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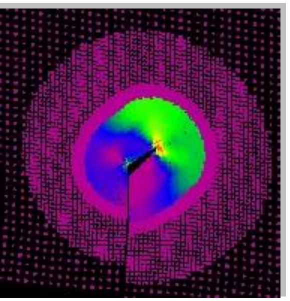
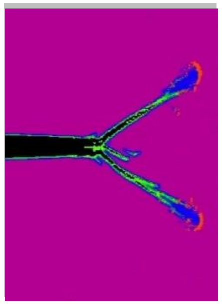
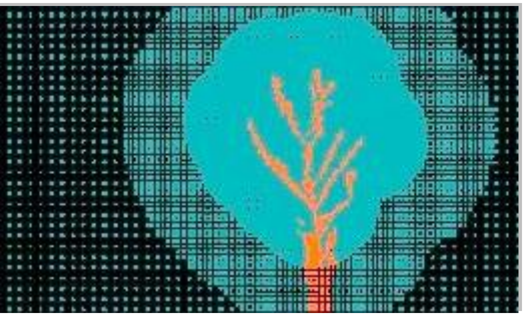

Predictivity in fracture modeling

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Workshop for Nonlocal Models in Mathematics, Computation, Science, and Engineering

Oak Ridge National Laboratory, TN, October 26, 2015

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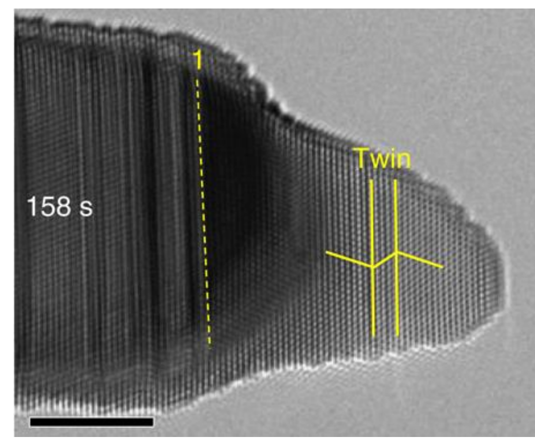
Outline

- Why is fracture a challenging problem?
- Treatment of fracture in the local theory and in peridynamics
- Reality and usefulness of nonlocality
- Material variability and the probabilistic nature of fracture

Physical aspects

- It involves many length and time scales.
- It can involve multiple mechanisms that lead to fracture only in combination with each other.
- It can involve many interacting defects.

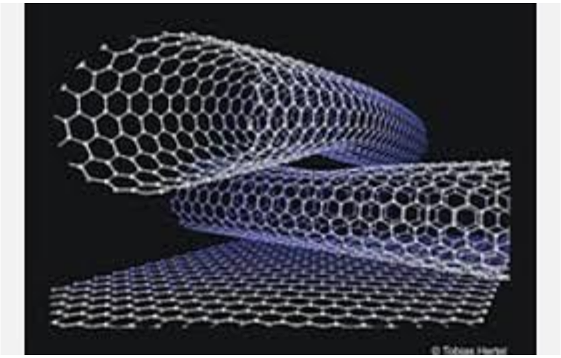
Fragmented glass
(image: Washington Glass School)



Nanoscale twins in fractured gold crystal
J. Wang et al, Nature Communications (2013)

Mathematical aspects

- The nature of fracture as a discontinuity is incompatible with the local theory.
- The Cauchy (local) theory assumes a continuous deformation.
- This leads to need to hack in extraneous mathematical relations (LEFM).
- Fracture processes are often physically nonlocal at some level.



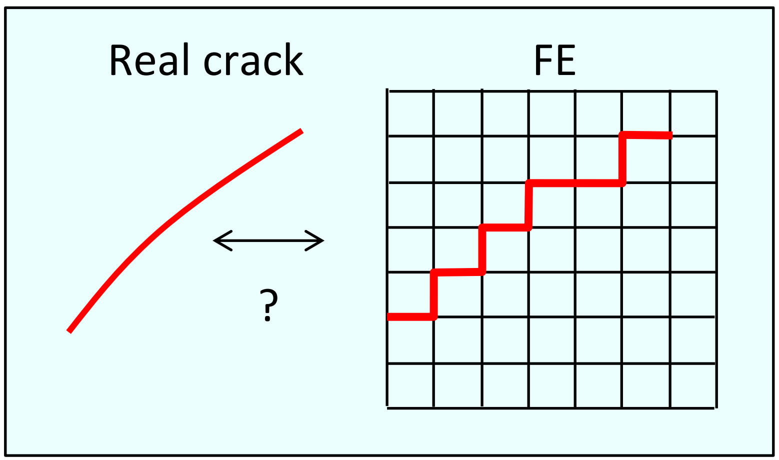
Carbon nanotubes (image: nsf.gov)

$$\nabla \cdot \sigma + b = 0$$

Augustin-Louis Cauchy, 1840
(image: Library of Congress)

Computational aspects

- Traditional FEM (e.g. displacement Galerkin) inherits the incompatibility of the local theory with fracture.
- This leads to the need to hack in a fix after discretization.
- MD is better but too slow.



Complex crack path in a composite

(b)

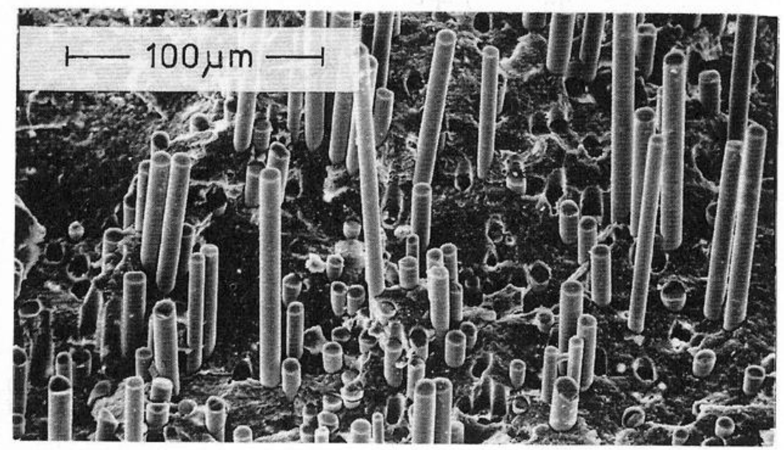


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of 'Silceram' glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

Fracture modeling in the local theory

- Smeared crack models, continuum damage mechanics
  - Attempt to adjust bulk material properties without addressing individual cracks.
  - Damage D at x evolves according to local conditions.

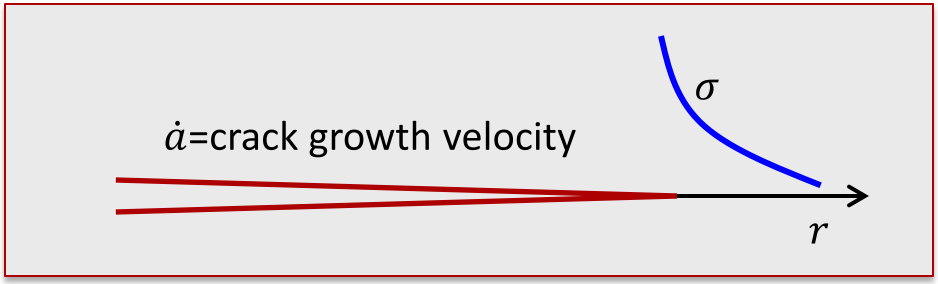
$$\dot{D} = \phi(F, \dot{F}, \theta, \dots)$$

    where F= deformation gradient tensor, θ= temperature.

  - Damage degrades the material properties. Examples:
    - $Y = (1-D)Y_0$ … flow stress (smeared crack model).
    - $E = (1-D)E_0$ … elastic modulus (CDM).
  - Advantage: Easy to include in FEM.
  - Disadvantage: Failure occurs in many elements rather than on 2D surfaces (discrete cracks).

Linear elastic fracture mechanics (LEFM)

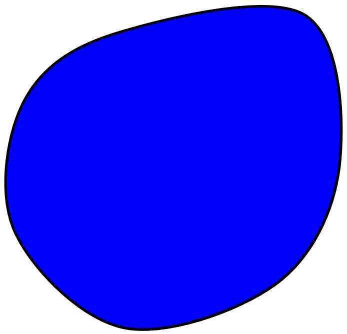
- Assumes that the classical asymptotic stress field ($\sigma = K/\sqrt{r}$) holds within a small region near the crack tip.
- Crack growth occurs according to a given function $\dot{a}(K)$ that is obtained empirically.



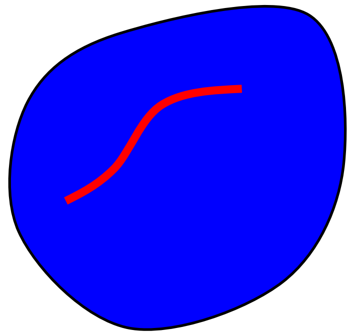
- Advantages:
  - Doesn't model the details of the process zone.
  - Compatible with energy balance concept of brittle fracture (Griffith).
- Disadvantages:
  - Doesn't model the details of the process zone.
  - The function $\dot{a}(K)$ can be measured only in ideal cases.
  - Assumes a pre-existing crack.

Purpose of peridynamics*

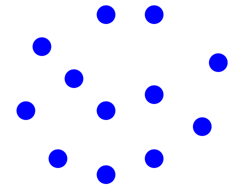
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body with a defect



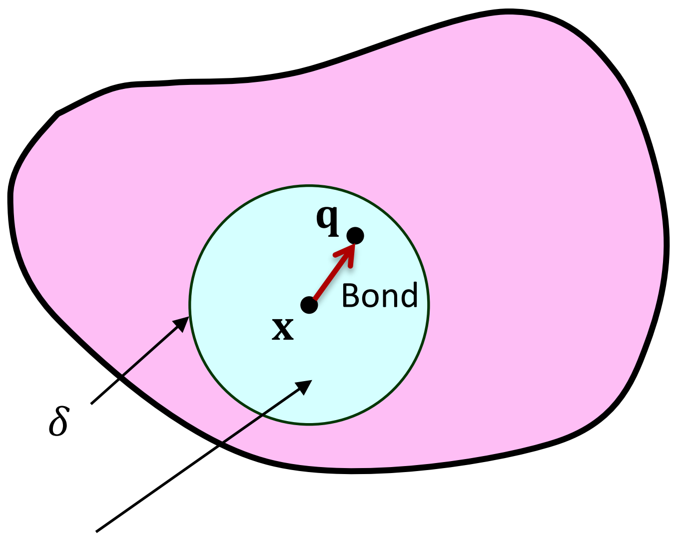
Discrete particles

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

* Peri (near) + dyn (force)

Peridynamics: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 $\mathbf{x}$, $\mathcal{H}_\mathbf{x}$.



$\mathcal{H}_\mathbf{x}$= family of $\mathbf{x}$

Equilibrium equation

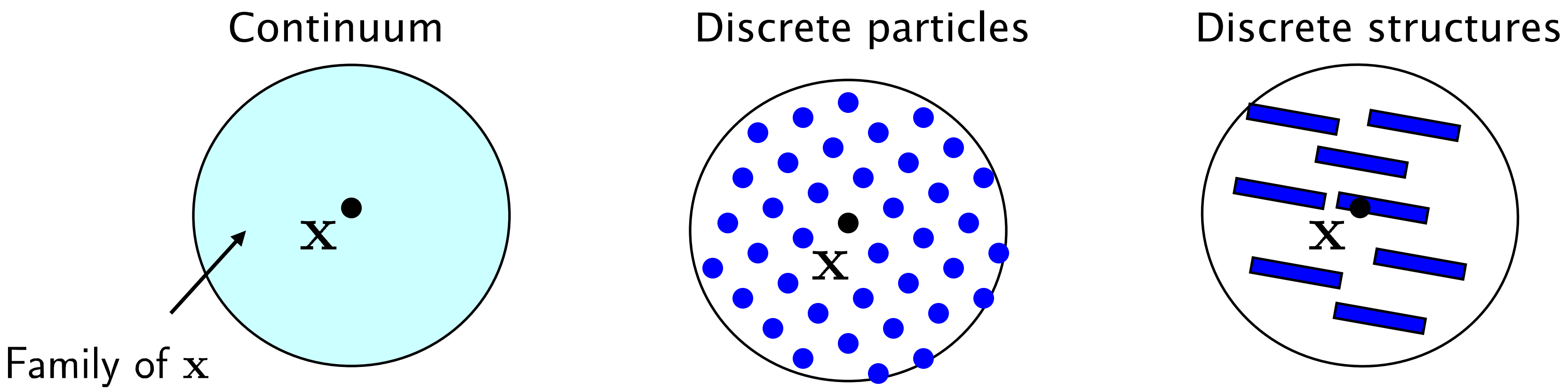
$$\int_{\mathcal{H}_\mathbf{x}} \mathbf{f}(\mathbf{q},\mathbf{x})\, dV_\mathbf{q} + \mathbf{b}(\mathbf{x}) = 0$$

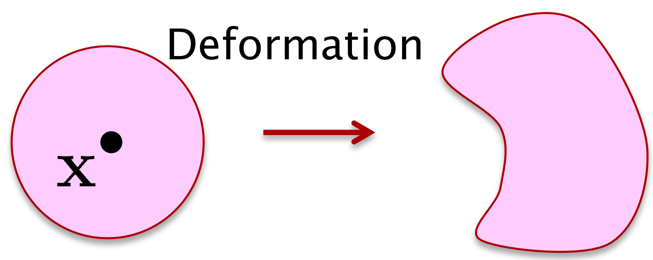
f = bond force density

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)

Peridynamics: Strain energy at a point





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

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Peridynamic vs. local equations

- State notation: State<bond>=vector

Relation	*Peridynamic theory*	*Standard theory*
Kinematics	$\underline{\mathbf{Y}}\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q}) - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
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	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + q + r$	$\dot{\varepsilon} = \boldsymbol{\sigma}\cdot\dot{\mathbf{F}} + q + r$

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

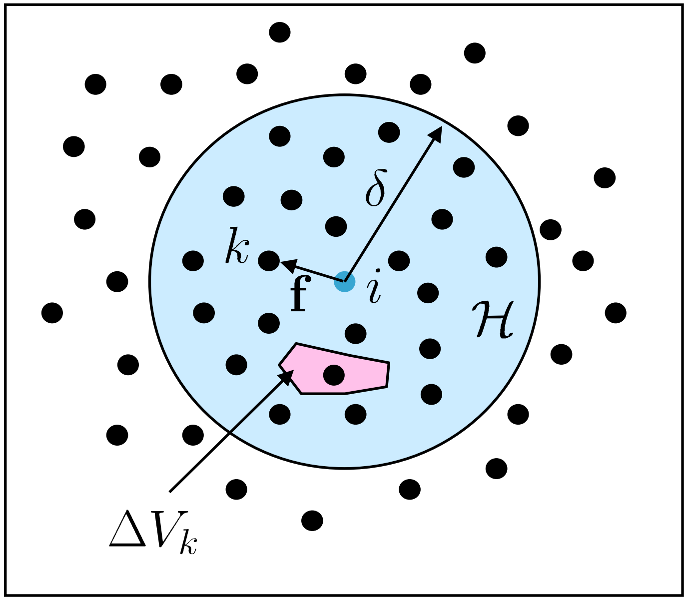
Peridynamics: EMU numerical method

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

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

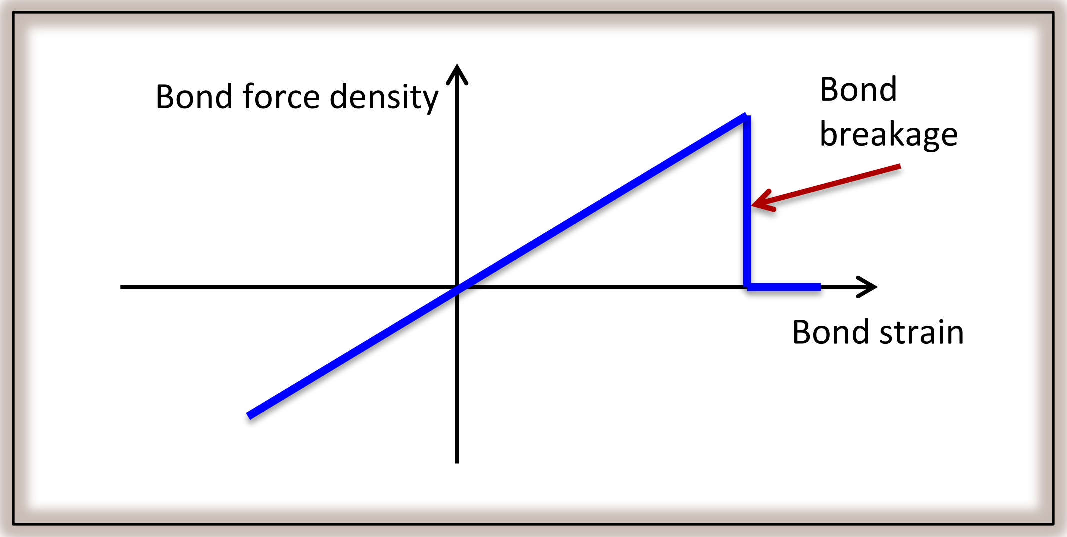
- Linearized model:

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

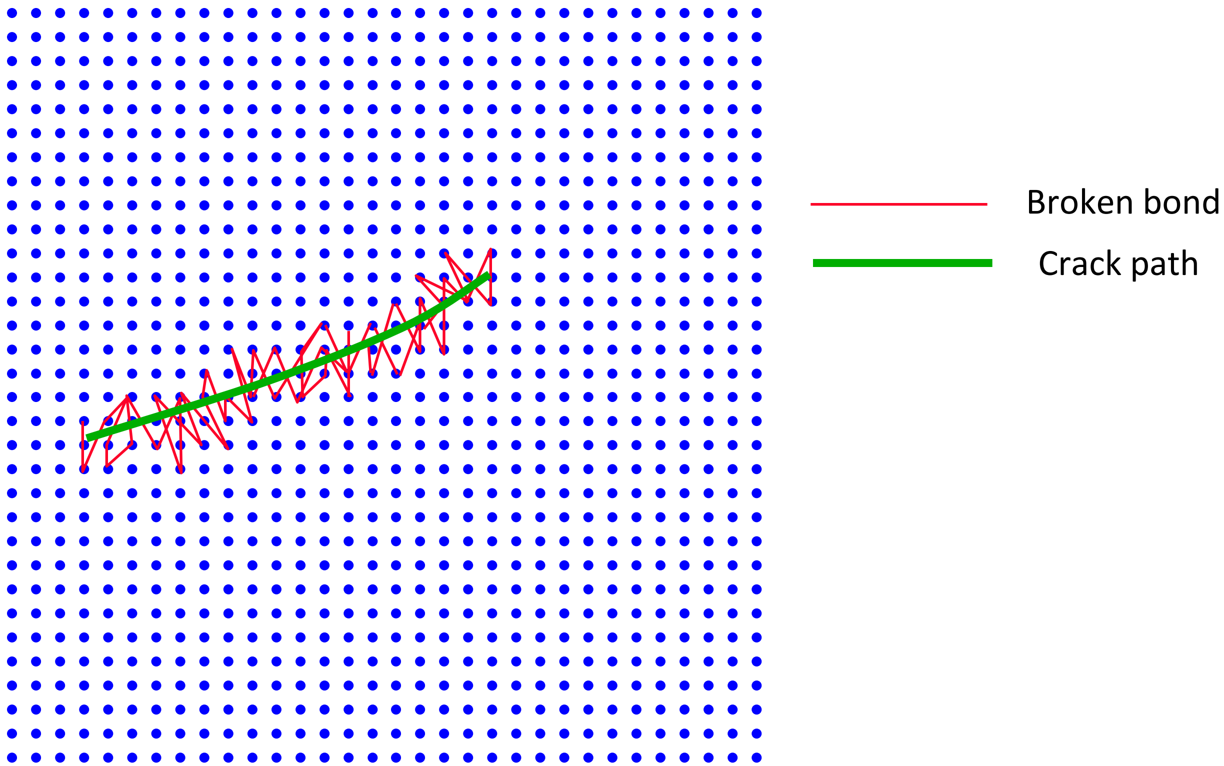


Bond based material models

- 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.

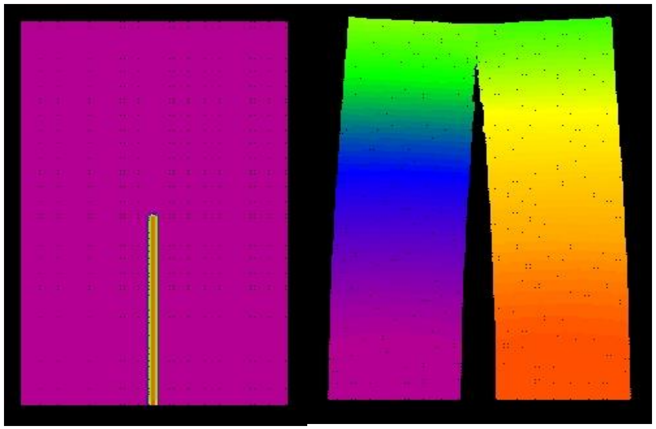


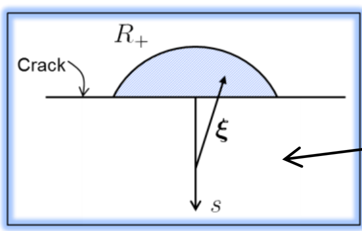
Autonomous crack growth



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

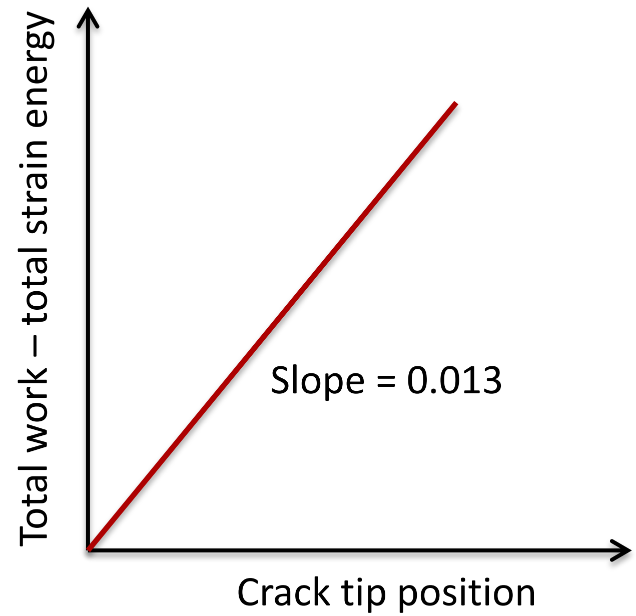
PD reproduces the Griffith crack energy





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.

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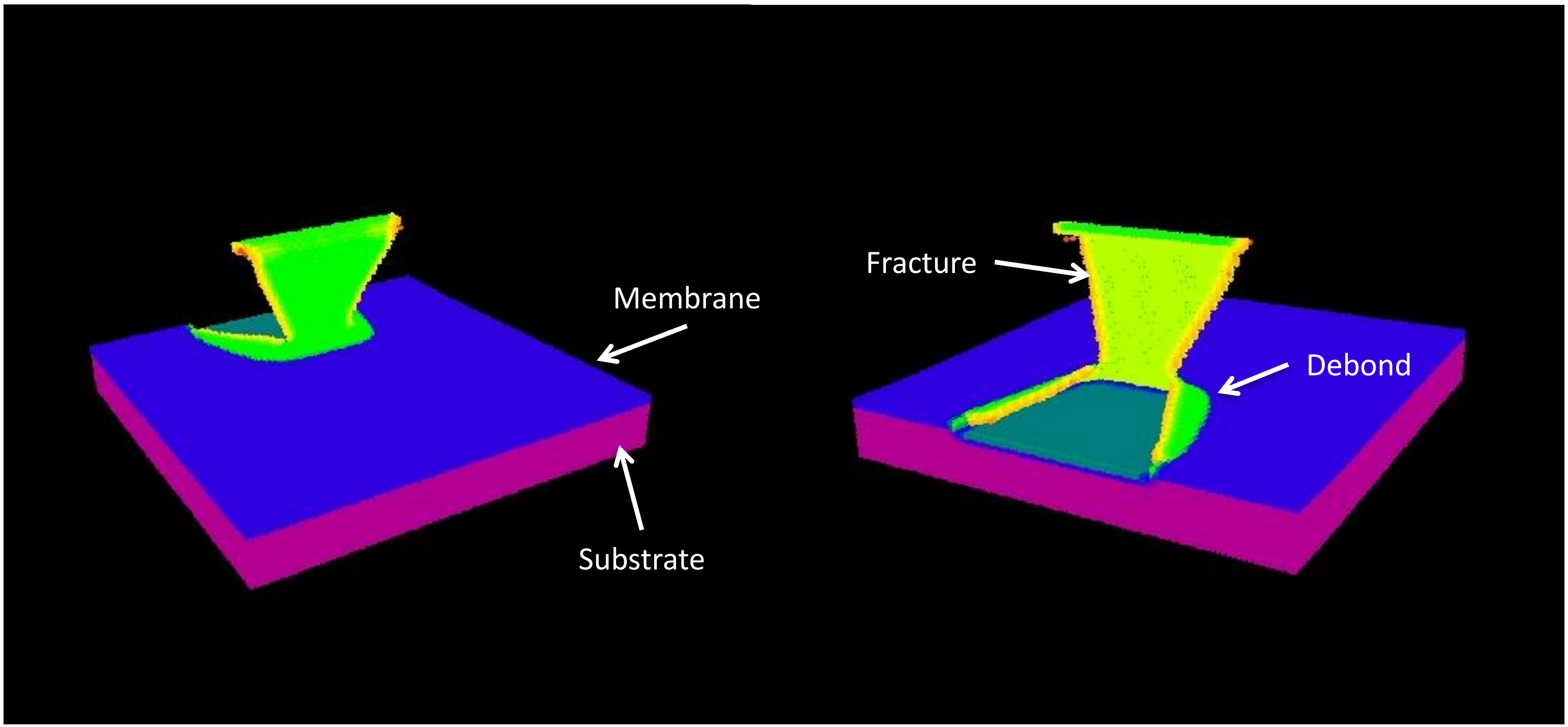
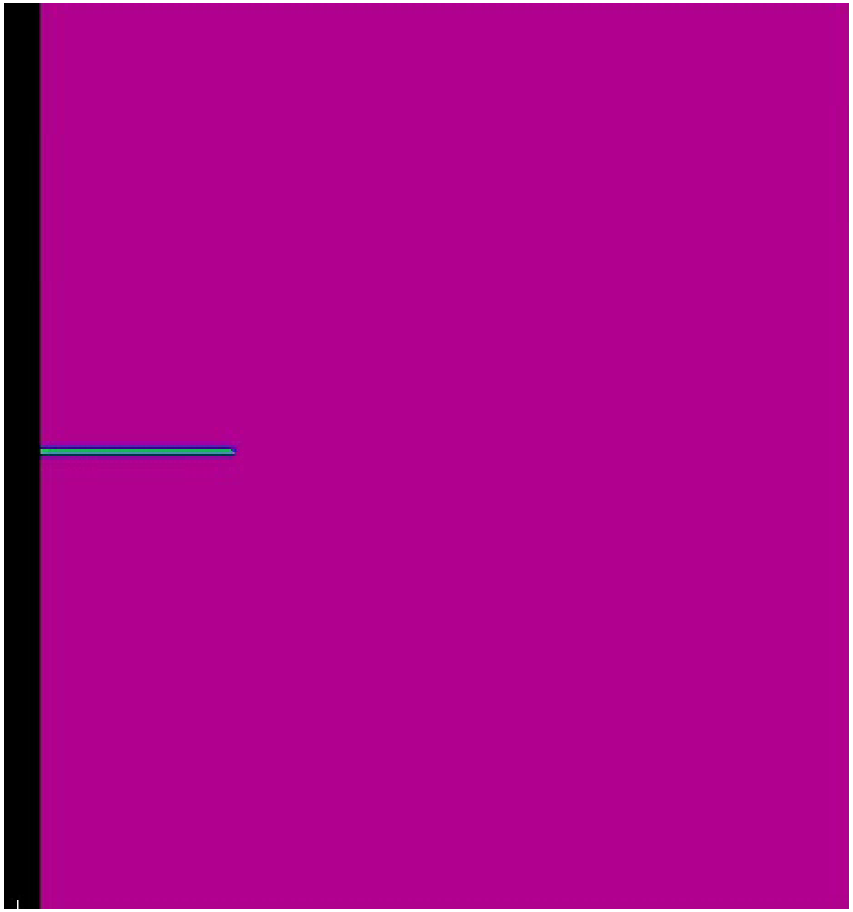
Fracture and debonding of membranes

- Simulation of peeling illustrates interplay between fracture (tearing) and debonding (peeling).



Dynamic crack branching

Video

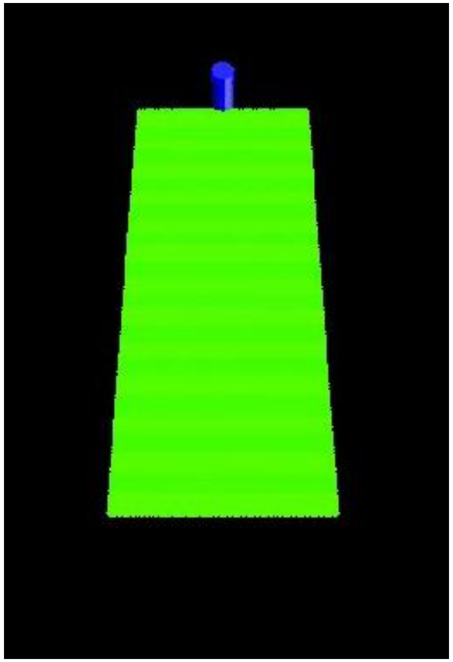


- Red indicates bonds currently undergoing damage.
- These appear ahead of the visible discontinuities.
- Blue/green indicate damage (broken bonds).
- More and more energy is being built up ahead of the crack – it can't keep up.
    - Leads to fragmentation.

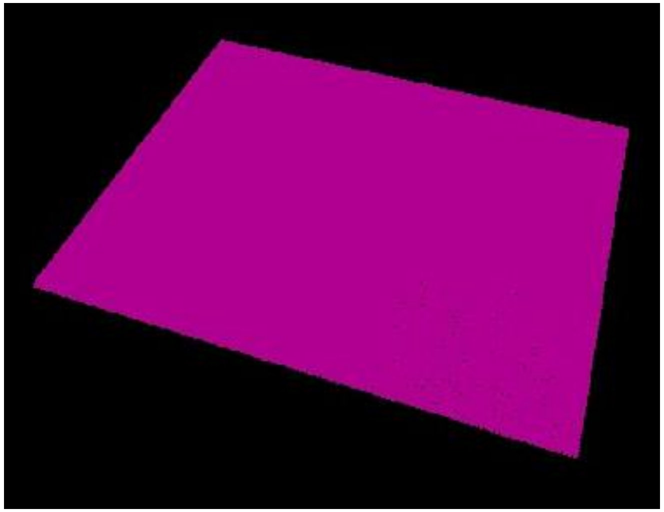
More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Membranes and thin films

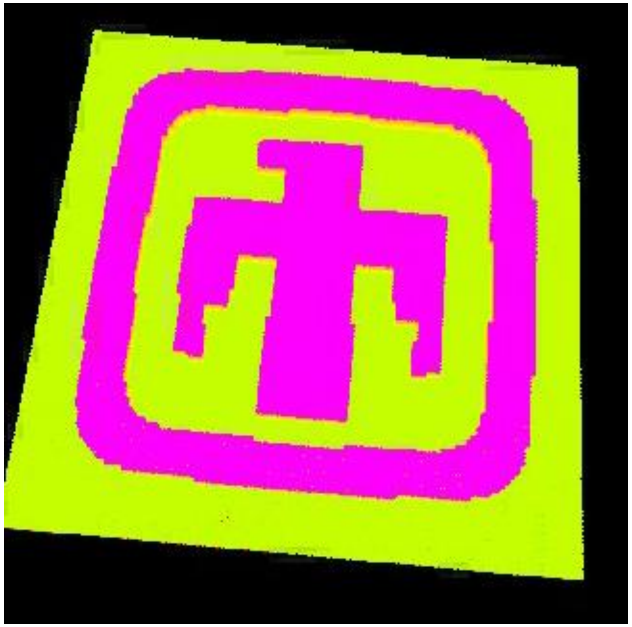
Videos



Oscillatory crack path



Crack interaction in a sheet



Aging of a film

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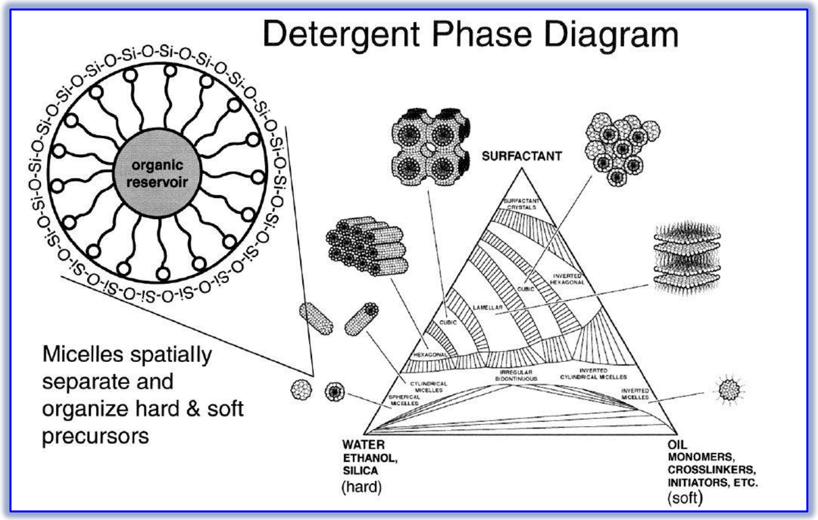
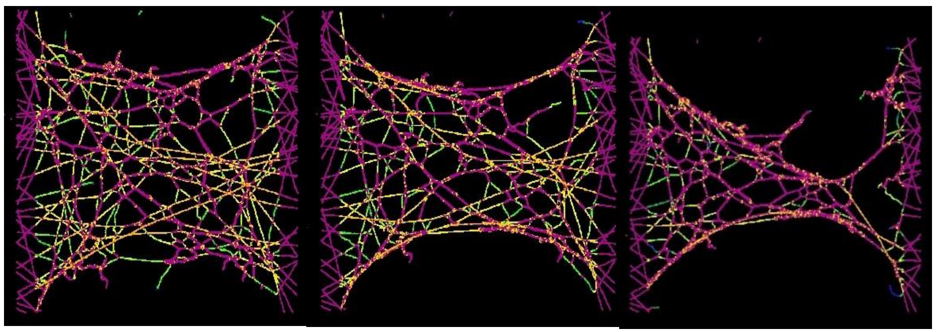
Physical nonlocality: Self-assembly and long-range forces

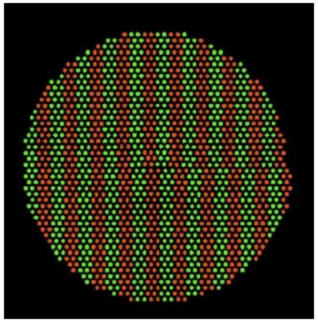
- Potential importance for self-assembled nanostructures.
- All forces are treated as long-range.



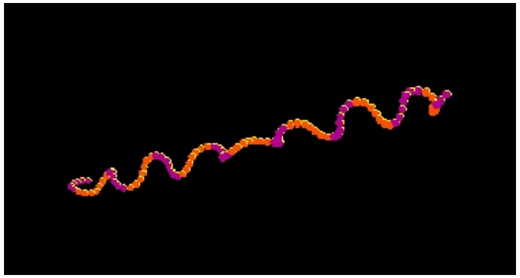
Self-assembly is driven by long-range forces
Image: Brinker, Lu, & Sellinger, Advanced Materials (1999)



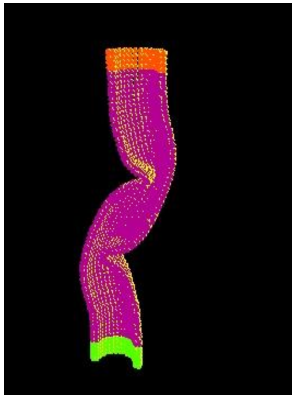
Failure in a nanofiber membrane
(F. Bobaru, Univ. of Nebraska)



Dislocation



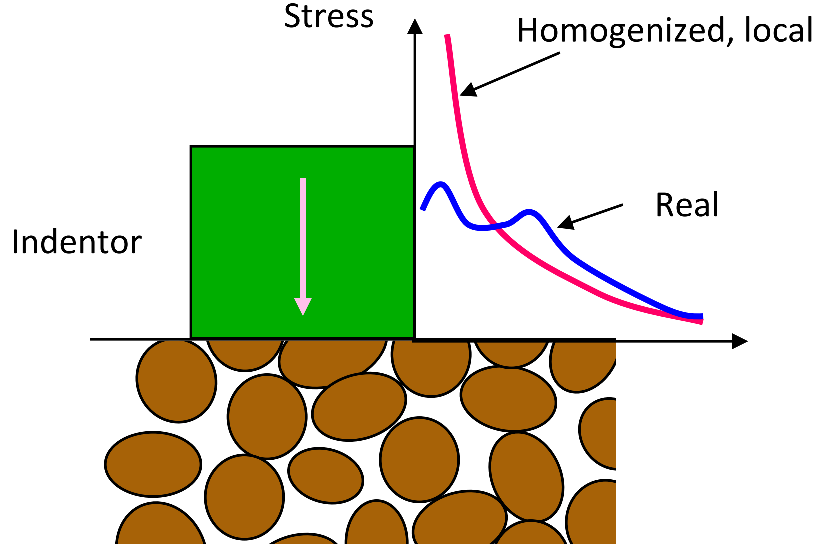
Nanofiber self-shaping



Carbon nanotube

Nonlocality can arise from the way we choose to model things

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



Concrete

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

Nonlocality in a composite

- When we use a “smoothed out” displacement field, nonlocality appears in the equations.
- Example: alternate stiff and compliant layers.
- Prescribe the mean displacement (1D) to be a step function of position.

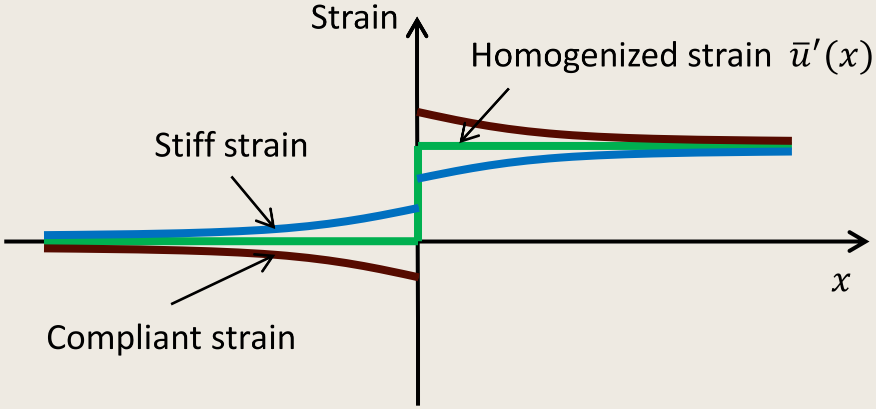
Nonlocality in a composite, ctd.

- The evolution equation for the mean displacement field is nonlocal.

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

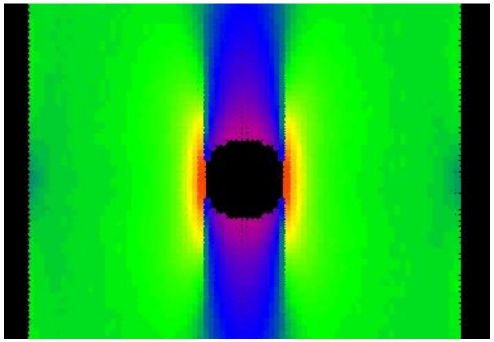
$$\frac{1}{\lambda} = \sqrt{\frac{E_s h_s h_c^2}{3\mu_c(h_s+h_c)}} = \text{length scale.}$$

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

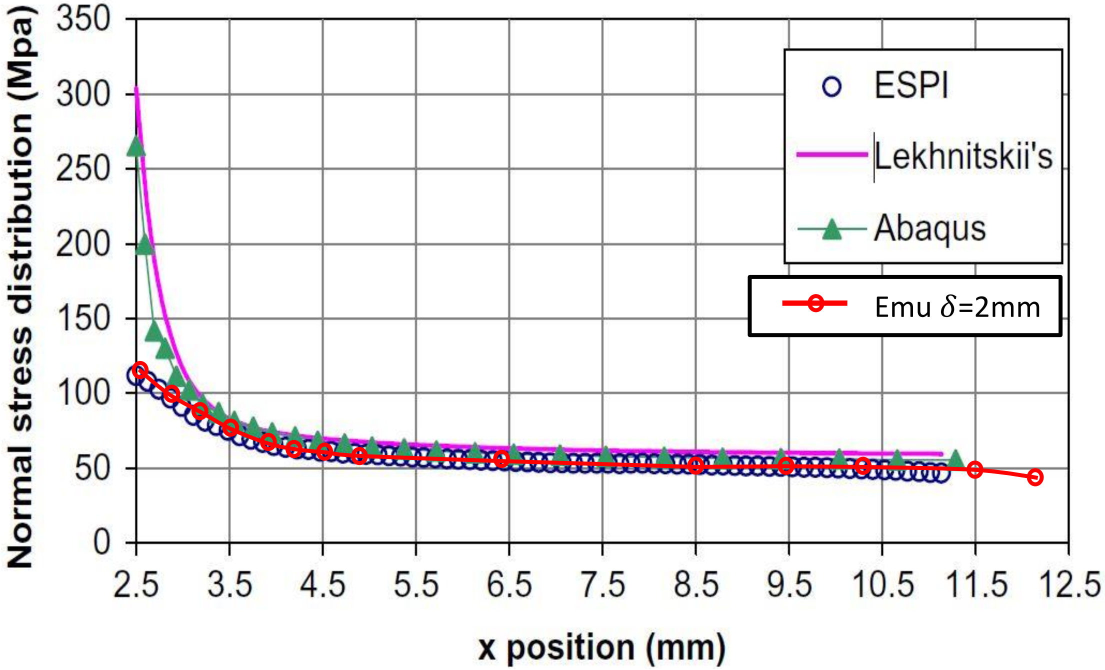


Are composites nonlocal?

- Peridynamic model is more accurate than the local model for predicting stress concentration in a laminate.
- $h_s = h_c$ =0.4mm, E_s = 150GPa, 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

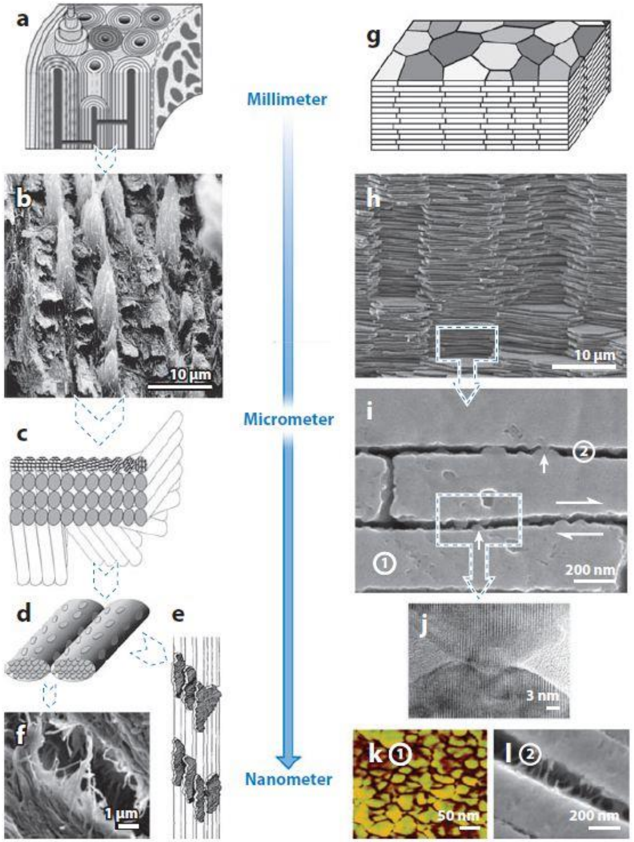
Survey of some nonlocal theories

- MD-like forces, Cauchy-Born kinematics (Navier).
- Add nonlocal terms to the standard local model (Kroner).
- Average the local stress and use this in the Cauchy equilibrium equation (Eringen).
- Average the damage and use this in a local material model (Belytschko, Bazant).
- Include rotational DOFs in a local model (Cosserat).
- Include second partial derivatives of displacement in a local model (Coleman).
- Strongly nonlocal, linear elastic, mechanical only (Kunin).

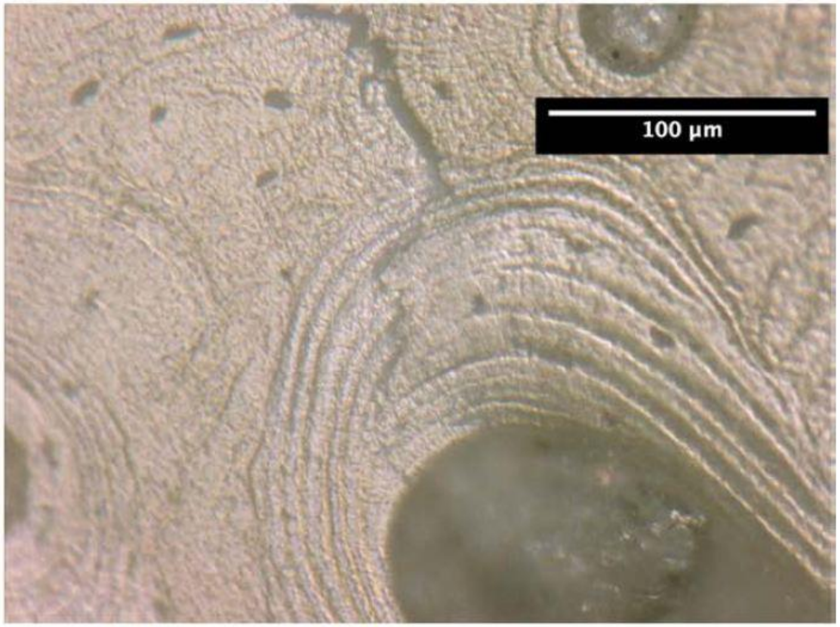
All of the above are unsuitable for modeling fracture.

- Strongly nonlocal, nonlinear, mechanical + consistent thermodynamics + diffusion + damage (peridynamics).

Bone: A composite material with many length scales



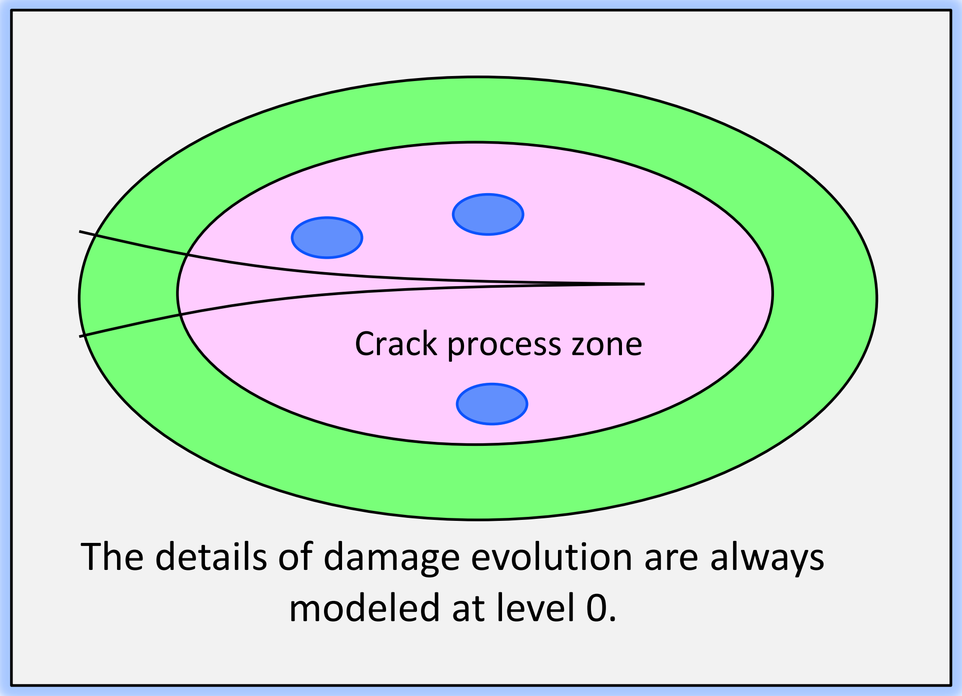
Bone contains a heirarchy of structures at many length scales. Image: Wang and Gupta, *Ann. Rev. Mat. Sci.* 41 (2011) 41-73



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

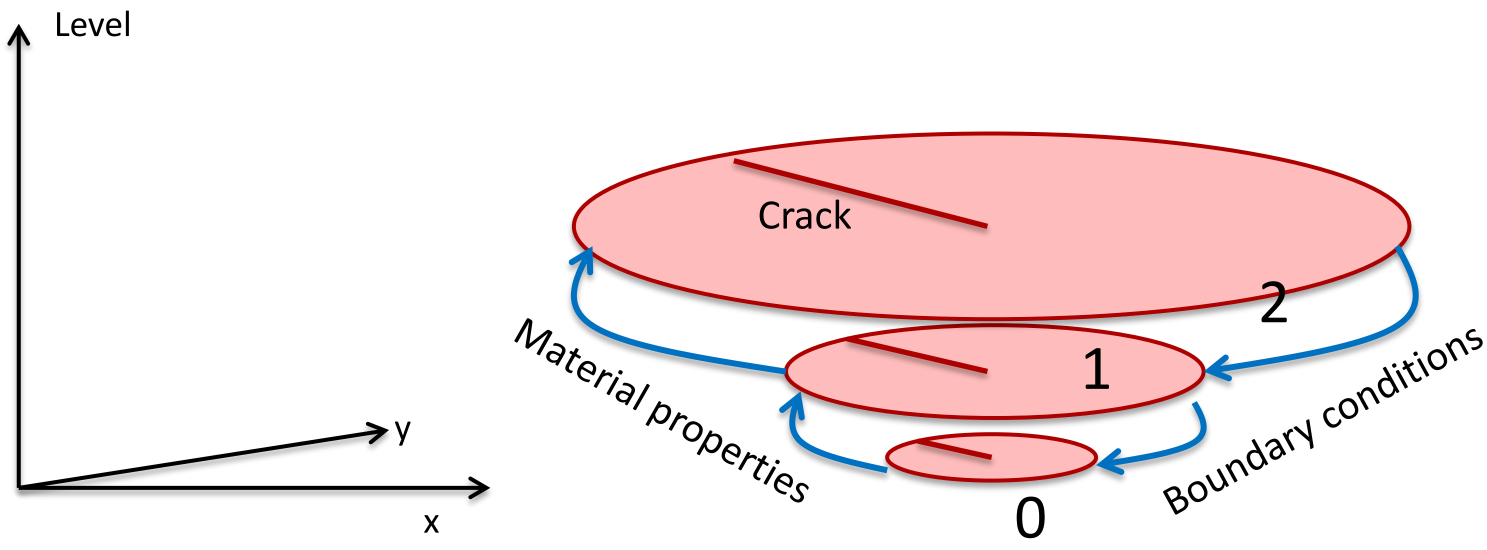
Concurrent multiscale method for defects

- 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

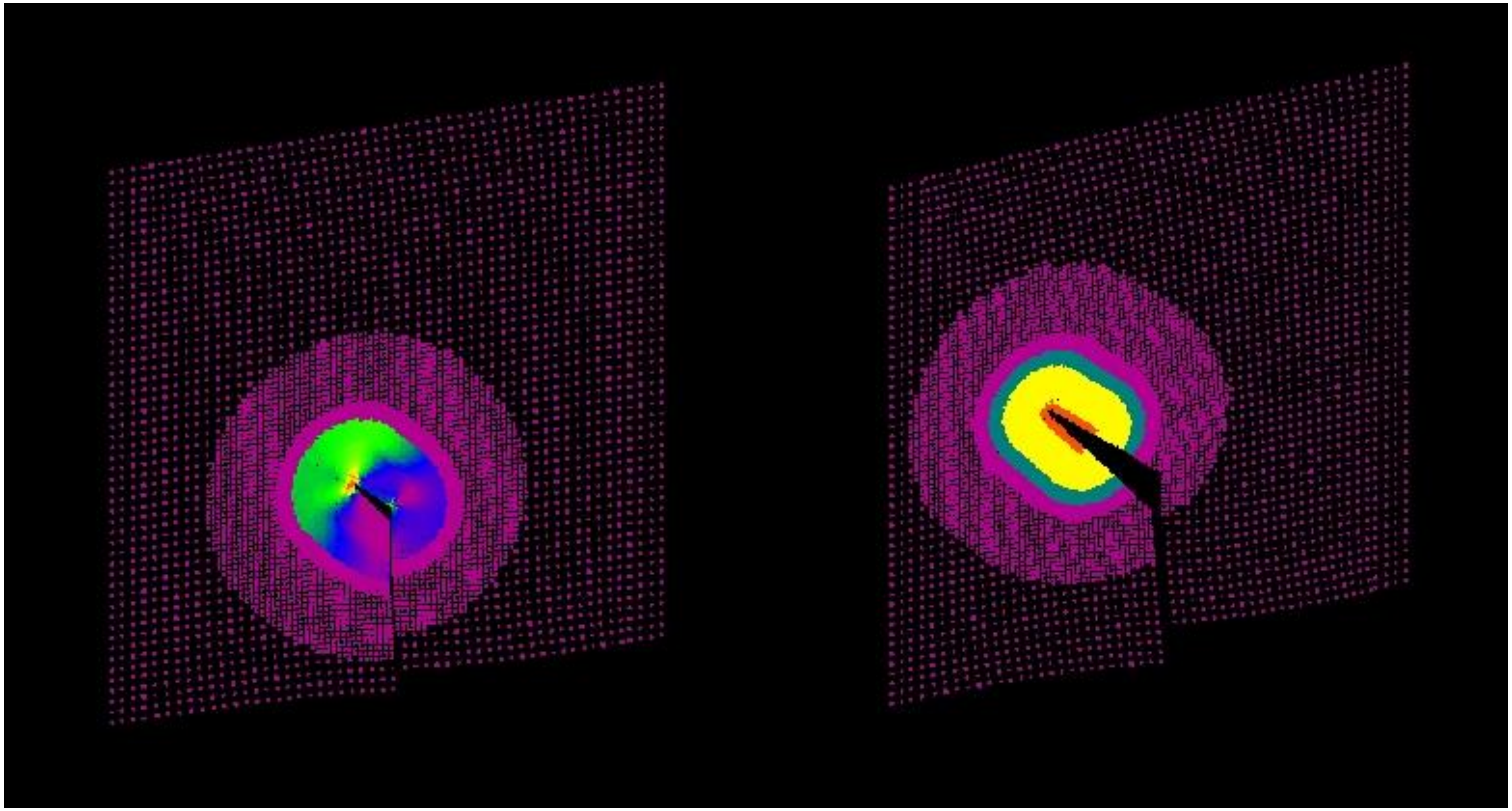
- The equation of motion is applied only within each level.
- Higher levels provide boundary conditions on lower levels.
- Lower levels provide coarsened material properties (including damage) to higher levels.
- In principle, a large number of levels can be used, all coupled in the same way: "scalable multiscale" method.



Schematic of communication between levels in a 2D body

Concurrent multiscale example: shear loading of a crack

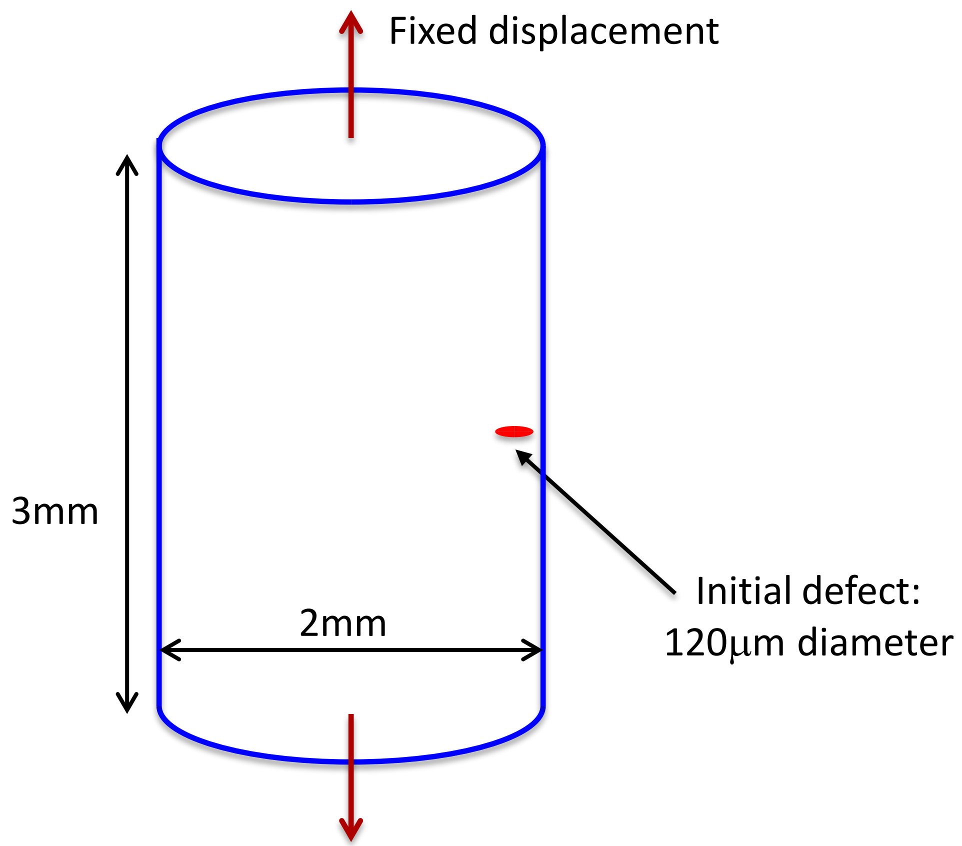
- Level 0 region adaptively follows the crack tip.



Bond strain | Damage process zone

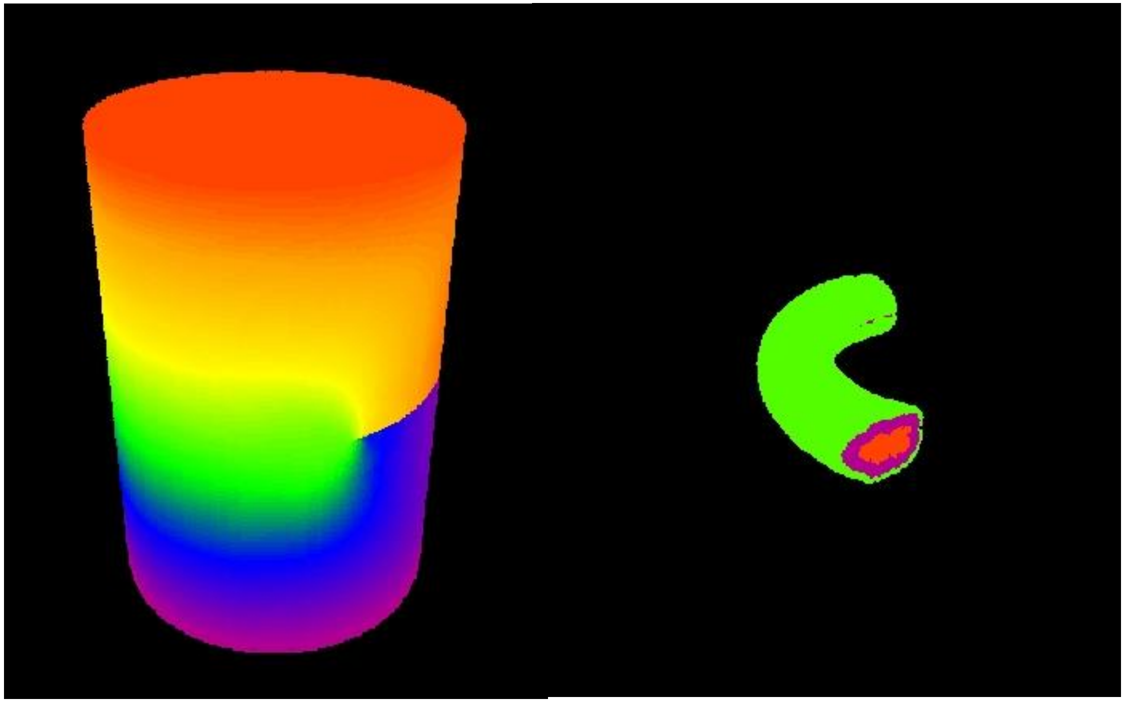
Failure of a glass rod in tension

- A classical test problem for fractography.
- We will try to reproduce key fractographic features.
- Multiscale approach allows us to make the horizon << geometric length scales.



ρ = 3000 kg/m^3
E = 70.5 GPa
ν= 0.25
G_{Ic} = 7.0 J/m^2
δ = 25μm

Failure of a glass rod in tension



Level 1 displacement   Level 0 surrounds the crack front

- Level 1 multiscale.
- 20,000,000 level 0 sites (most are never used).
- Level 0 horizon is 25μm.

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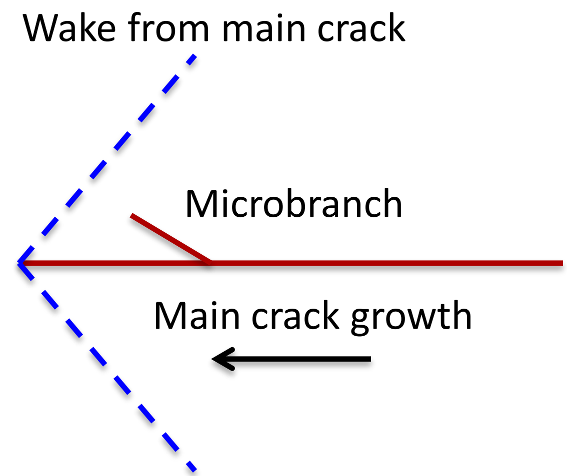
Failure of a glass rod in tension (movie)

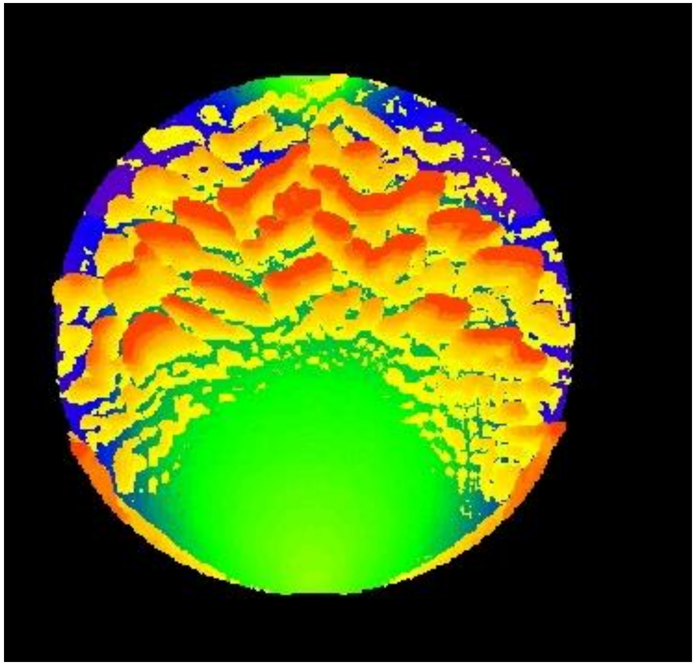
Evolution of surface roughness (movie)



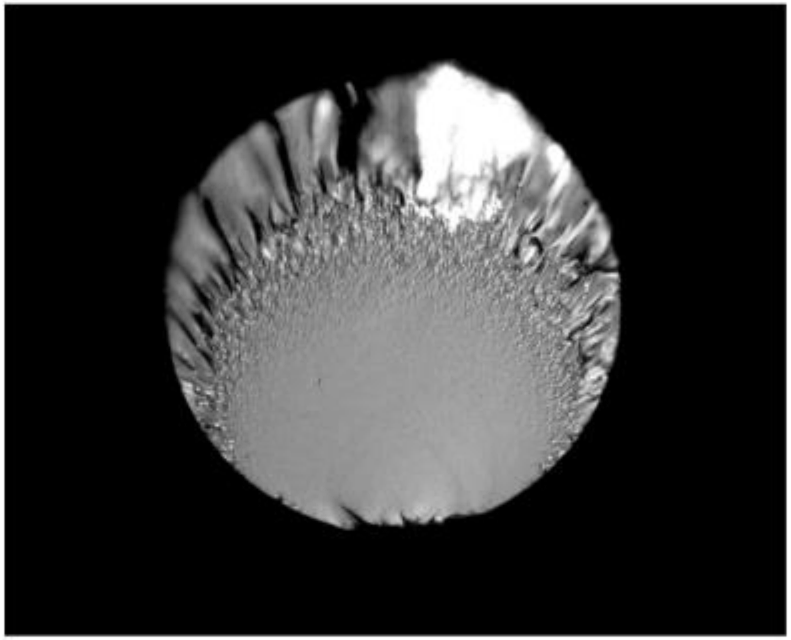
- Rough features branch off from the main crack.
- Each one grows slower than the main crack and eventually dies.

Mirror-mist-hackle

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



3D peridynamic model



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

Composite fracture features

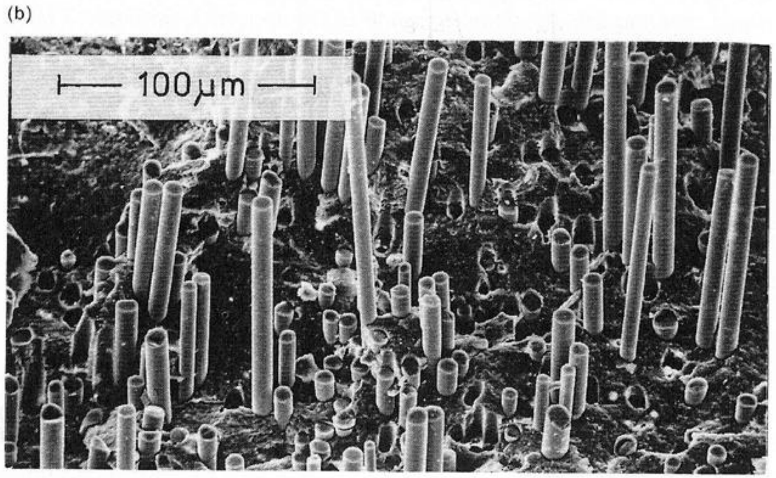
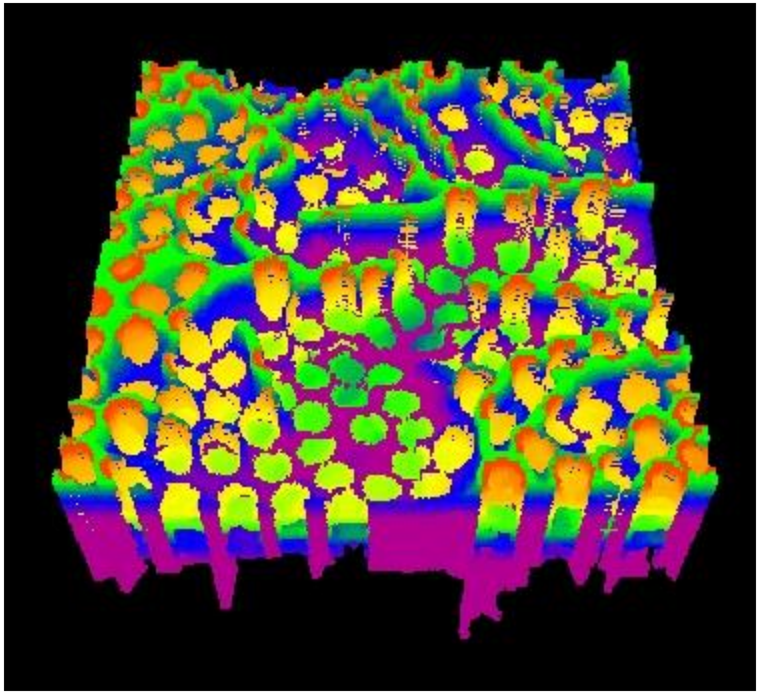


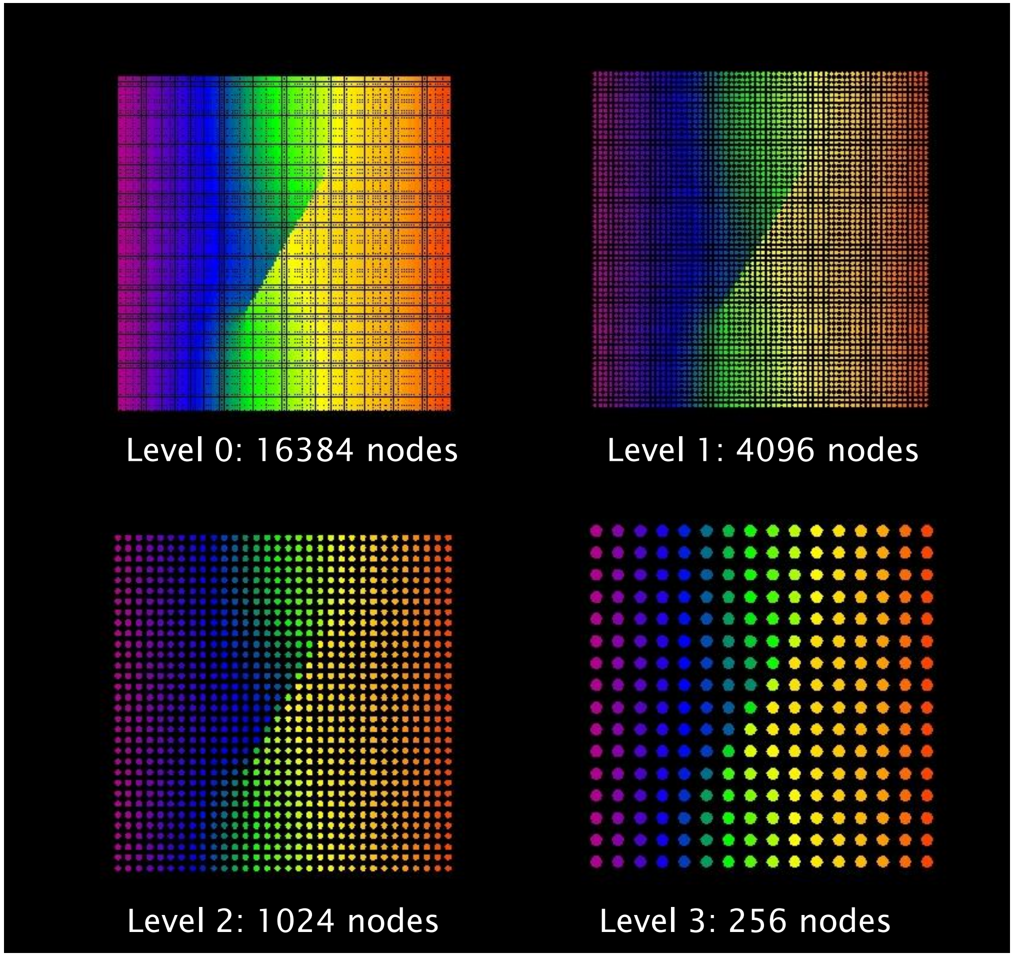
Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of 'Silceram' glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

Complex crack path in a composite



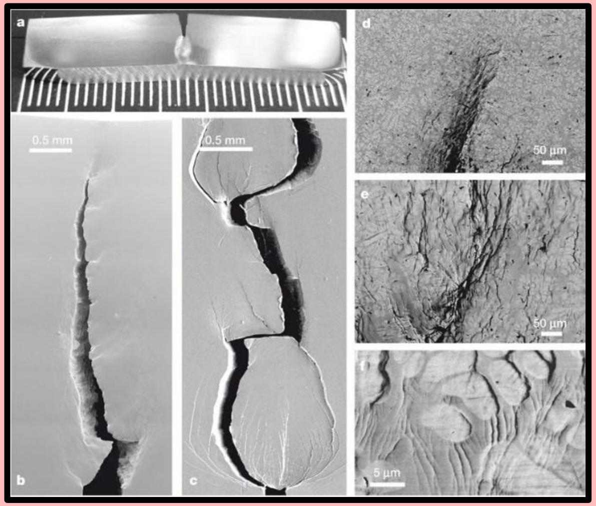
Multiscale verification: crack in a plate

- Example: Solve the same problem in four different levels using the successively upscaled material properties – results are the same.



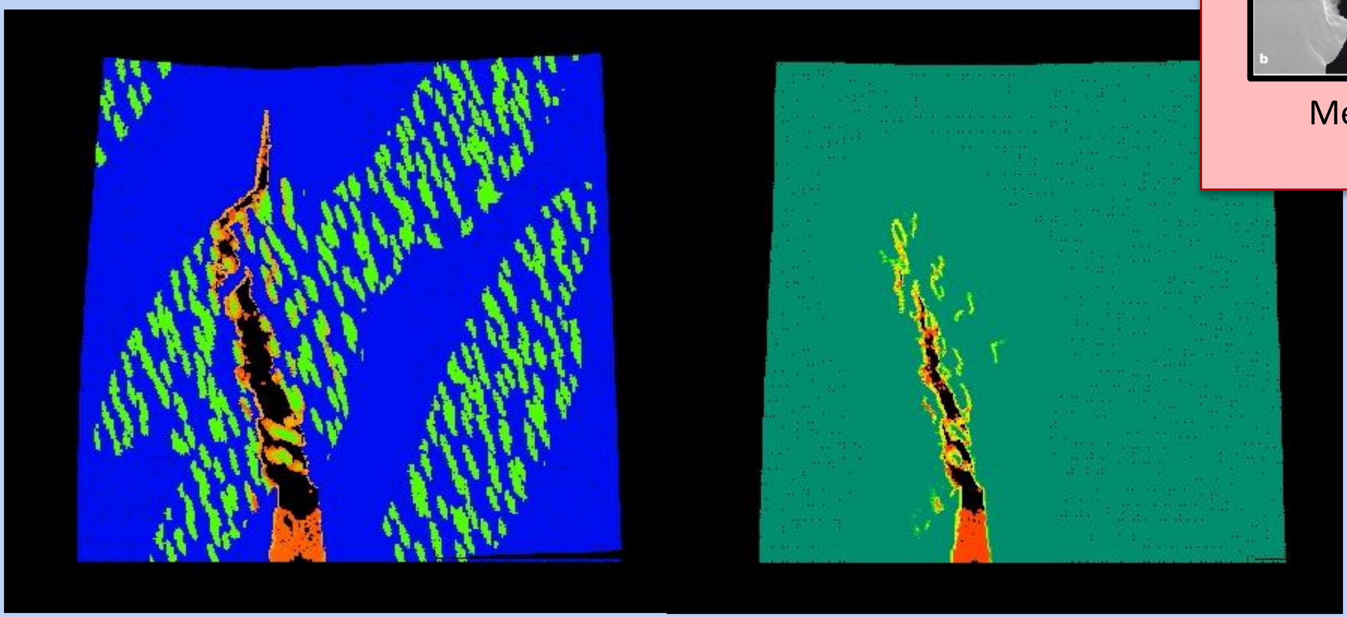
Multiscale modeling reveals the structure of brittle cracks

- Material design requires understanding of how morphology at multiple length scales affects strength.
- This is a key to material reliability.



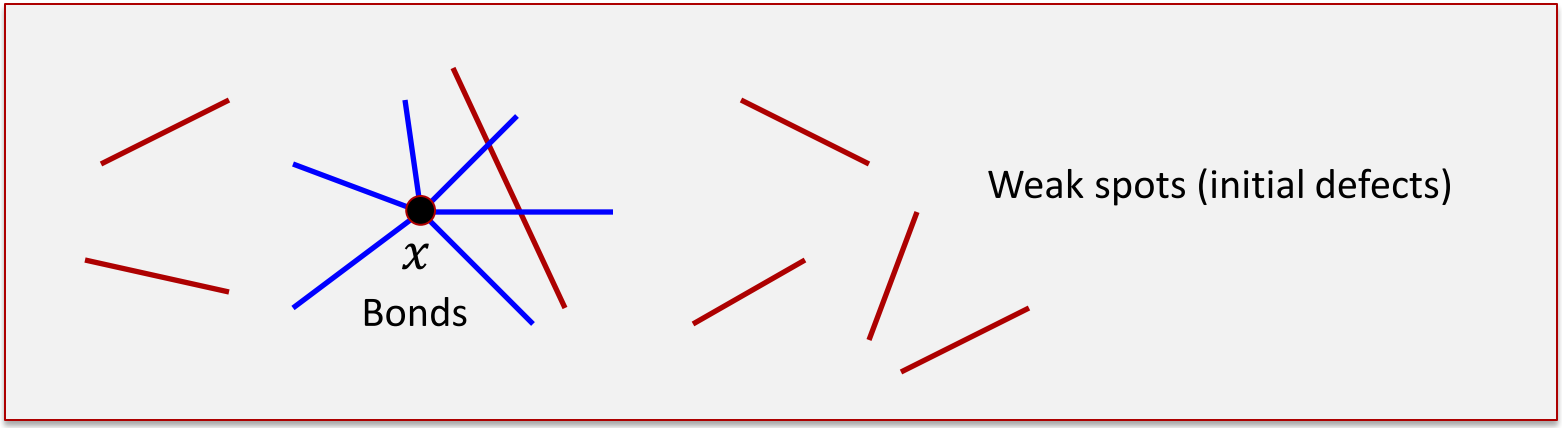
Metallic glass fracture (Hofmann et al, Nature 2008)

Multiscale model of crack growth through a brittle material with distributed defects



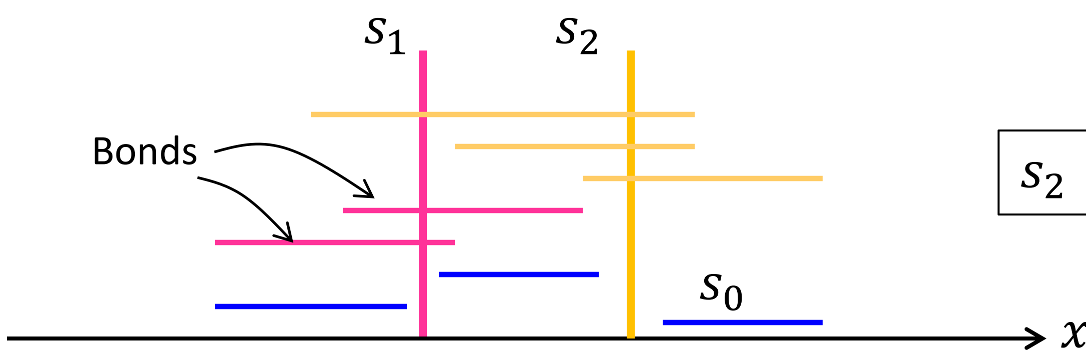
How should we treat a random distribution of defects?

- Can the random nature of fracture be reflected in continuum level properties?
  - Wrong ways:
    - Local: randomly assign element properties.
    - Peridynamic: randomly assign critical strains to bonds.
- Right way:
  - Start with a realization of a random distribution of initial defects.
  - Assign critical bonds strains that reflect each realization.



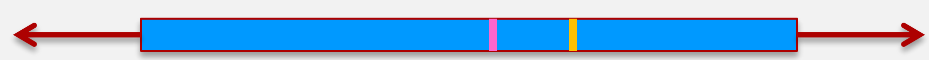
Modeling randomness in fracture

- Assign a critical strain to each defect s_i.
- Set each bond critical strain to the minimum of those of the defects it crosses.



$$s_2 < s_1 < s_0$$

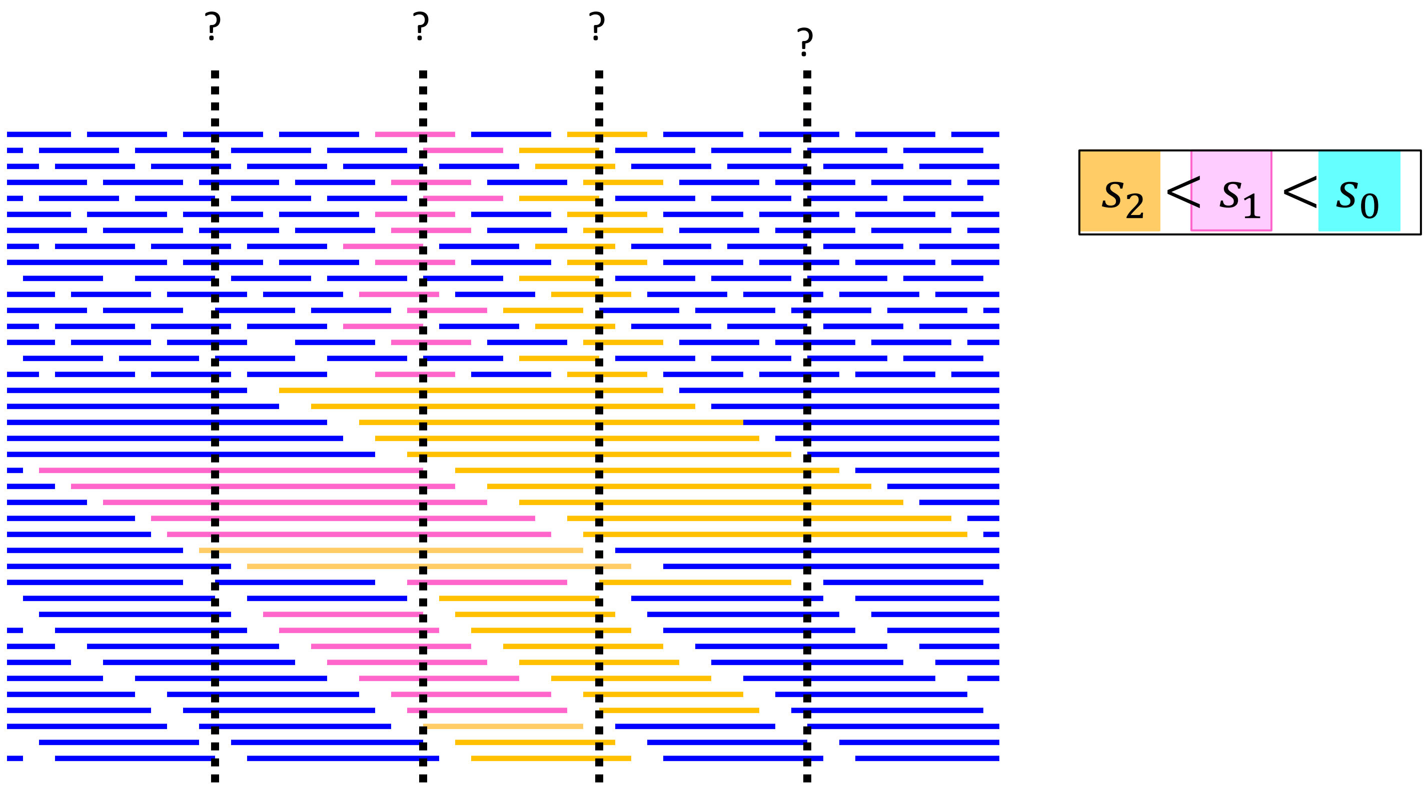
$s_0 \ldots$ undamaged critical strain
$s_1 \ldots$ defect 1 critical strain
$s_2 \ldots$ defect 2 critical strain



Bar containing two defects

Where would fracture occur in this model?

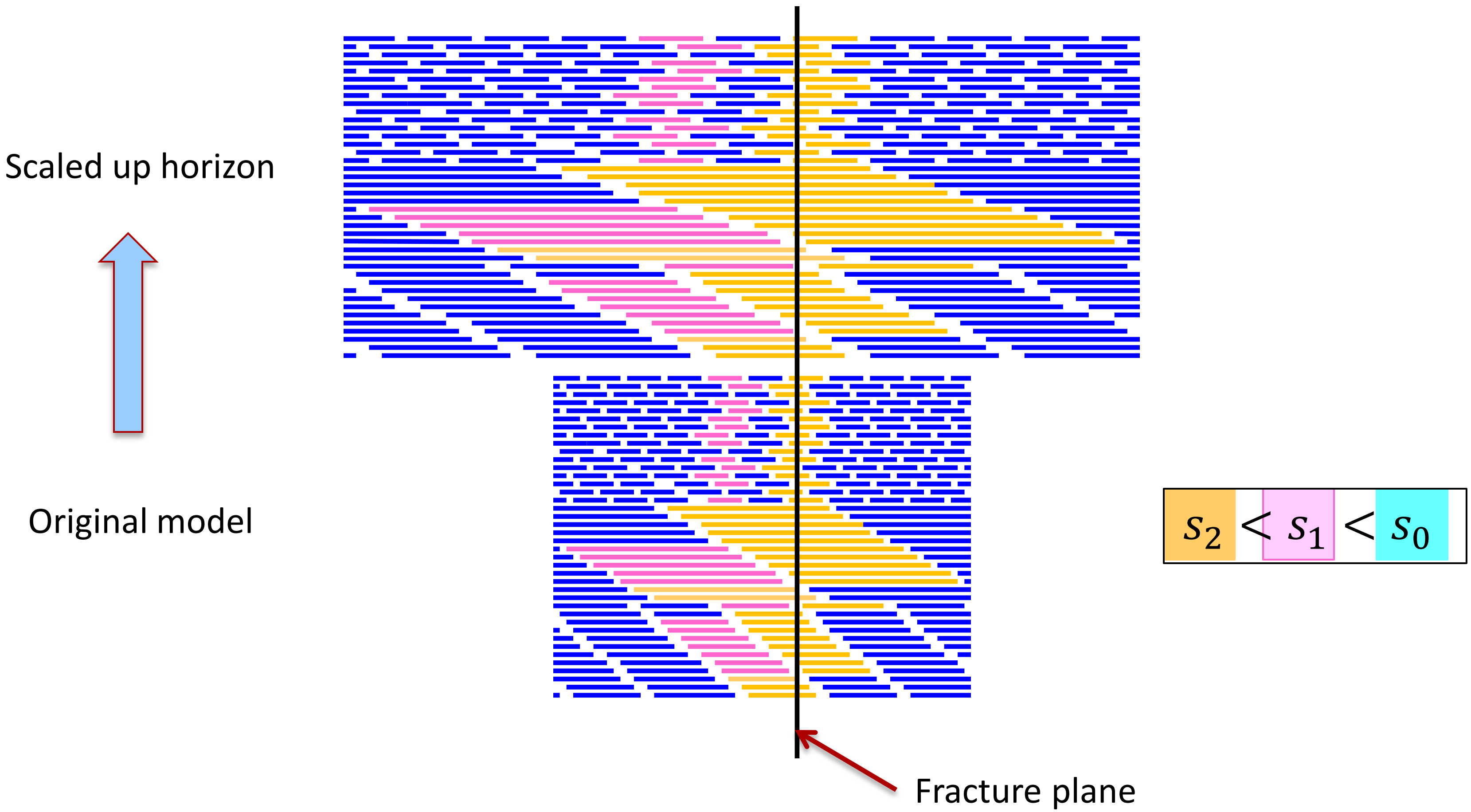
- Assign a critical strain to each defect s_i.
- Set each bond critical strain to the minimum of those of the defects it crosses.



Colors show critical strain in some bonds

Rescaling the critical strains

- Set each new bond critical strain to the minimum of those of the original bonds it intersects.
- The rescaled model still fractures at the weakest spot.



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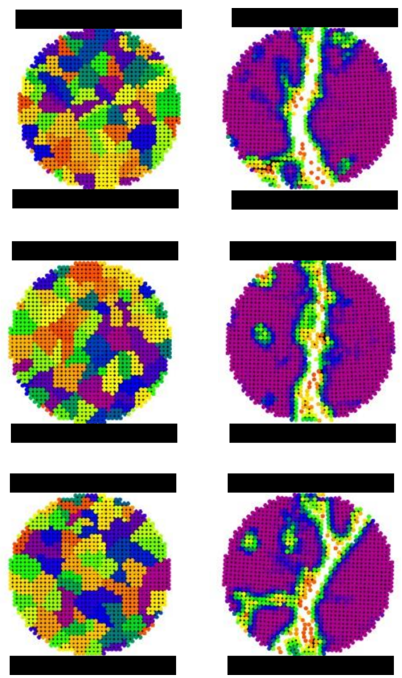
Strategy for treating randomness in fracture due to material variability

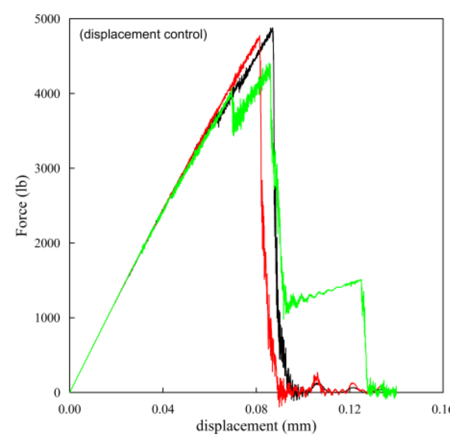
- Define a set of realizations of randomly distributed initial defects.
- Assign level 0 bond strains.
- Scale up to any desired length scale The scaled up model contains the defects.

material realization 1

material realization 2

material realization 3





Brazilian test: J Bishop & J. Holland

Discussion

- It’s fairly clear that nonlocality is an essential feature of any mechanics theory that seeks to accomplish what peridynamics seeks to accomplish.
- Nonlocal interactions can arise due to the way we choose to model things.
    - Especially heterogeneous media.
- Nonlocality may also be an essential feature of a scalable multiscale approach to treating large numbers of small defects.

Do we need a different word for nonlocal continuum mechanics?