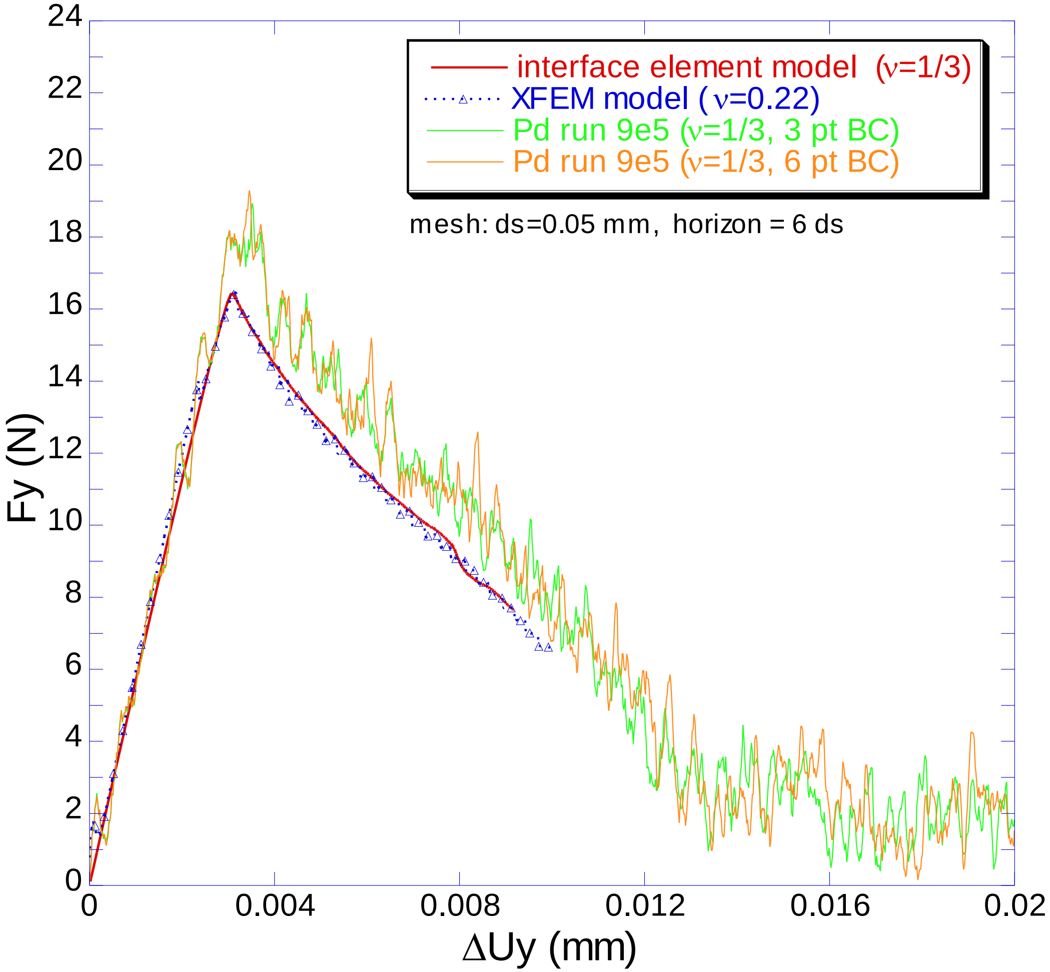
$$(E_\delta(\underline{\mathbf{Y}}))\langle\boldsymbol{\xi}\rangle = r\underline{\mathbf{Y}}\langle\boldsymbol{\xi}/r\rangle, \qquad r = \frac{\delta_1}{\delta} \leq 1$$

- Then set

$$W_\delta(\underline{\mathbf{Y}}) = W_1(E_\delta(\underline{\mathbf{Y}}))$$



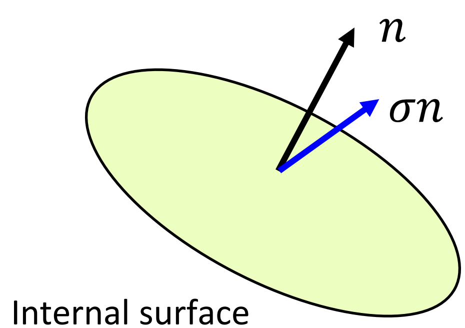
Comparison with XFEM, interface elements



Peridynamics basics:
The nature of internal forces

Standard theory

Stress tensor field
(assumes contact forces and smooth deformation)

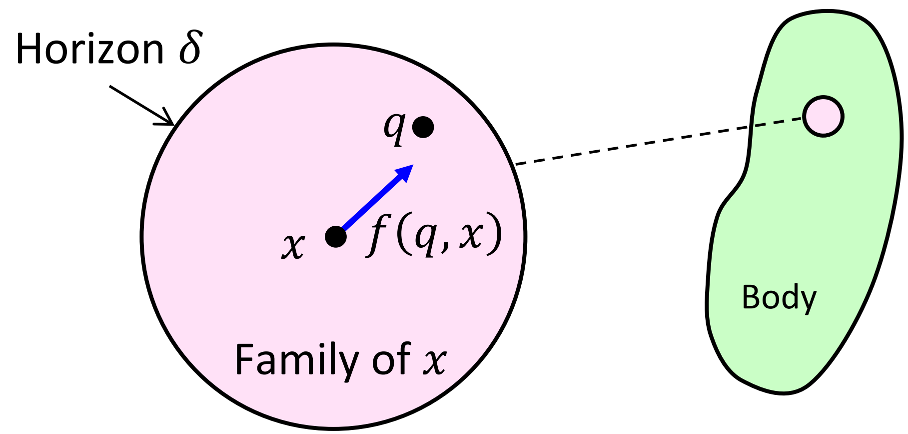


$$\rho \ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t)$$

Differentiation of contact forces

Peridynamics

Bond forces within small neighborhoods
(allow discontinuity)



$$\rho \ddot{u}(x,t) = \int_{H_x} f(q,x) dV_q + b(x,t)$$

Summation over bond forces

Peridynamics basics: States

- A *peridynamic state* is a mapping on bonds in a family.
- We write:

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

  where $\boldsymbol{\xi}$ is a bond, $\underline{\mathbf{A}}$ is a state, and $\mathbf{u}$ is some vector.

- States play a role in peridynamics similar to that of second order tensors in the local theory.

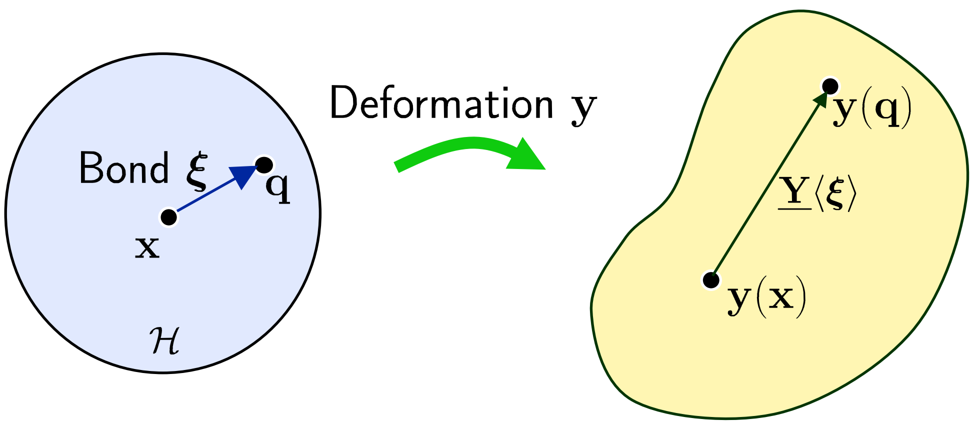
Peridynamics basics: Kinematics

- The *deformation state* is the function that maps each bond $\boldsymbol{\xi}$ into its deformed image:

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

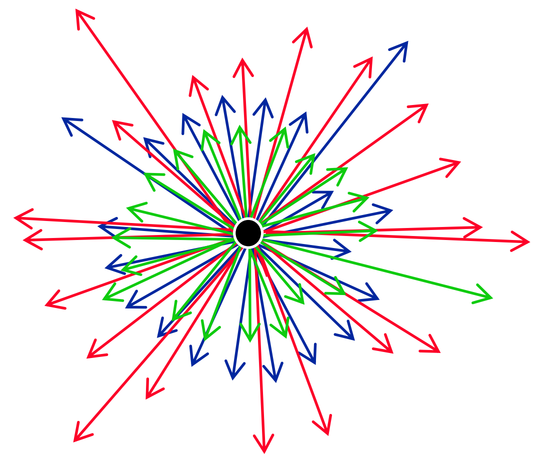
where $\mathbf{y}$ is the deformation and

$$\boldsymbol{\xi} = \mathbf{q} - \mathbf{x}.$$



Undeformed family of $\mathbf{x}$

Deformed family of $\mathbf{x}$



Deformed images of bonds:
State description allows complexity

Peridynamics basics: Force state

- $\mathbf{f}(\mathbf{x},\mathbf{q})$ has contributions from the material models at both $\mathbf{x}$ and $\mathbf{q}$.

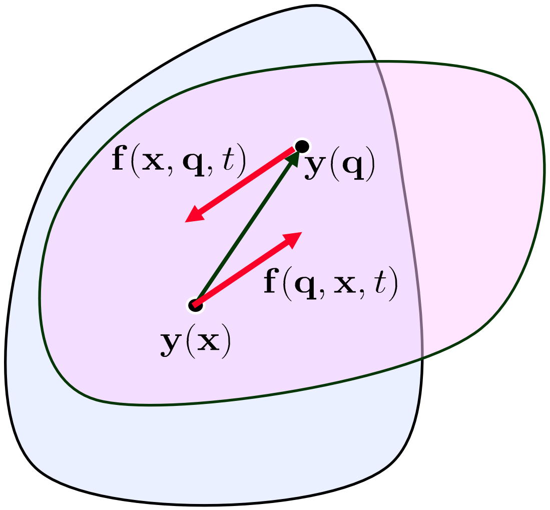
$$\mathbf{f}(\mathbf{x},\mathbf{q}) = \mathbf{t}(\mathbf{x},\mathbf{q}) - \mathbf{t}(\mathbf{q},\mathbf{x})$$

$$\mathbf{t}(\mathbf{x},\mathbf{q}) = \underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{q}-\mathbf{x}\rangle, \qquad \mathbf{t}(\mathbf{x},\mathbf{q}) = \underline{\mathbf{T}}[\mathbf{q}]\langle \mathbf{x}-\mathbf{q}\rangle$$

- $\underline{\mathbf{T}}[\mathbf{x}]$ is the *force state*: maps bonds onto bond force densities. It is found from the constitutive model:

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

where $\hat{\underline{\mathbf{T}}}$ maps the deformation state to the force state.



Peridynamics basics: Elastic materials

- A peridynamic elastic material has strain energy density given by

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

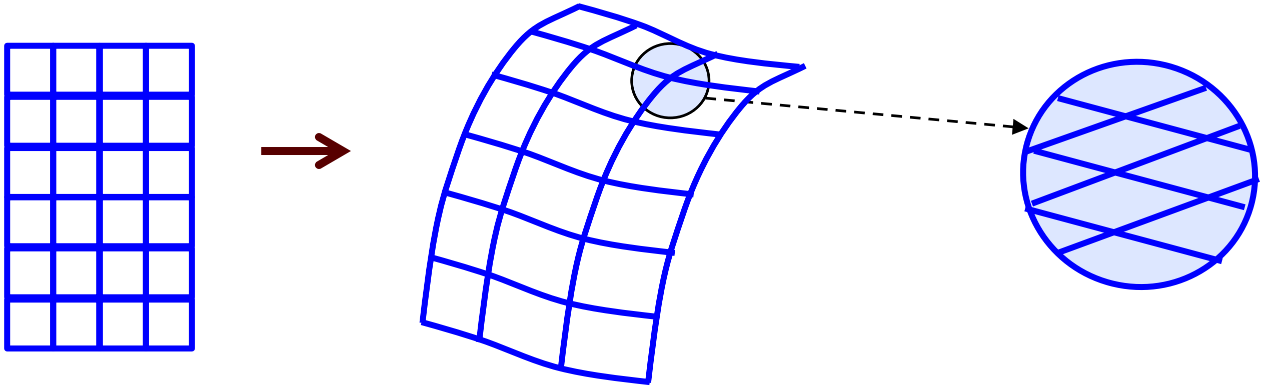
- The force state is given by

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

where $W_{\underline{\mathbf{Y}}}$ is the Frechet derivative of the strain energy density.

Peridynamics converges to the local theory

- Can prove that if the deformation is smooth, then in the limit $\delta \to 0$ while holding the bulk material properties constant, for any bond $\boldsymbol{\xi}$:
- $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \to \mathbf{F}\boldsymbol{\xi}$, where $\mathbf{F}$=deformation gradient tensor
- There exists a tensor field $\boldsymbol{\sigma}$ such that $\int \mathbf{f} \to \nabla \cdot \boldsymbol{\sigma}$, so the standard PDE is recovered.



In this sense, the standard theory is a subset of peridynamics.

*Joint work with R. Lehoucq

Some results about peridynamics

- For any choice of horizon, we can fit material model parameters to match the bulk properties and energy release rate.
  - Using nonlocality, can obtain material model parameters from wave dispersion curves (Weckner).
- Coupled coarse scale and fine scale evolution equations can be derived for composites (Lipton and Alali).
- A set of discrete particles interacting through any multibody potential can be represented exactly as a peridynamic body.
- Well posedness has been established under certain conditions (Mangesha, Du, Gunzburger, Lehoucq).

EMU numerical method

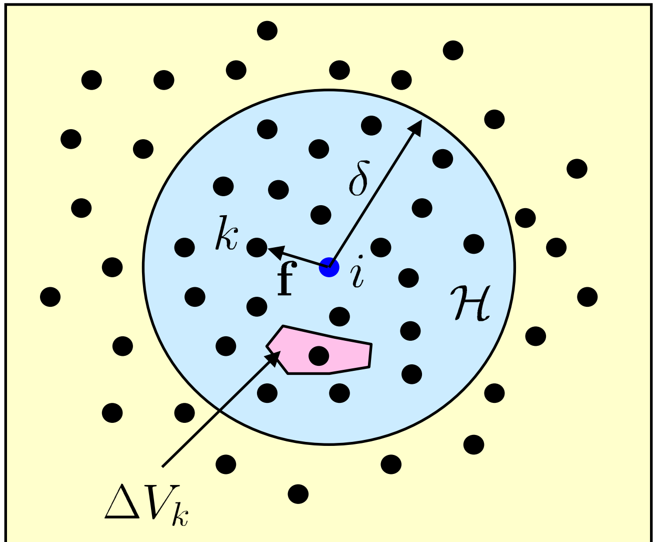
- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

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

$$\downarrow$$

$$\rho\ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\,\Delta V_k + \mathbf{b}_i^n$$

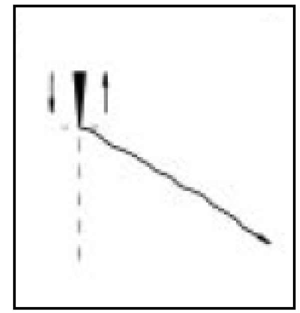
- Looks a lot like MD.
- Unrelated to Smoothed Particle Hydrodynamics
  - SPH solves the local equations by fitting spatial derivatives to the current node values.



Discretized model in the reference configuration

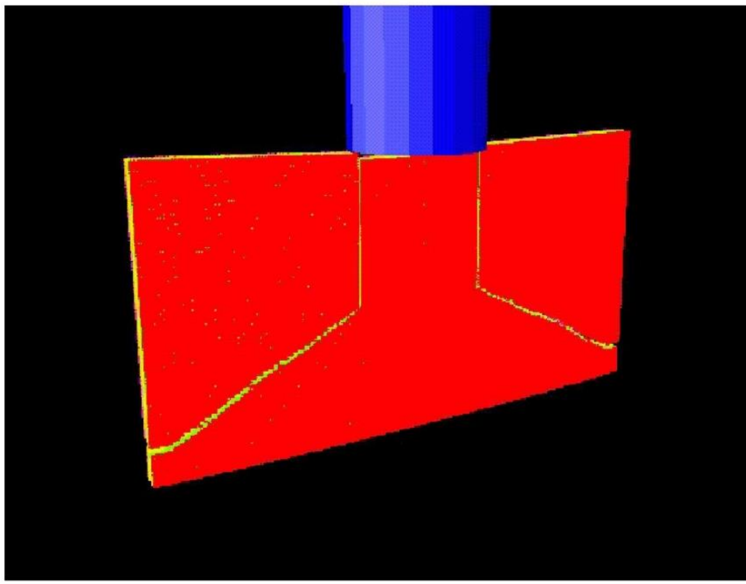
Example: Dynamic fracture

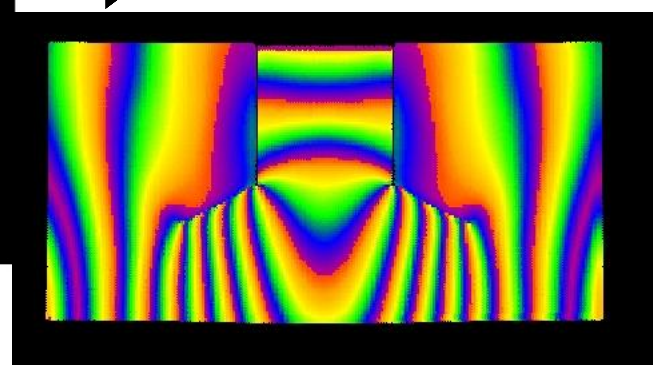
- Dynamic fracture in maraging steel (Kalthoff & Winkler, 1988)
- Mode-II loading at notch tips results in mode-I cracks at 70deg angle.
- 3D EMU model reproduces the crack angle.



Experiment

EMU*

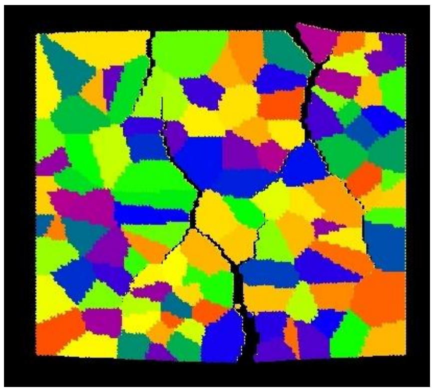




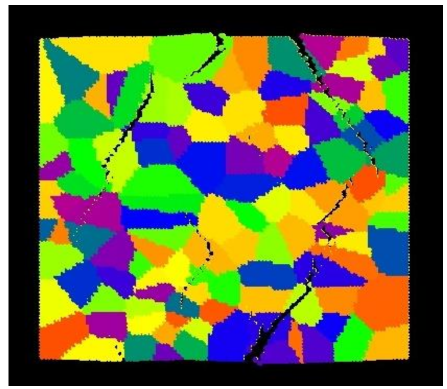
S. A. Silling, Dynamic fracture modeling with a meshfree peridynamic code, in *Computational Fluid and Solid Mechanics 2003*, K.J. Bathe, ed., Elsevier, pp. 641-644.

Polycrystals: Mesoscale model*

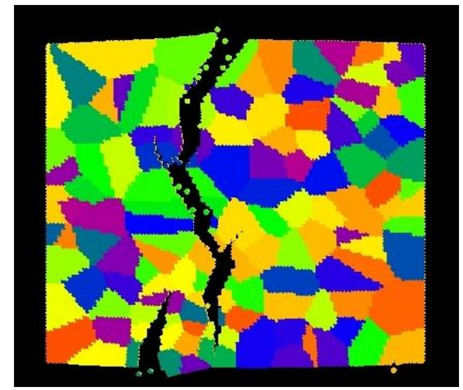
- What is the effect of grain boundaries on the fracture of a polycrystal?



$\beta = 0.25$



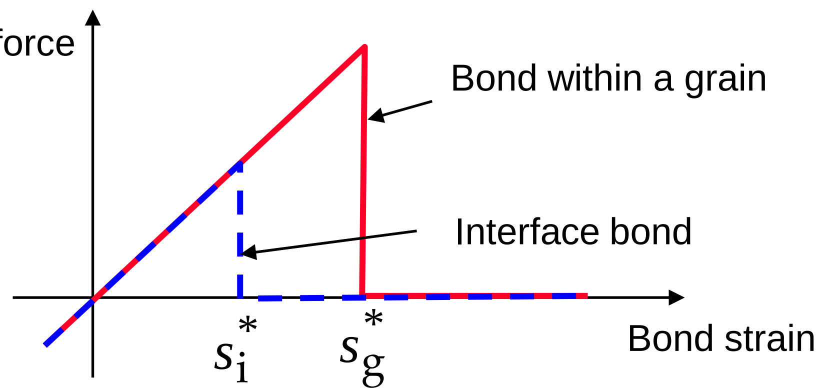
$\beta = 1$



$\beta = 4$

$$\beta = \frac{s_{\mathrm{i}}^{*}}{s_{\mathrm{g}}^{*}}$$

Large β favors trans-granular fracture.



* Work by F. Bobaru & students

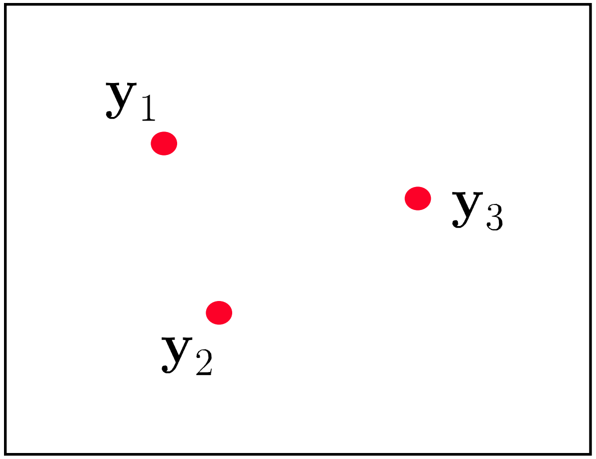
Discrete particles and PD states

- Consider a set of atoms that interact through an $N-$body potential:

$$U(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N),$$

  $\mathbf{y}_1, \dots, \mathbf{y}_N$ = deformed positions, $\mathbf{x}_1, \dots, \mathbf{x}_N$ = reference positions.

- This can be represented exactly as a peridynamic body.



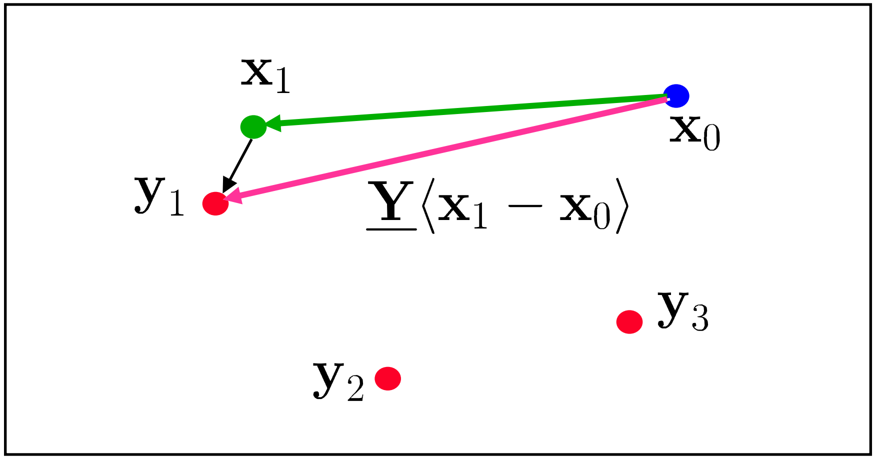
Sandia National Laboratories

Discrete particles and PD states, ctd.

Define a peridynamic body by:

$$\hat{W}(\underline{\mathbf{Y}}, \mathbf{x}) = \Delta(\mathbf{x}-\mathbf{x}_0)U(\underline{\mathbf{Y}}\langle\mathbf{x}_1-\mathbf{x}_0\rangle, \underline{\mathbf{Y}}\langle\mathbf{x}_2-\mathbf{x}_0\rangle, \ldots, \underline{\mathbf{Y}}\langle\mathbf{x}_N-\mathbf{x}_0\rangle),$$

$$\rho(\mathbf{x}) = \sum_i \Delta(\mathbf{x}-\mathbf{x}_i)M_i$$



Discrete particles and PD states, ctd.

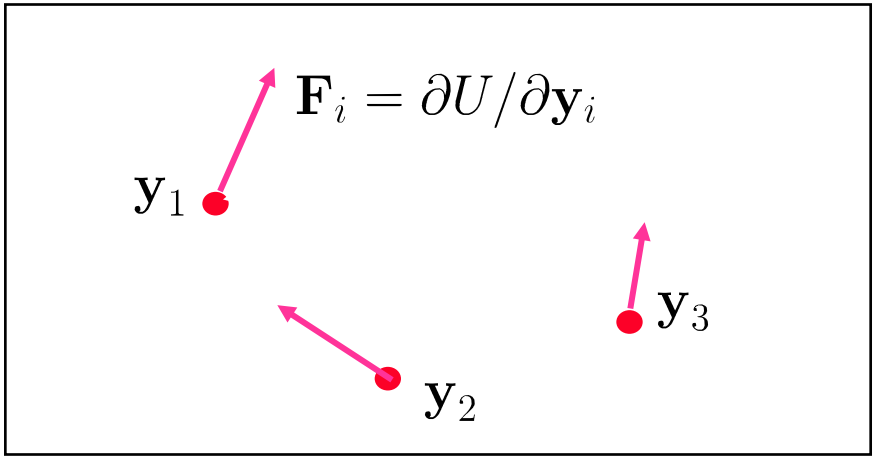
After evaluating the Frechet derivative $\underline{\mathbf{T}}$, find

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \int \mathbf{f}(\mathbf{x}', \mathbf{x}, t)\, dV_{\mathbf{x}'}$$

implies

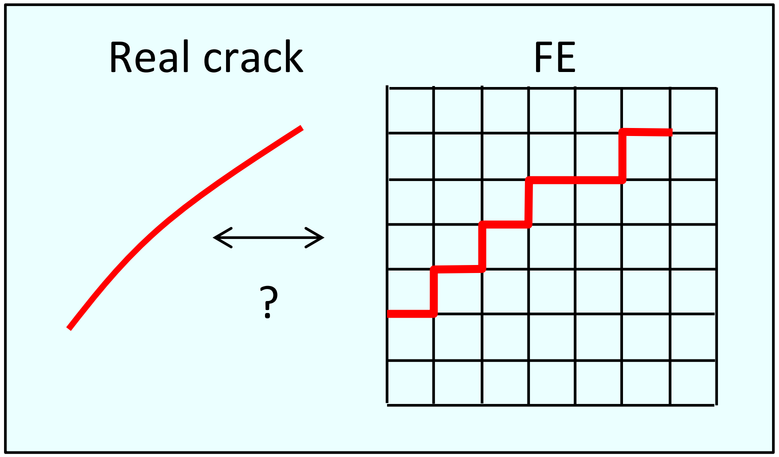
$$M_i \ddot{\mathbf{y}}(\mathbf{x}_i, t) = -\frac{\partial U}{\partial \mathbf{y}_i}, \qquad i = 1, \dots, N$$

In other words, the PD equation of motion reduces to Newton's second law.



Why this is important

- The standard PDEs are incompatible with the essential physical nature of cracks.
  - Can’t apply PDEs on a discontinuity.
- Typical FE approaches implement a fracture model <u>after</u> numerical discretization.
  - Need supplemental kinetic relations that are understood only in idealized cases.



Complex crack path in a composite

(b)

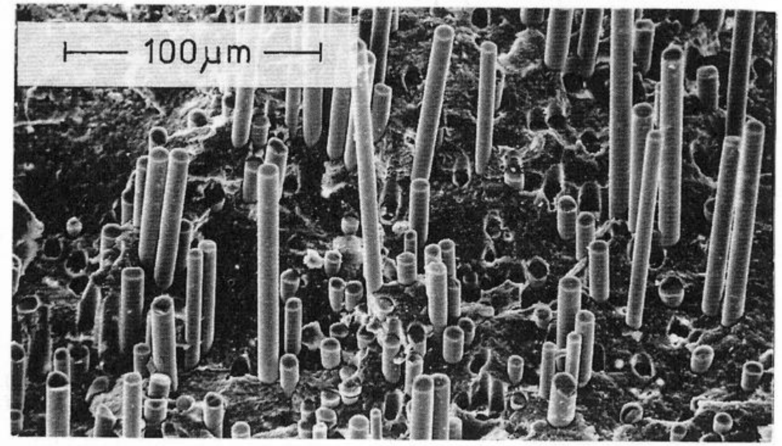
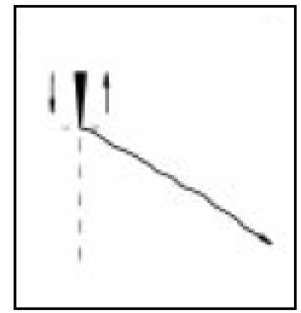


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of ‘Silceram’ glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

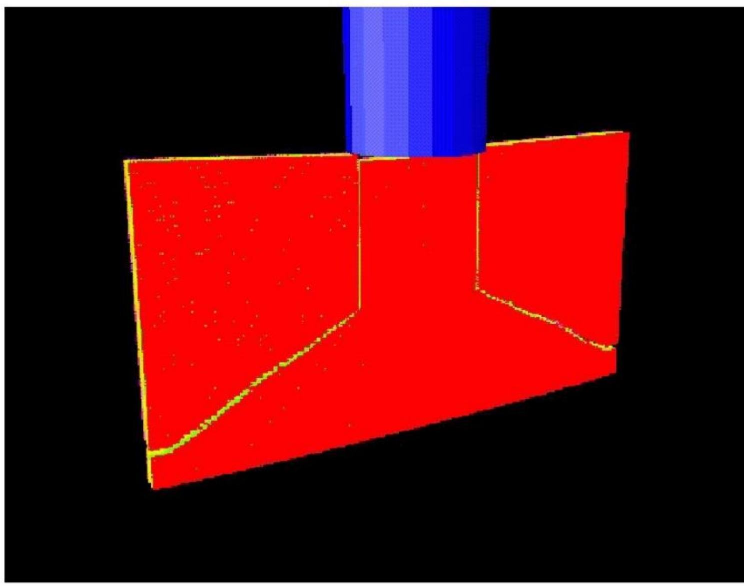
Dynamic fracture in a hard steel plate

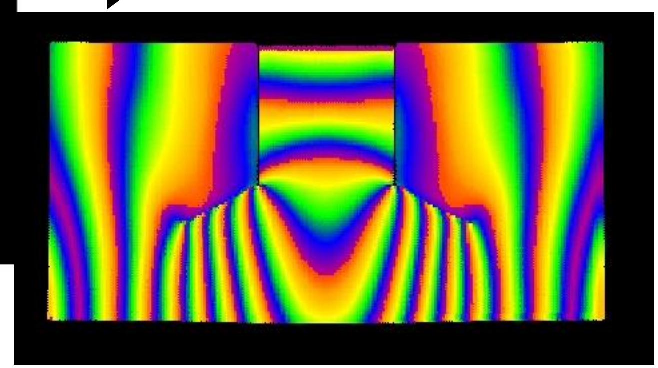
- Dynamic fracture in maraging steel (Kalthoff & Winkler, 1988)
  - Mode-II loading at notch tips results in mode-I cracks at 70deg angle.
  - 3D EMU model reproduces the crack angle.



Experiment

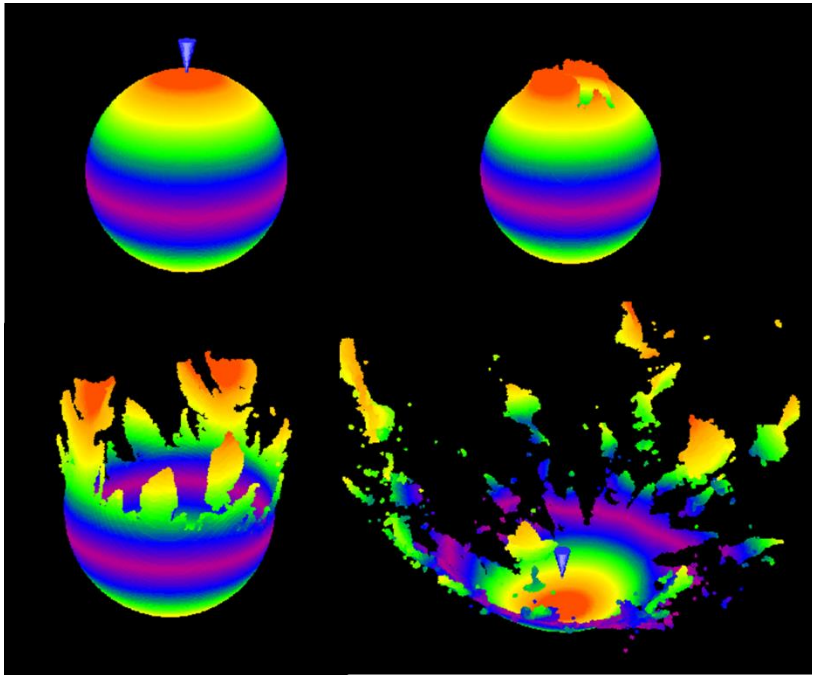
EMU*



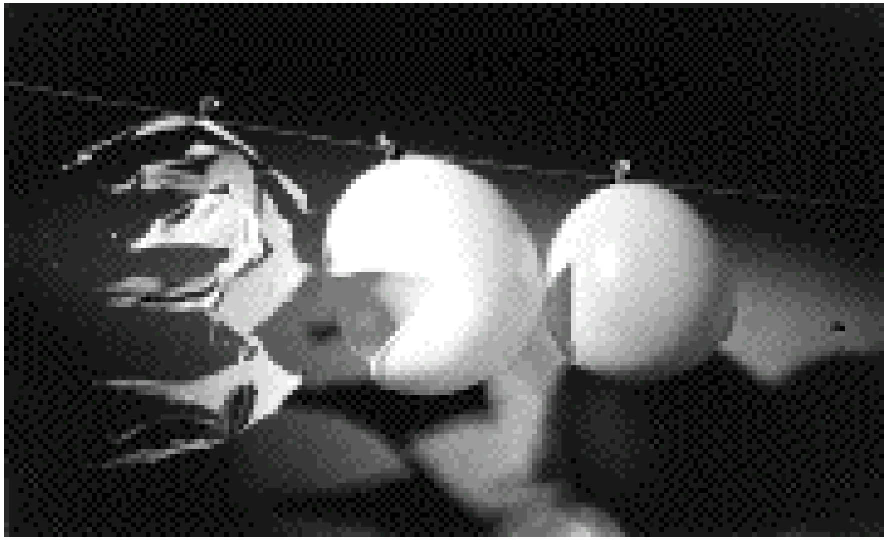


S. A. Silling, Dynamic fracture modeling with a meshfree peridynamic code, in *Computational Fluid and Solid Mechanics 2003*, K.J. Bathe, ed., Elsevier, pp. 641–644.

Dynamic fracture in membranes



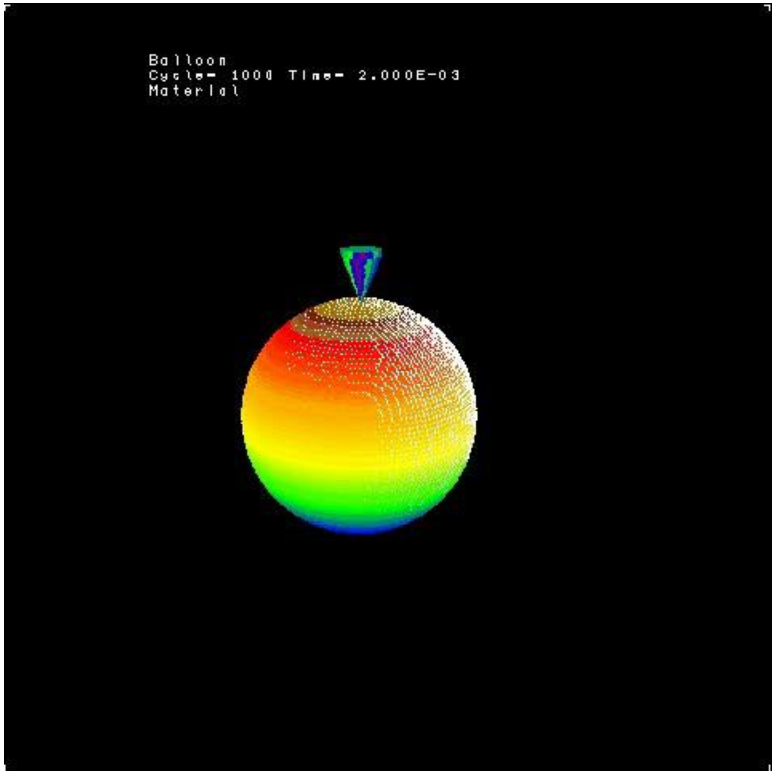
EMU model of a balloon penetrated by a fragment



Early high speed photograph by Harold Edgerton (MIT collection)
http://mit.edu/6.933/www/Fall2000/edgerton/edgerton.ppt

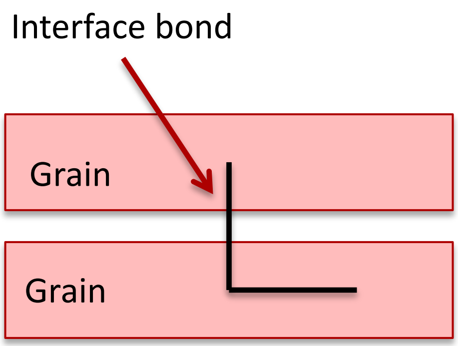
Pressurized shell struck by a fragment

Video

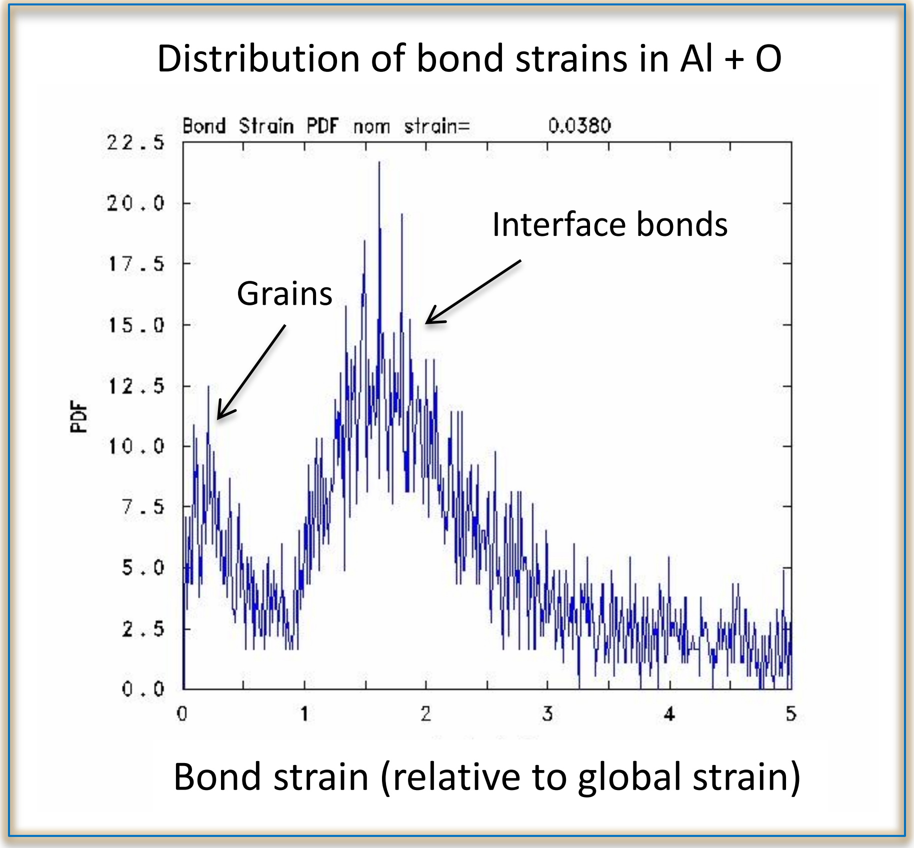


Determining the continuum properties of grain boundaries

- MD shows that with oxide present, grain boundaries are much more compliant than the grains.
- How to translate this into peridynamic properties?

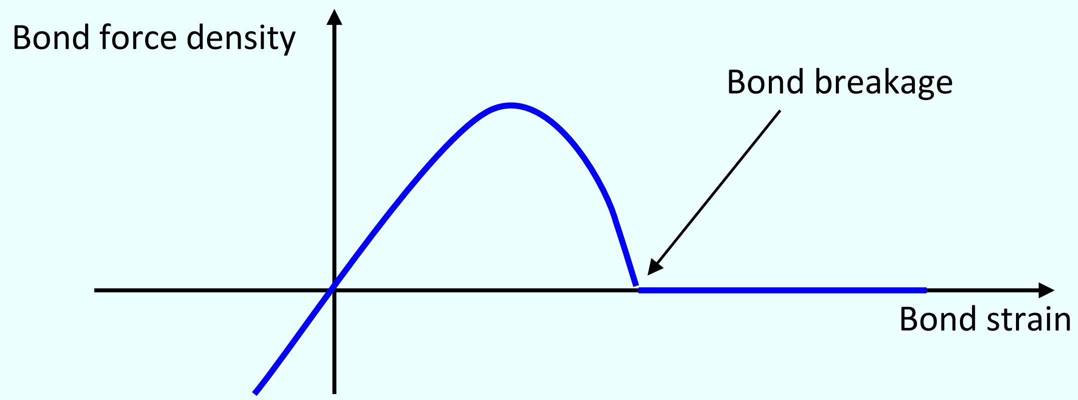


Conclude from this distribution that interface bonds are 10 times more compliant than bonds within grains.



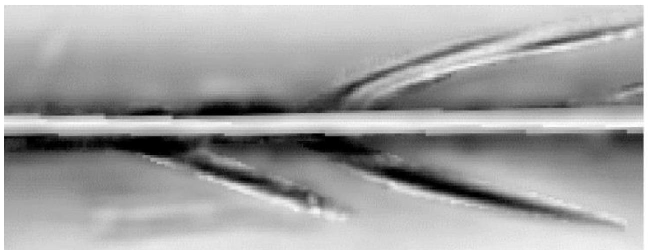
Damage due to bond breakage

- Recall: each bond carries a force.
- Damage is implemented at the bond level.
  - Bonds break irreversibly according to some criterion.
  - Broken bonds carry no force.
- Examples of criteria:
  - Critical bond strain (brittle).
  - Hashin failure criterion (composites).
  - Gurson (ductile metals).

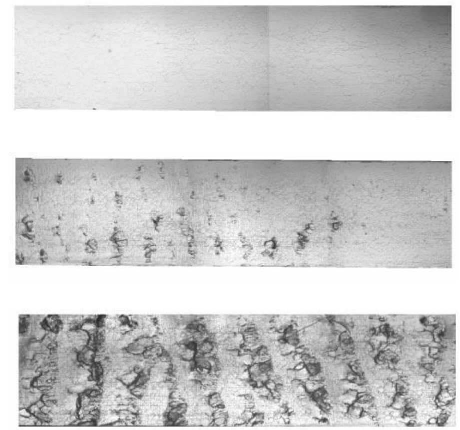


Critical bond strain damage model

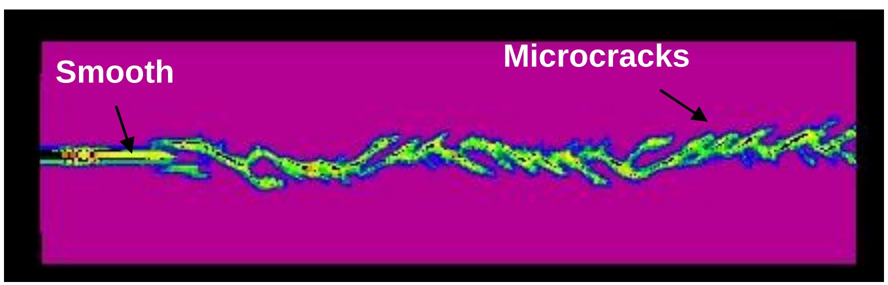
Dynamic fracture in PMMA: Damage features



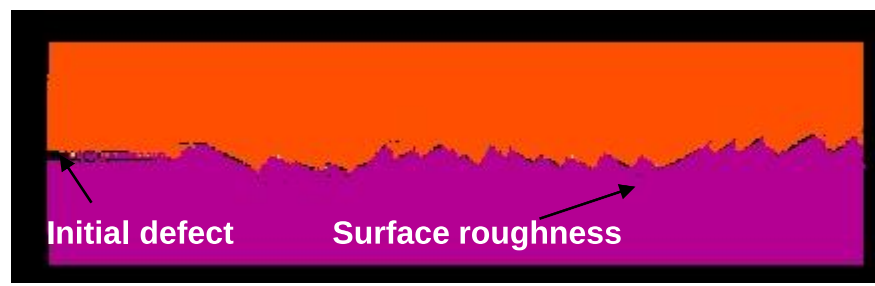
Microbranching



Mirror-mist-hackle transition*



EMU damage

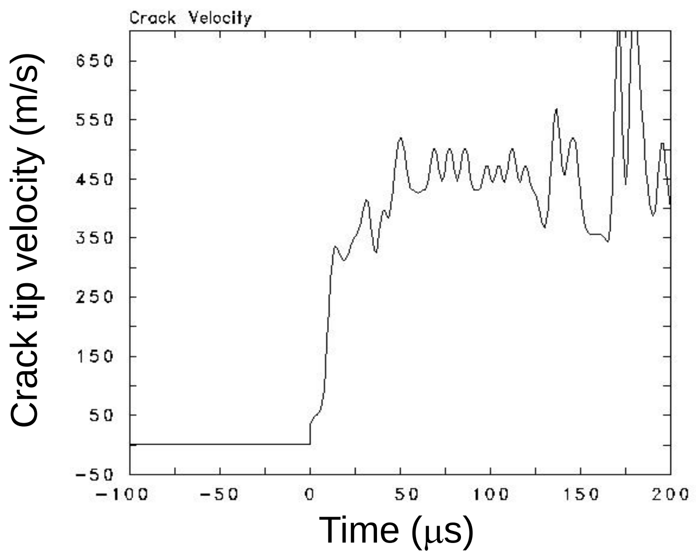


EMU crack surfaces

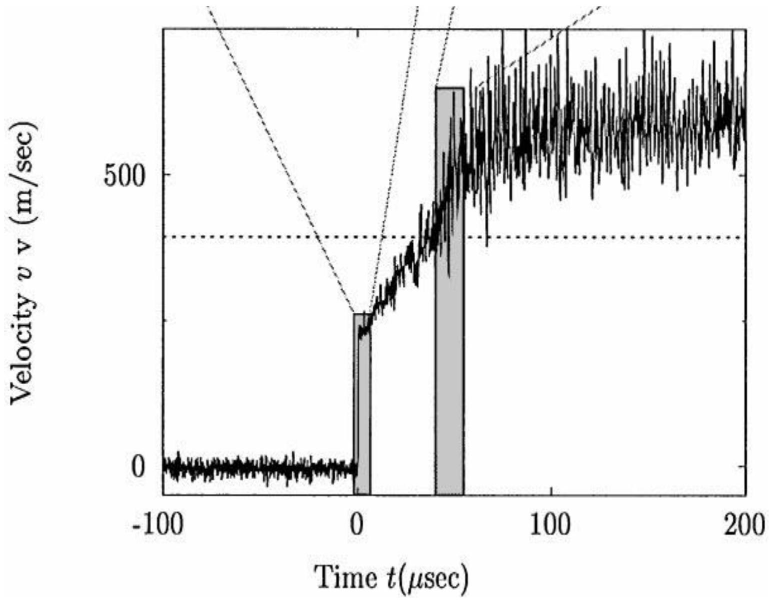
* J. Fineberg & M. Marder, *Physics Reports* 313 (1999) 1-108

Dynamic fracture in PMMA: Crack tip velocity

- Crack velocity increases to a critical value, then oscillates.



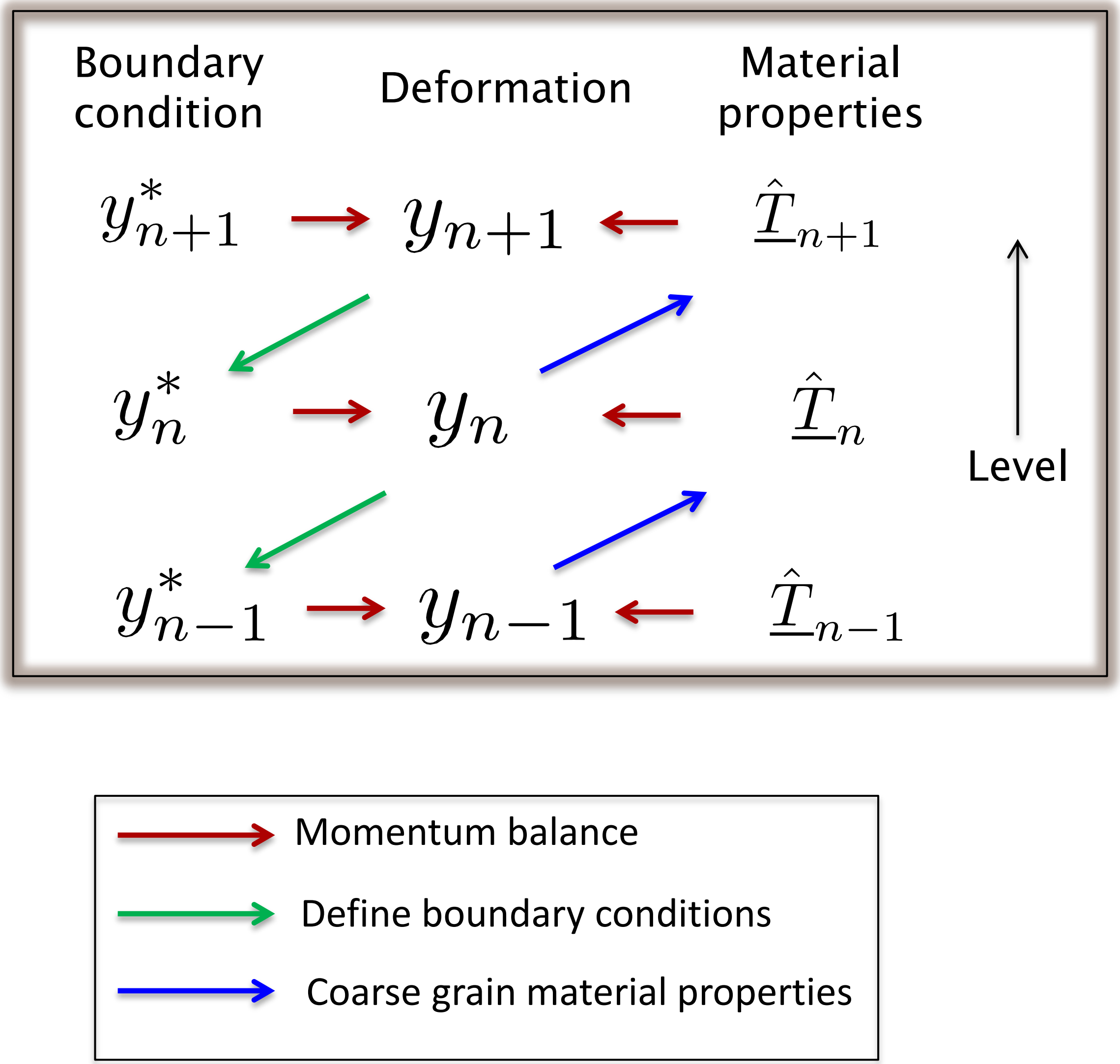
EMU

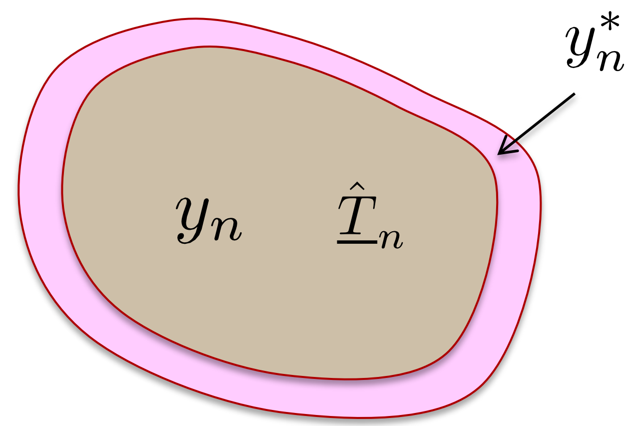


Experiment*

* J. Fineberg & M. Marder, *Physics Reports* 313 (1999) 1-108

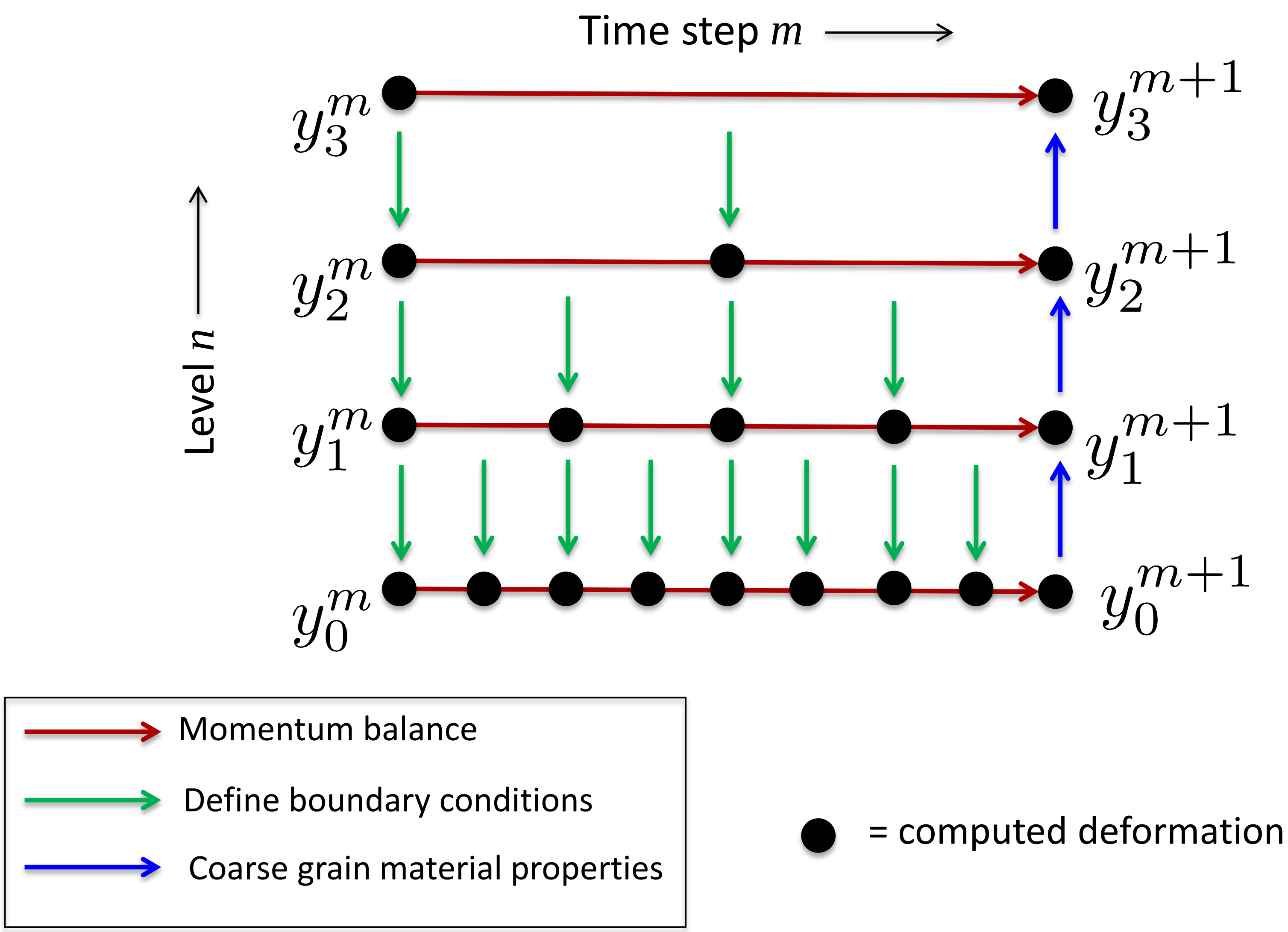
Dependencies between levels





Level n problem

Flow of information in a time step



Peridynamics basics: Bonds and bond force density

- The vector from $\mathbf{x}$ to any point $\mathbf{q}$ in its family in the reference configuration is called a *bond*.

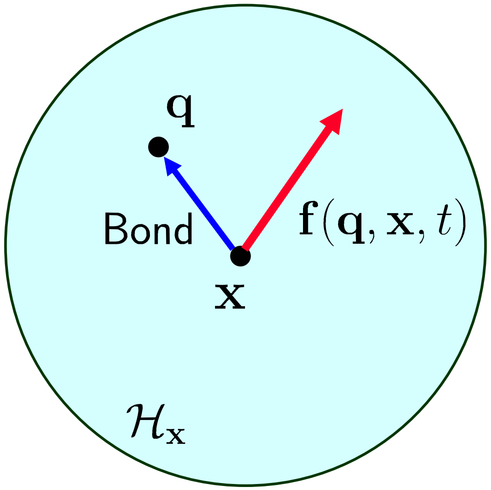
$$\boldsymbol{\xi} = \mathbf{q} - \mathbf{x}$$

- Each bond has a *pairwise force density* vector that is applied at both points:

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

- Equation of motion is an integro-differential equation, not a PDE:

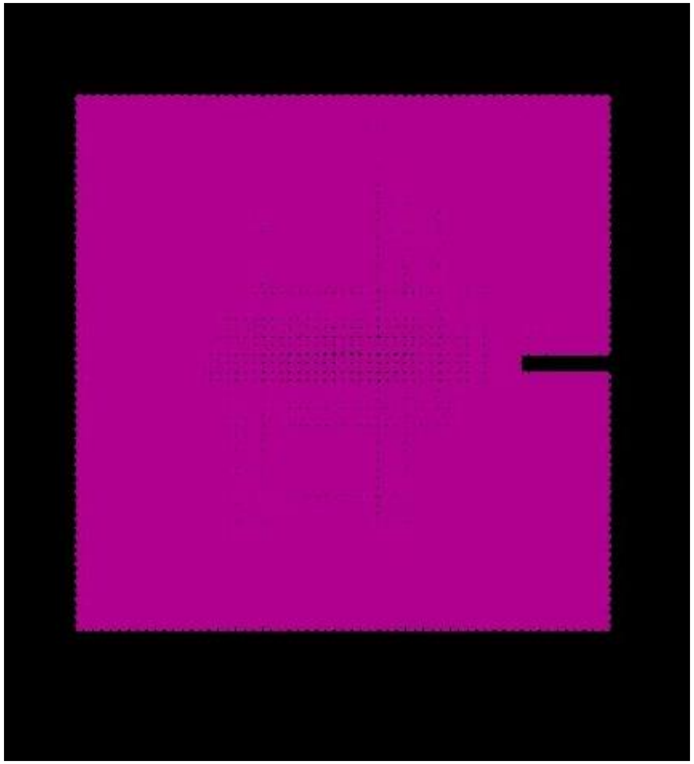
$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{q}, \mathbf{x}, t)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}, t).$$



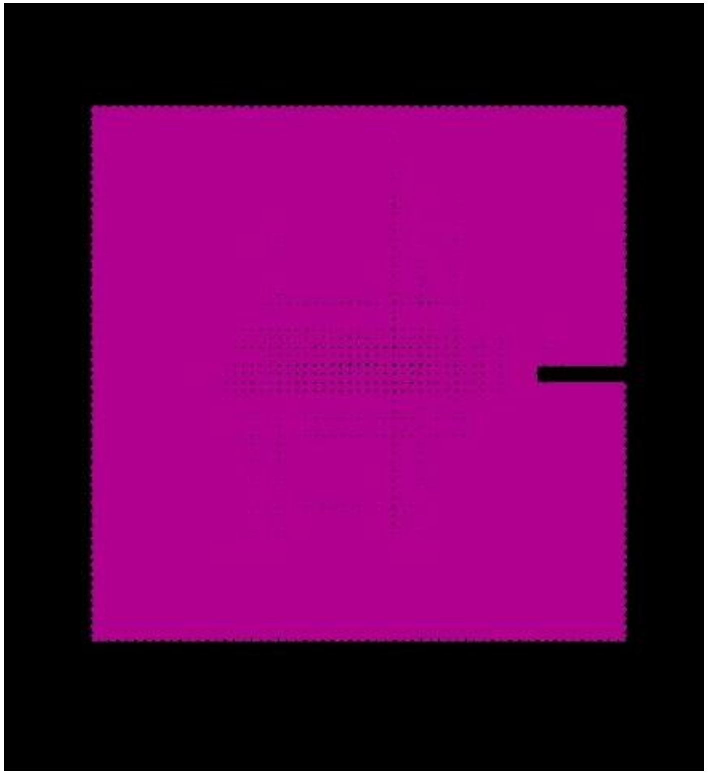
Calibrated peridynamic continuum model (videos)

- Simulations accurately reflect the embrittlement due to oxide.
- Note greater ductility (deformation prior to failure) in Al compared with Al + O.

Videos



Al



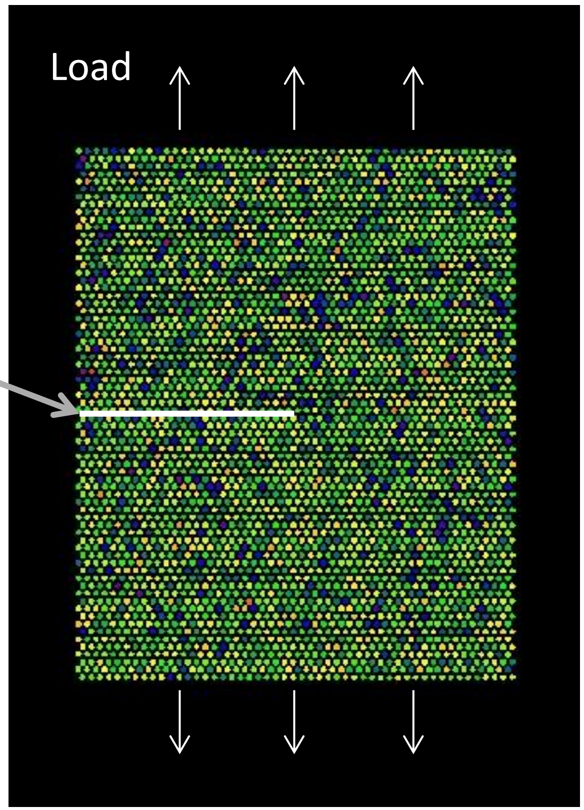
Al + O

Colors indicate bond strain (range is 0 – 3)

Identifying a nucleating crack in MD

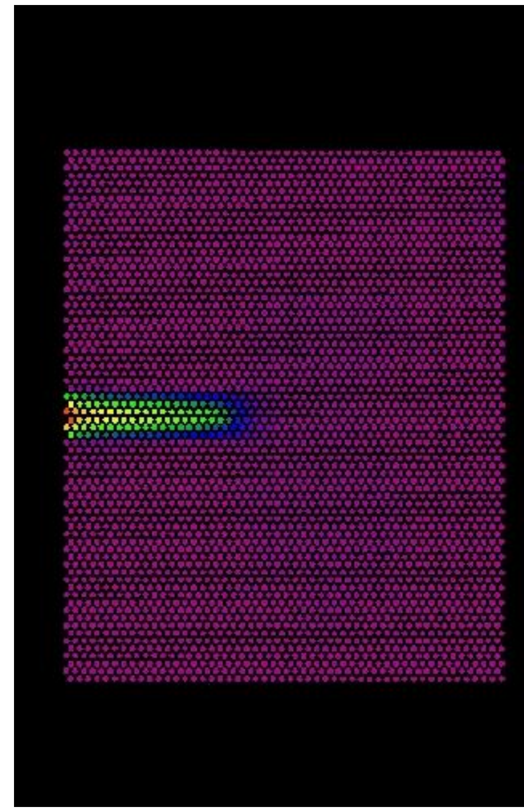
- Look for large peridynamic bond strains in a smoothed grid.
- To test: try to correctly identify when an artificial crack appears and grows.

Artificial crack:
atoms on opposite
sides do not interact



Atomic velocities in Al
(mostly thermal, T=20degC)

Smoothing →



Continuum model:
Peridynamic bond strains

Determining the failure properties of grain boundaries

- MD shows that failure mostly occurs at grain boundaries.
- How to determine the peridynamic bond failure strain?
- Bond failure strain is defined to be the bond strain at the time the bond strain rate starts increasing.