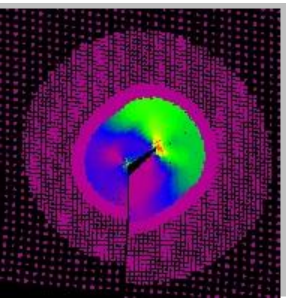
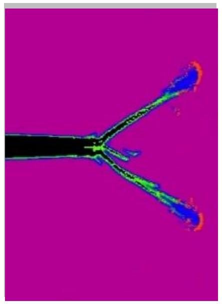
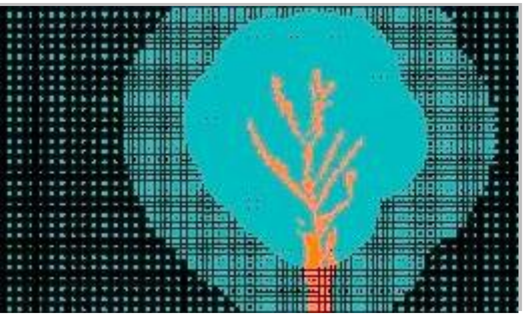
SAND2015-8881C







Three-Dimensional Simulation of Fractographic Features with Multiscale Peridynamics

Stewart Silling

Multiscale Science Department
Sandia National Laboratories
Albuquerque, New Mexico

Florin Bobaru, Yenan Wang

Department of Mechanical Engineering
University of Nebraska
Lincoln, Nebraska

MS&T Conference, Columbus, OH, October 7, 2015

Exceptional service in the national interest

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Outline

- Background
- Peridynamics: what it is
- Impact and fragmentation
- Hierarchical concurrent multiscale method
- Results: Computer simulation of crack surface features
  - Mirror-mist-hackle
  - Interaction of a crack with a bending stress field
  - Multiple defects -- gull wing fracture surface

Background

- Fractographic features are important in failure analysis. They help to:
  - Locate site of critical defects.
  - Figure out what the stress conditions at time of failure were.
- Sample of computational methods that have been applied to crack instability (mainly 2D):
  - Lattice method: Marder & Gross (1995)
  - MD: Abraham, Brodbeck & Rudge (1994, 1997), Buehler & Gao (2006)
  - VIB: Klein & Gao (2002)
  - CZ: Zhou, Molinari & Shioya (2005)
  - Cracking particle method: Rabczuk, Song & Belytschko (2009)
  - XFEM: Menouillard & Belytschko (2010)
  - Phase field: Karma & Kobkovsky (2004), Spatschek et al (2006)

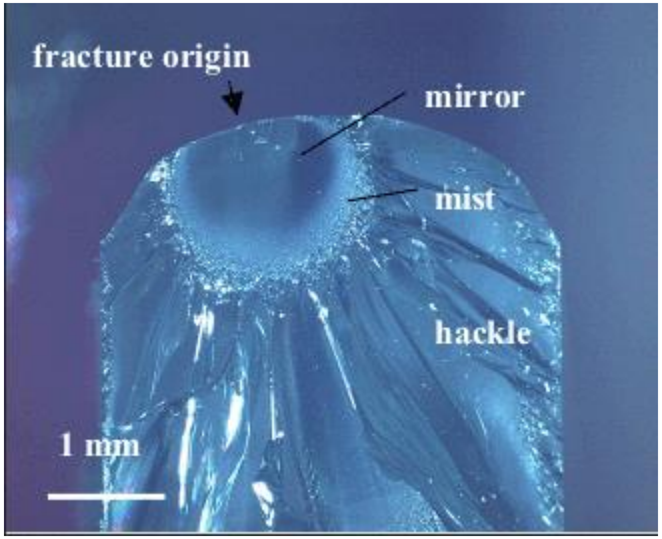
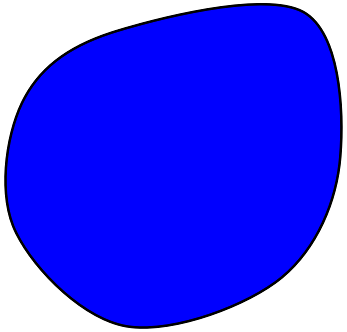


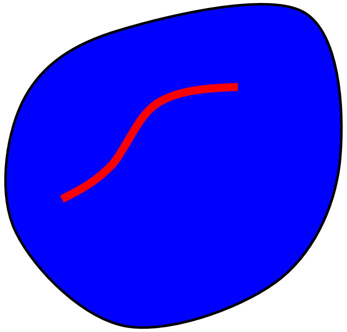
Image: Weissmann, Univ. Erlangen-Nurnberg

Purpose of peridynamics*

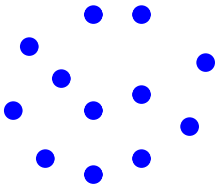
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body with a defect



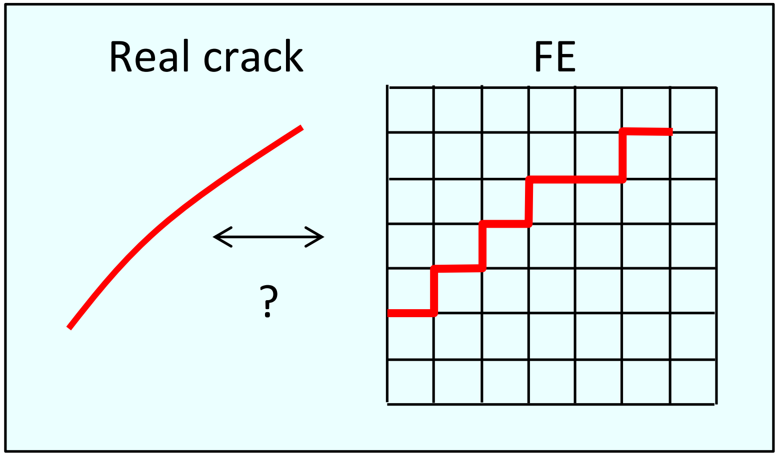
Discrete particles

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

* Peri (near) + dyn (force)

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 after numerical discretization.
  - Need supplemental kinetic relations that are understood only in idealized cases.



Complex crack path in a composite

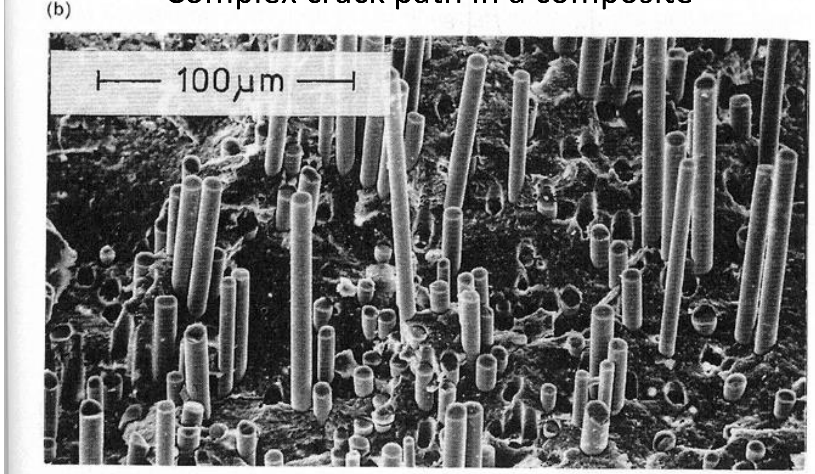
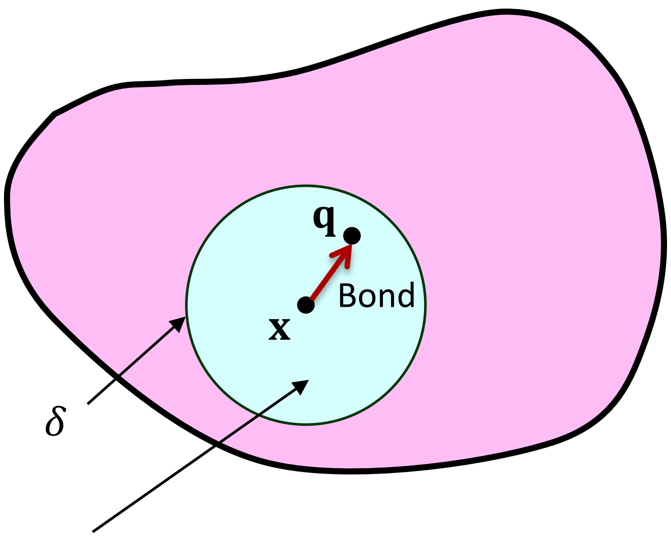


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of ‘Silceram’ glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

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



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

Equilibrium equation

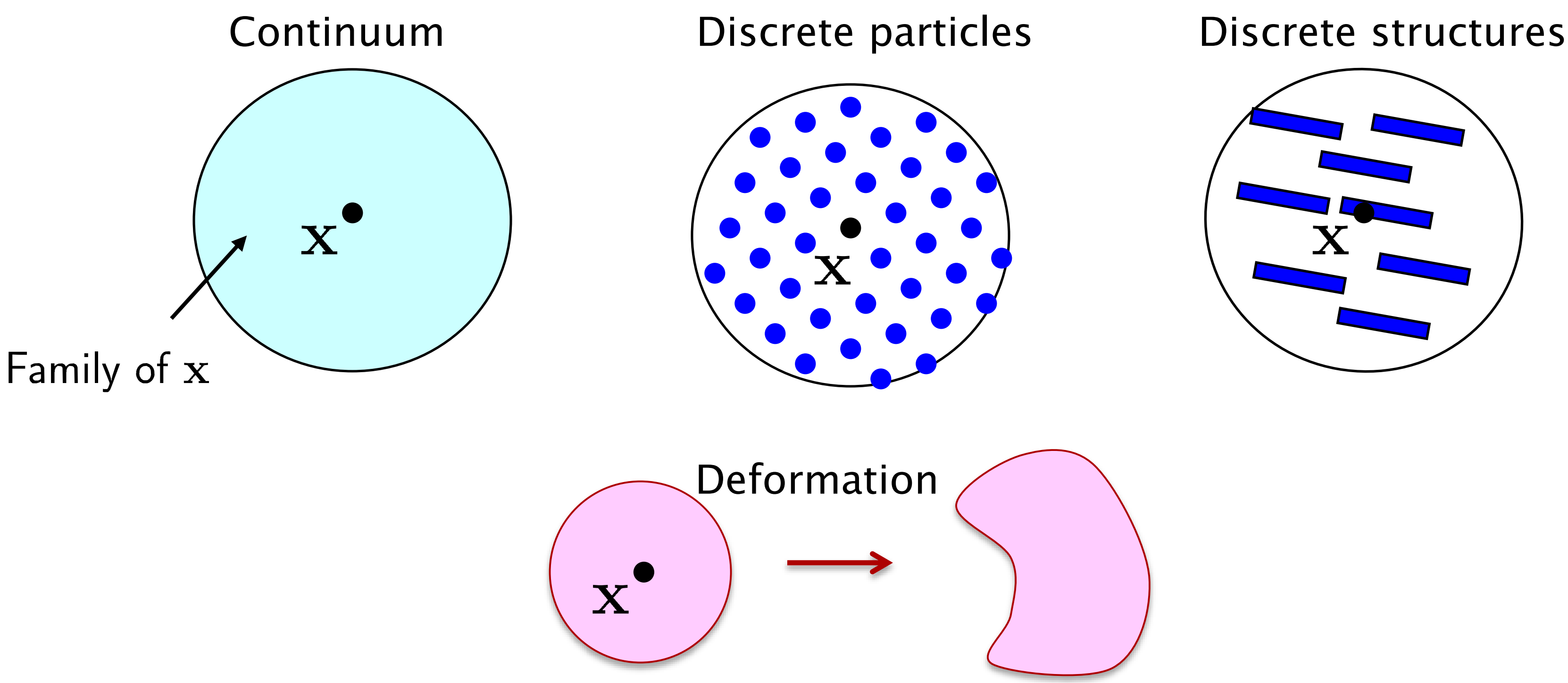
$$\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q}, \mathbf{x})\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}) = 0$$

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)

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.

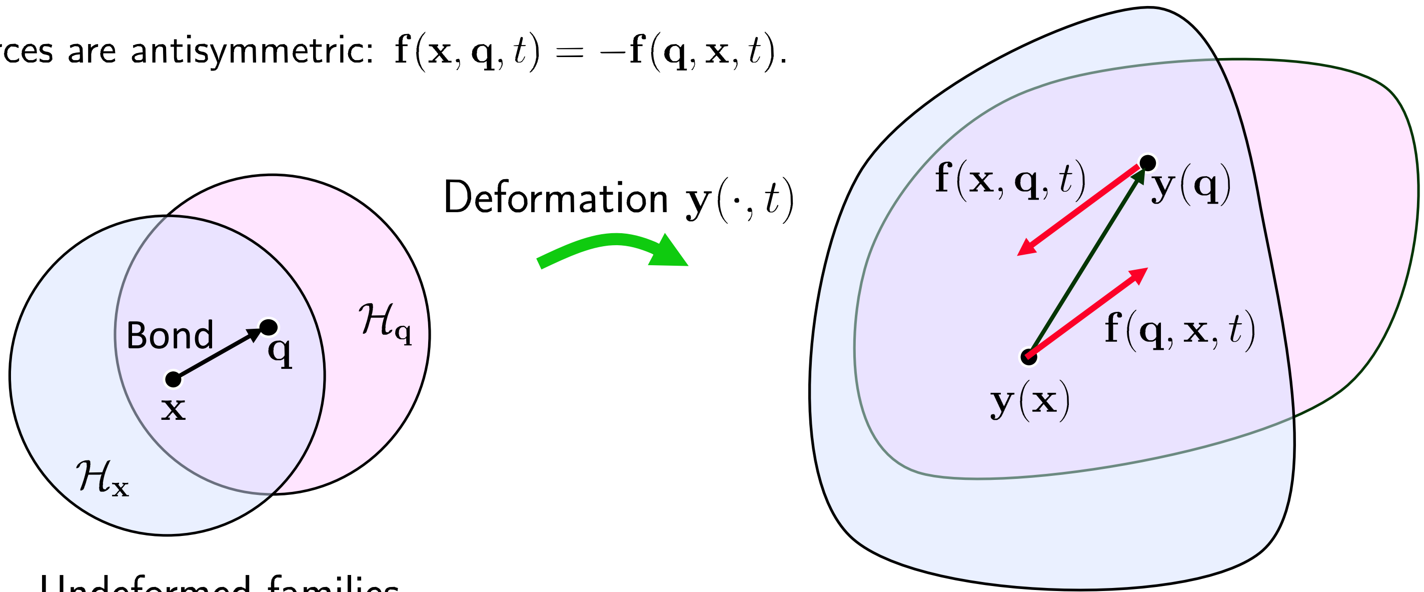
- Euler-Lagrange equation is the equilibrium equation:

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

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.
  - 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	$\dot{\varepsilon}=\underline{\mathbf{T}}\bullet\dot{\underline{\mathbf{Y}}}+q+r$	$\dot{\varepsilon}=\boldsymbol{\sigma}\cdot\dot{\mathbf{F}}+q+r$

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

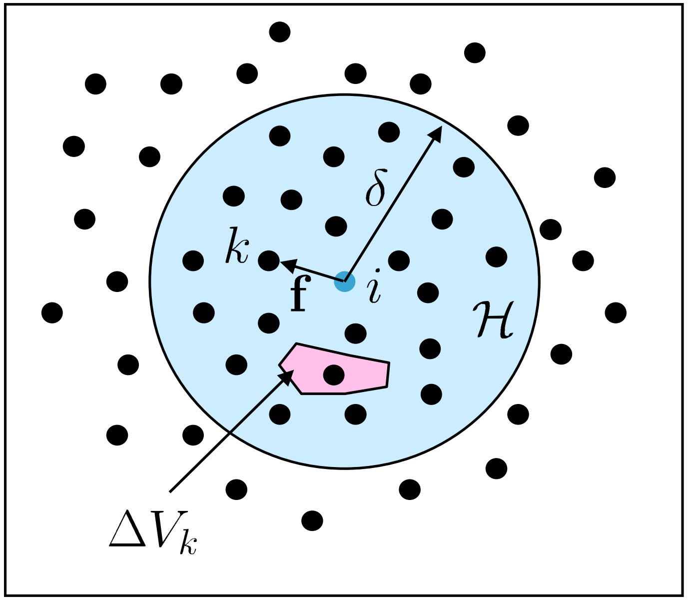
EMU numerical method

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

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

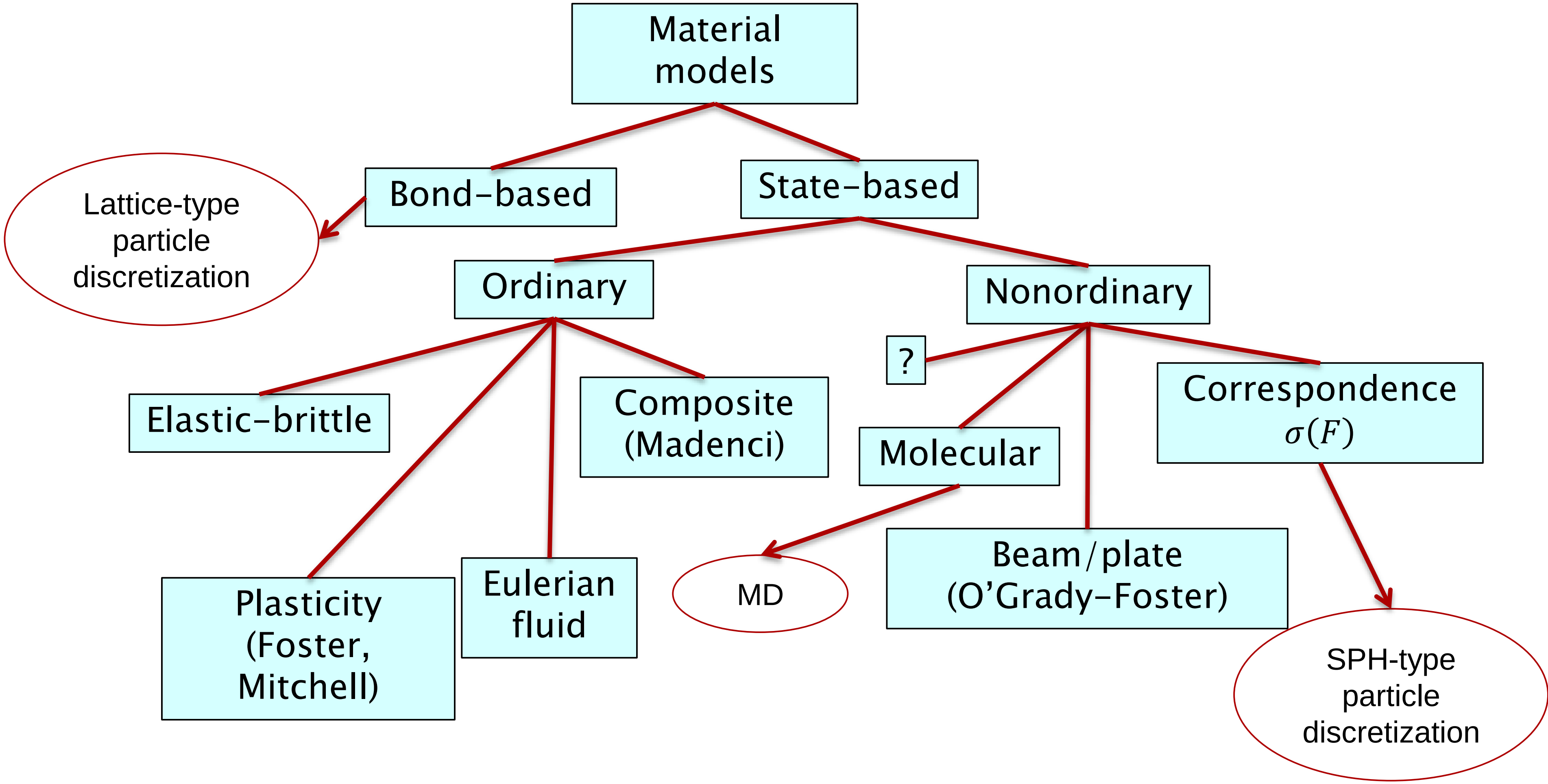
- Linearized model:

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



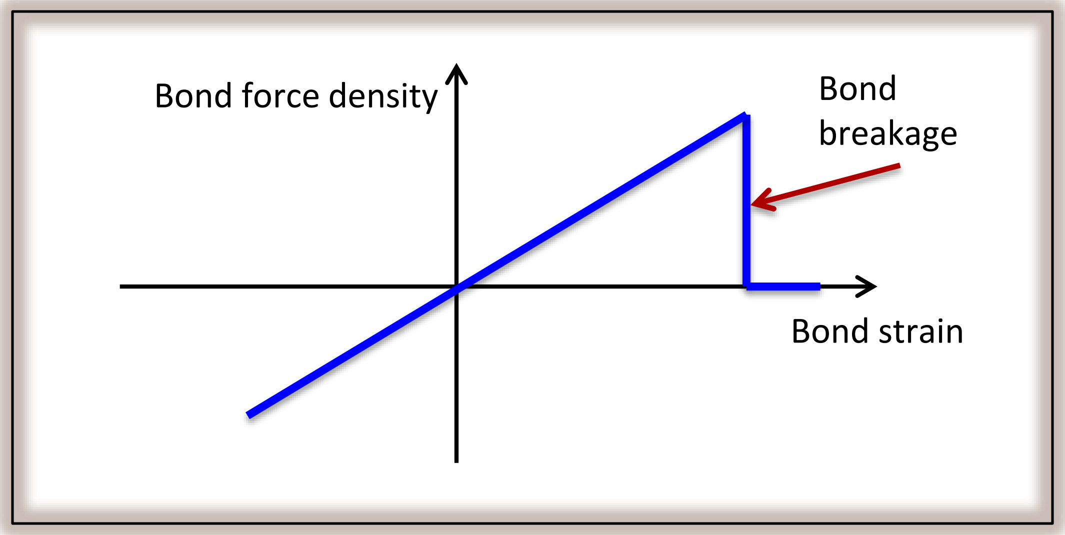
Types of material models

- A material model determines the bond forces in the family according to the deformation of the family.

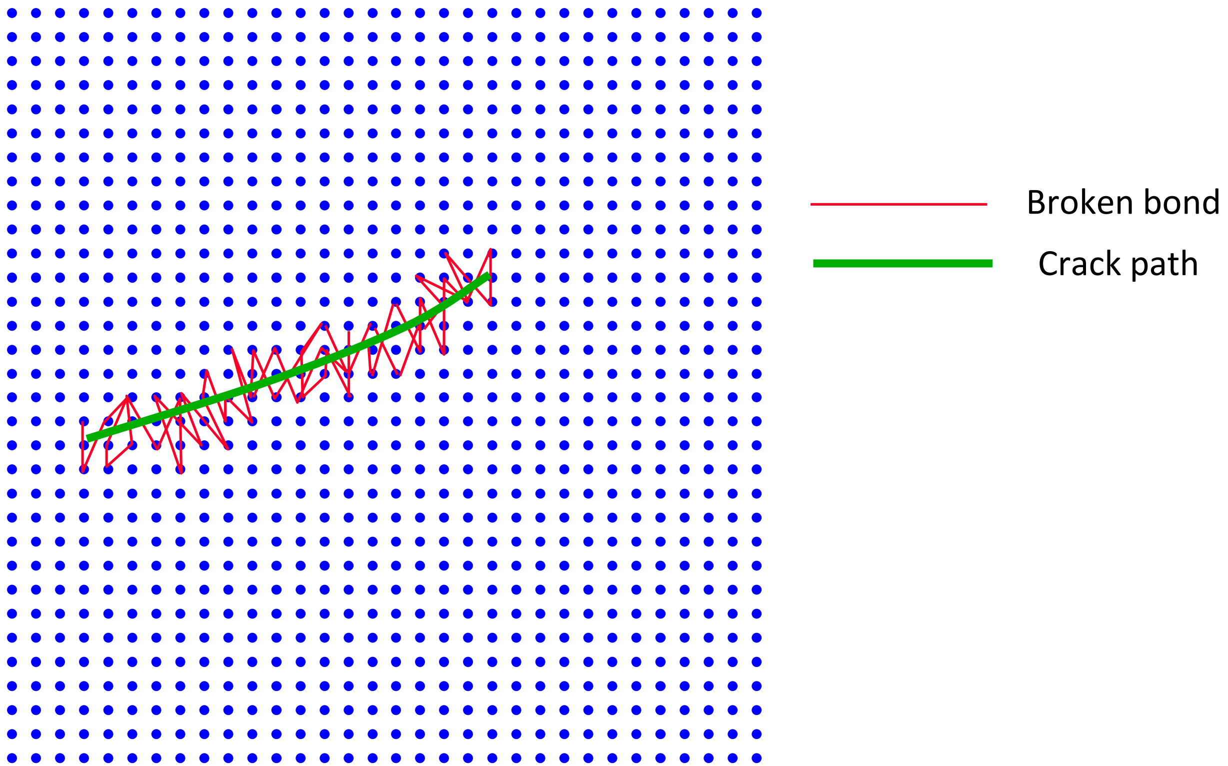


Bond based material models

- 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.

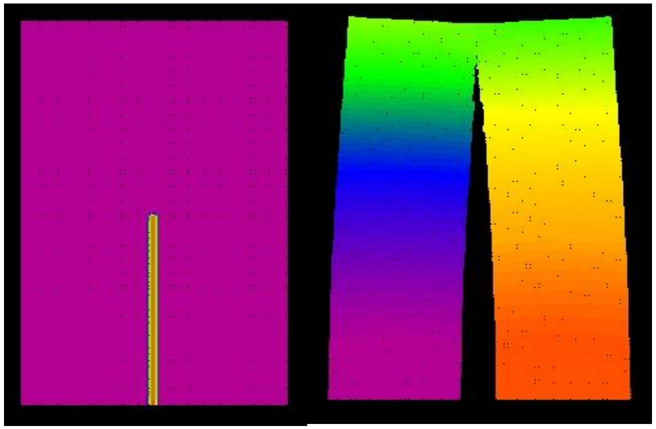


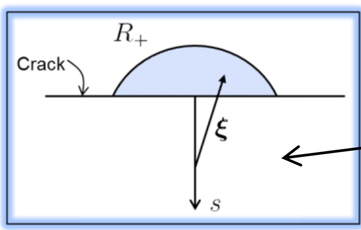
Autonomous crack growth



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

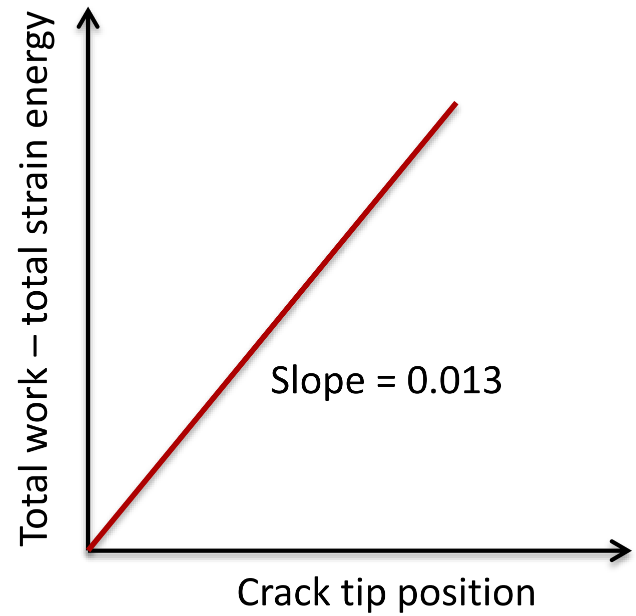
Constant bond failure strain reproduces the Griffith crack growth criterion





From bond properties, energy release rate should be

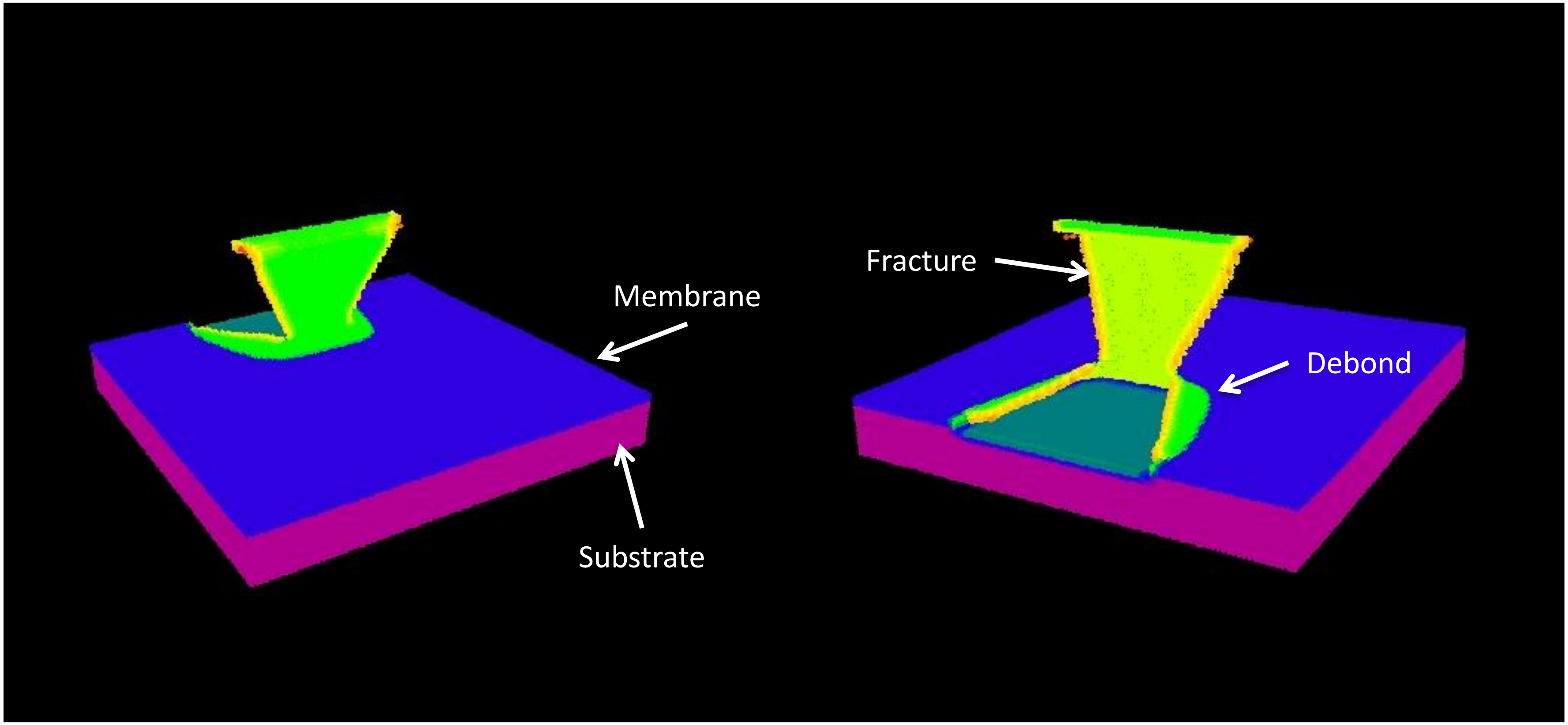
G = 0.013



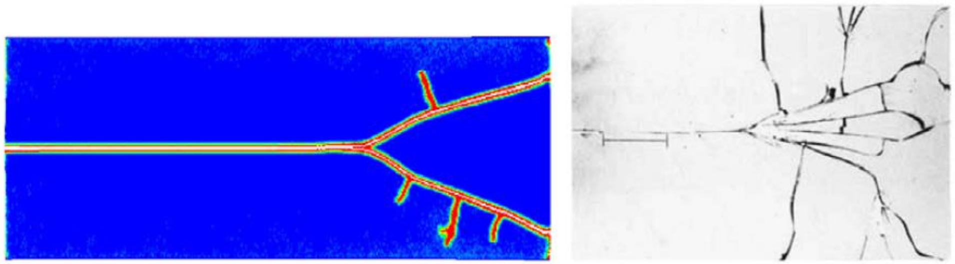
- This confirms that the energy consumed per unit crack growth area equals the expected value from bond breakage properties.

Fracture and debonding of membranes

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

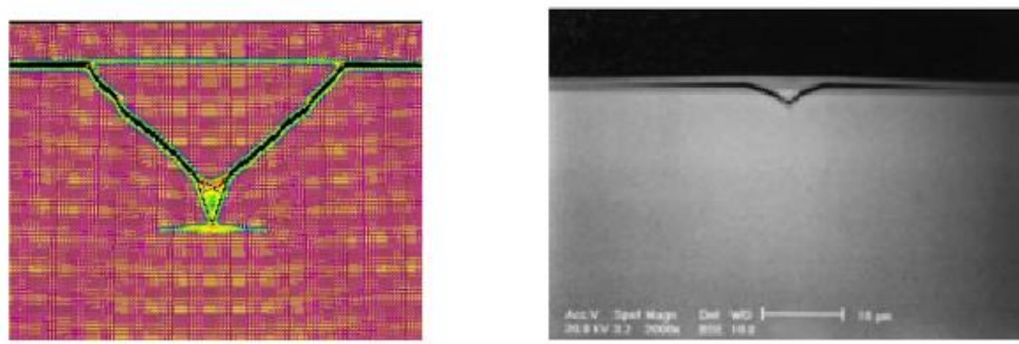


2D studies of brittle fracture with peridynamics: examples



(a) (b)

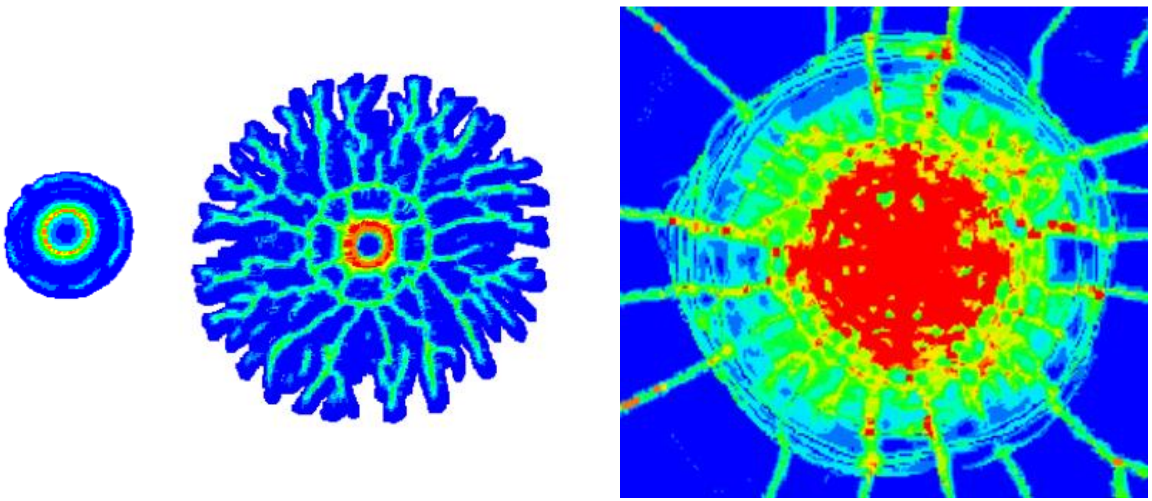
Crack branching in a glass plate with effect of reflected waves:
Ha & Bobaru, Engin Fract Mech (2011)



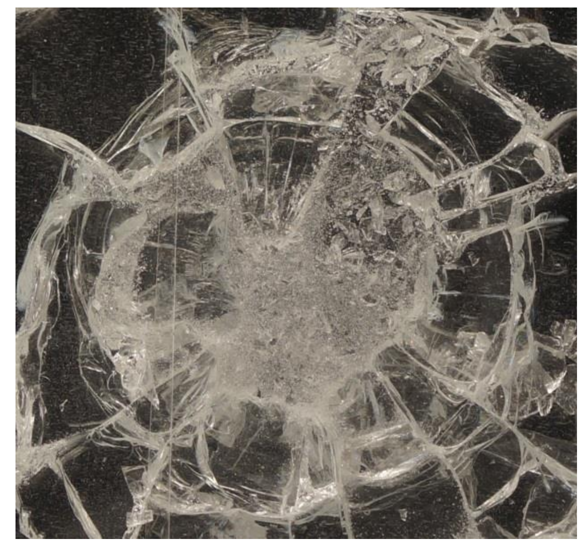
Delamination in SiO_2/Si_xN_y electronic components:
Agwai, Guven, & Madenci, IEEE (2008)

3D peridynamic model of impact on glass

- Steel sphere strikes a glass plate.
- The model predicts the evolution of some important features.



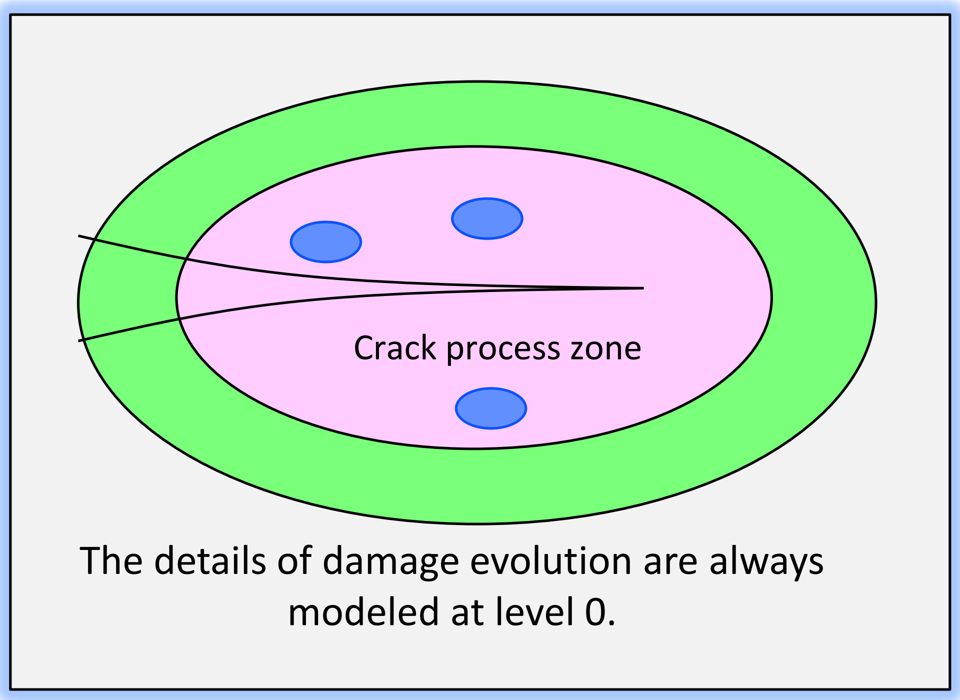
Transition from Hertz cone to fragmentation



Photograph from impact side

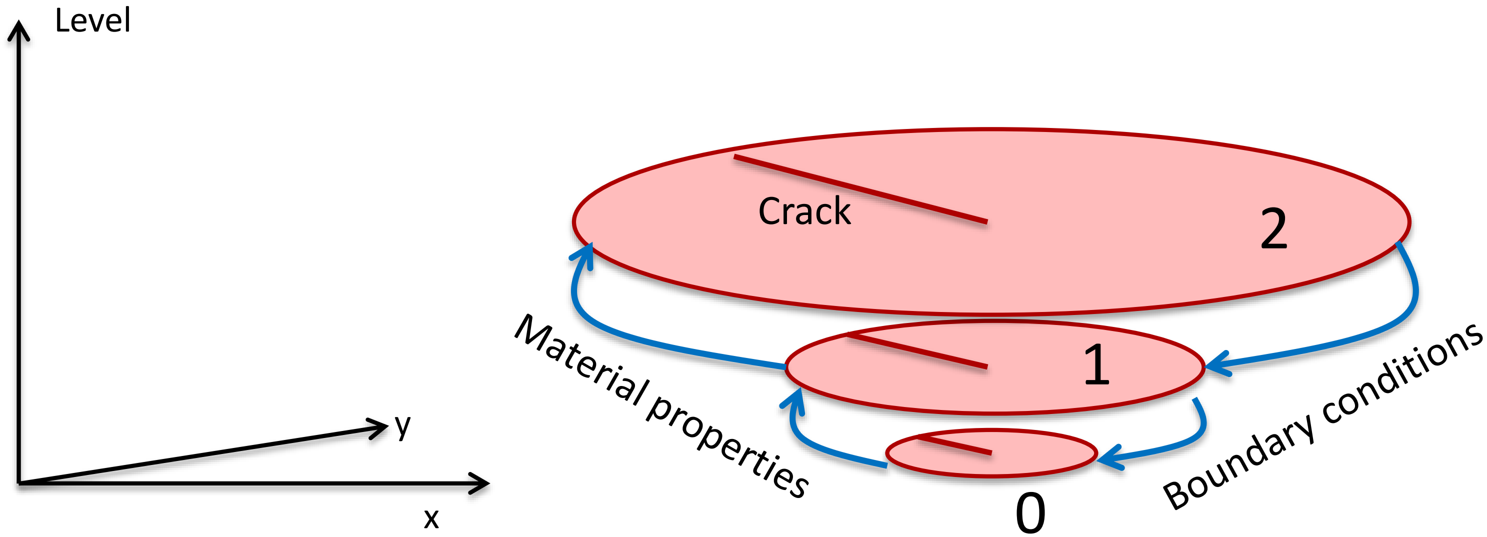
Concurrent multiscale method for defects

- 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

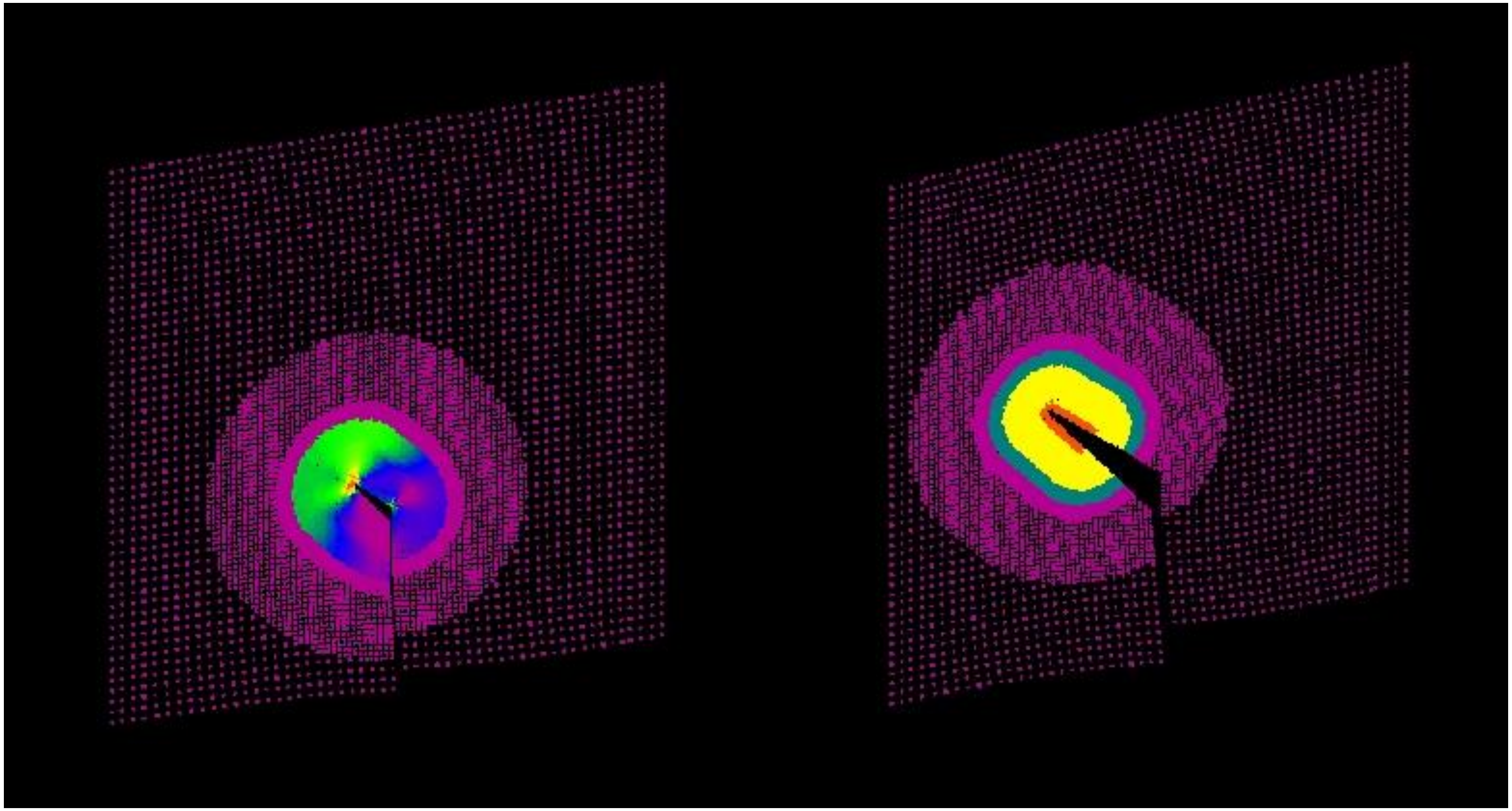
- The equation of motion is applied only within each level.
- Higher levels provide boundary conditions on lower levels.
- Lower levels provide coarsened material properties (including damage) to higher levels.
- In principle, a large number of levels can be used, all coupled in the same way: “scalable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

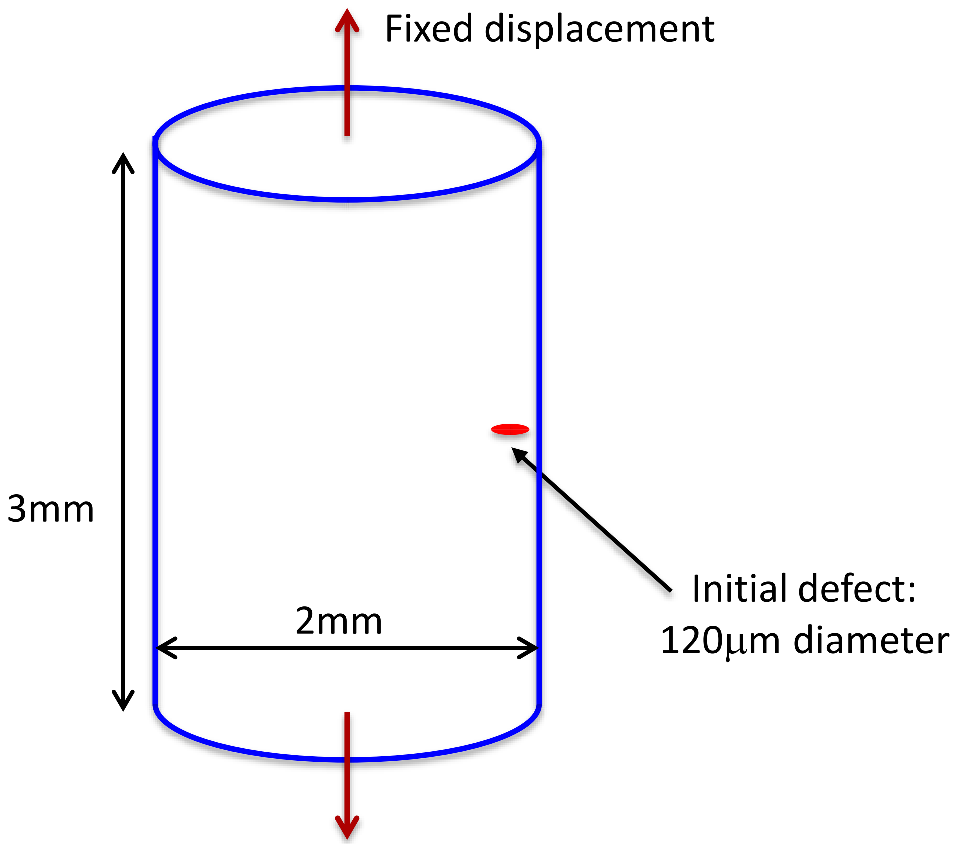


Bond strain

Damage process zone

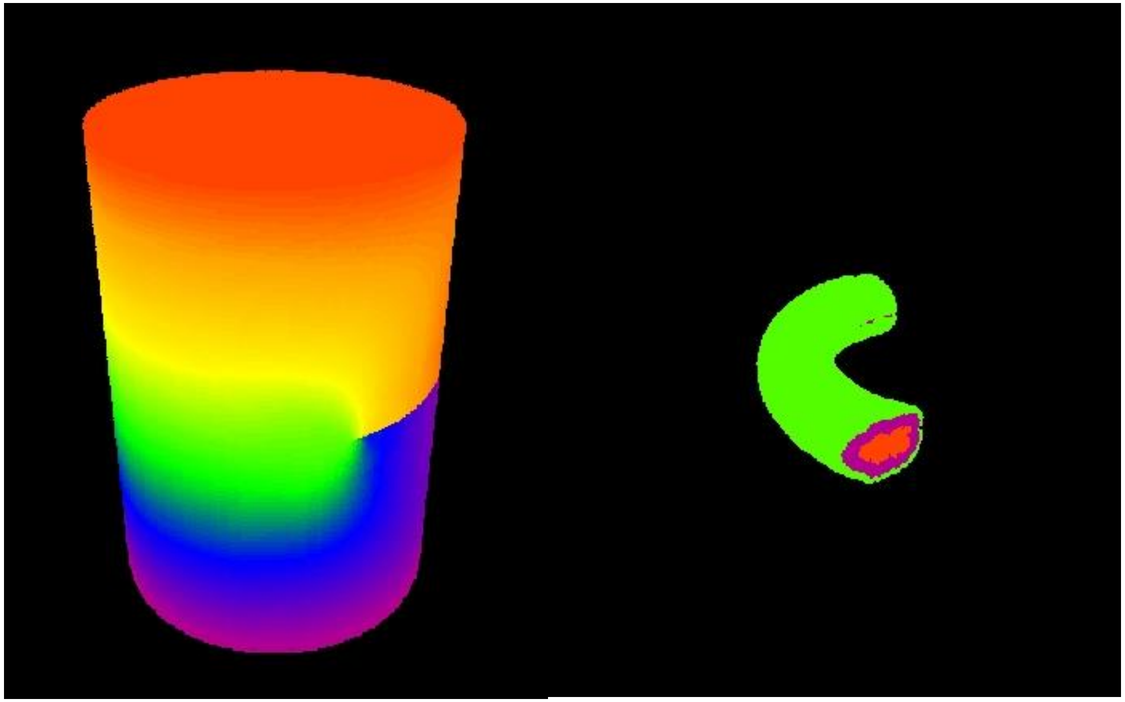
Failure of a glass rod in tension

- 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

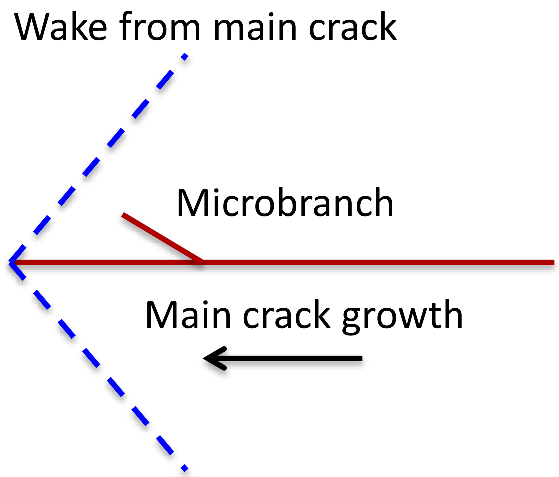


Level 1 displacement   Level 0 surrounds the crack front

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

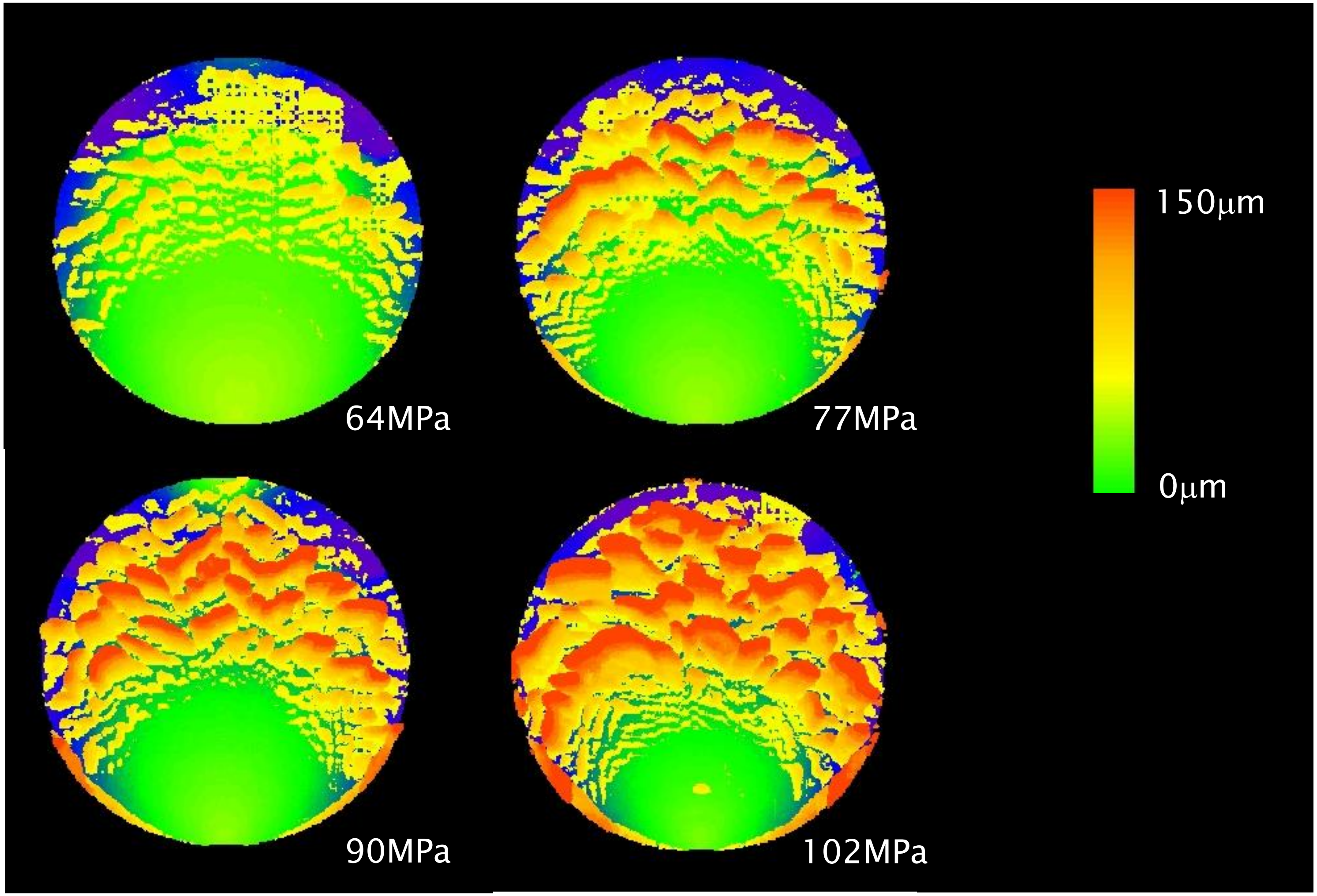
Failure of a glass rod in tension (movie)

Evolution of surface roughness (movie)



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

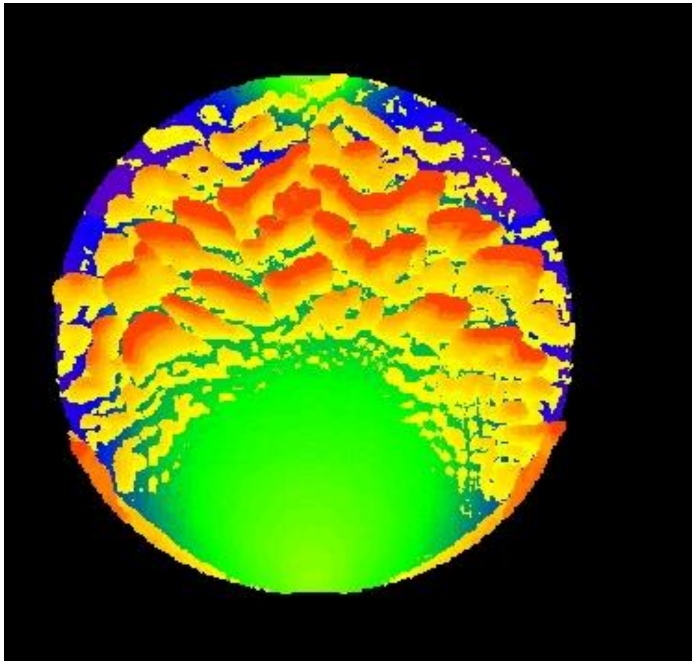
Crack surface for four values of initial stress: mirror-mist-hackle



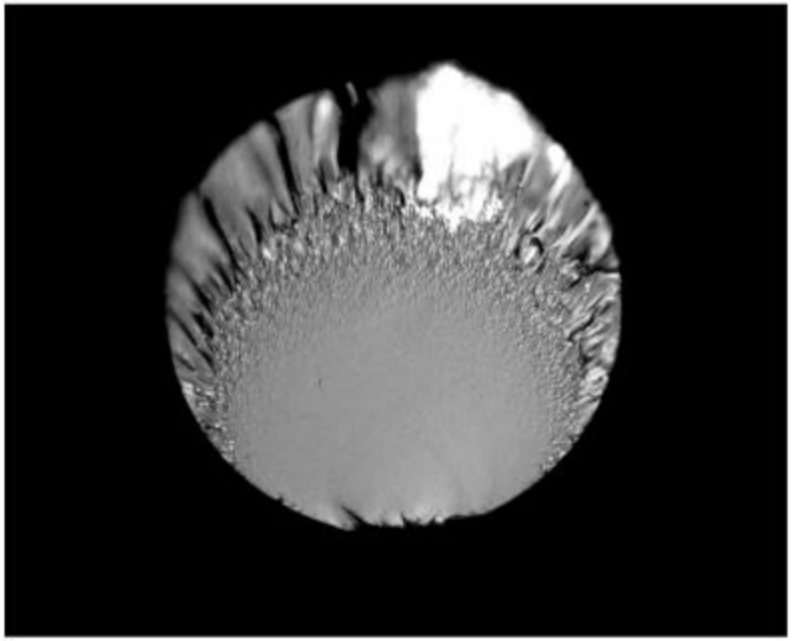
Colors show elevation of the fracture surface above the initial defect position.

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.

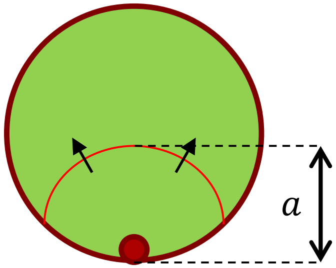


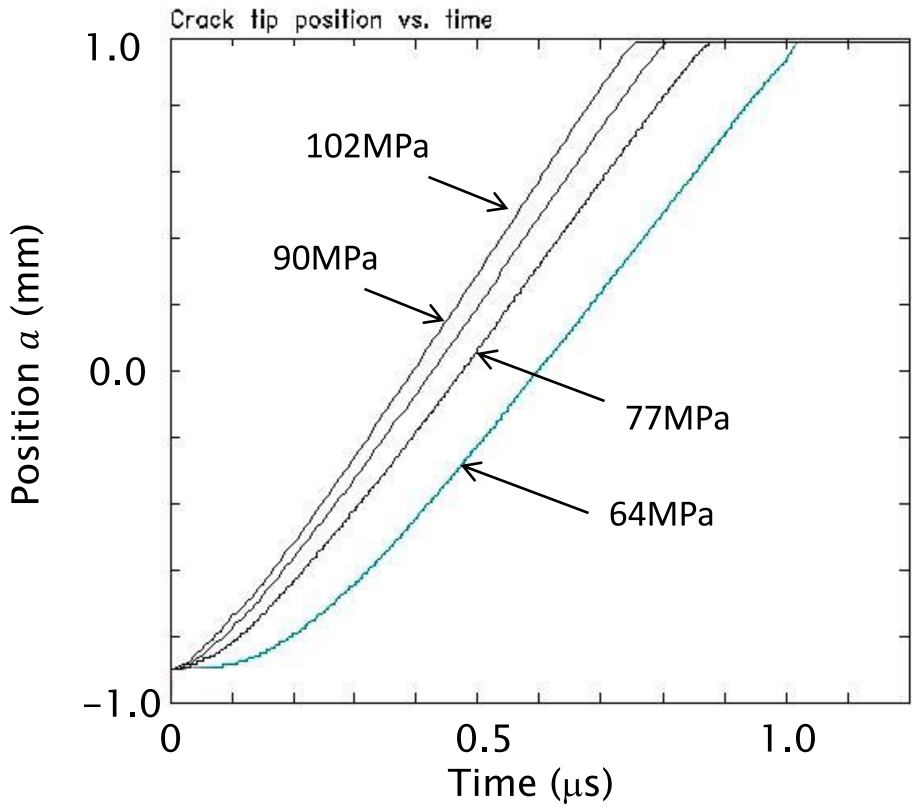
3D peridynamic model



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

Crack front position vs. time



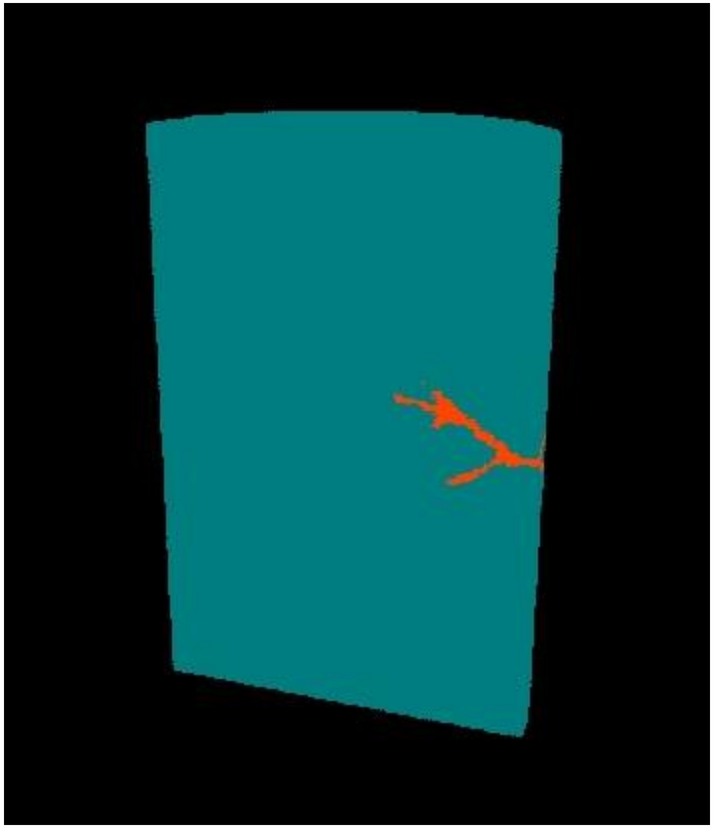


- The crack speeds up to a limiting velocity that depends on the stress.
- Higher stress leads to higher crack speed.
- 64MPa stress:

$$\dot{a} = 2500 \text{ m/s} \approx 0.81\ c_s$$

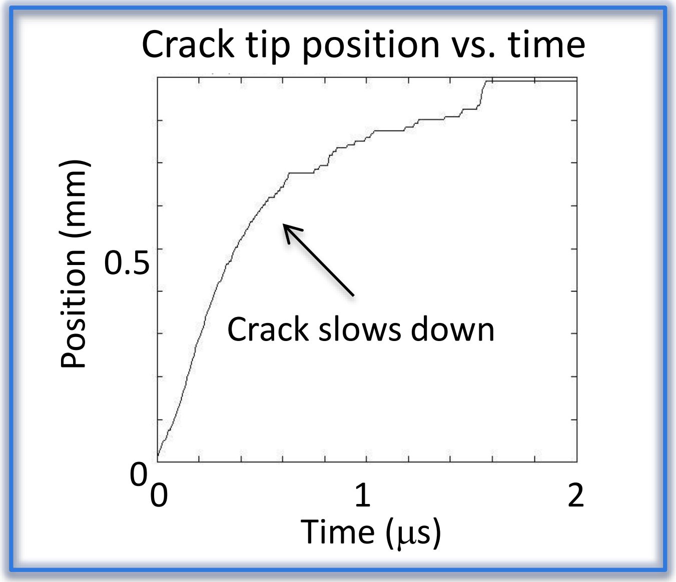
Higher stress causes branching

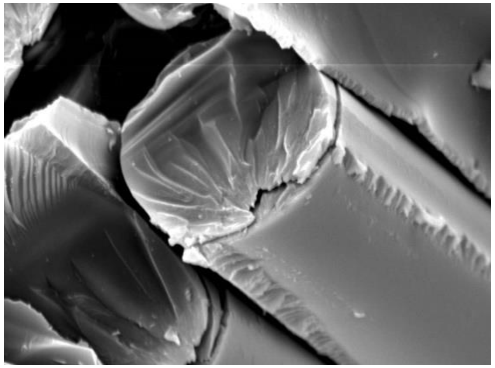
- 115 MPa



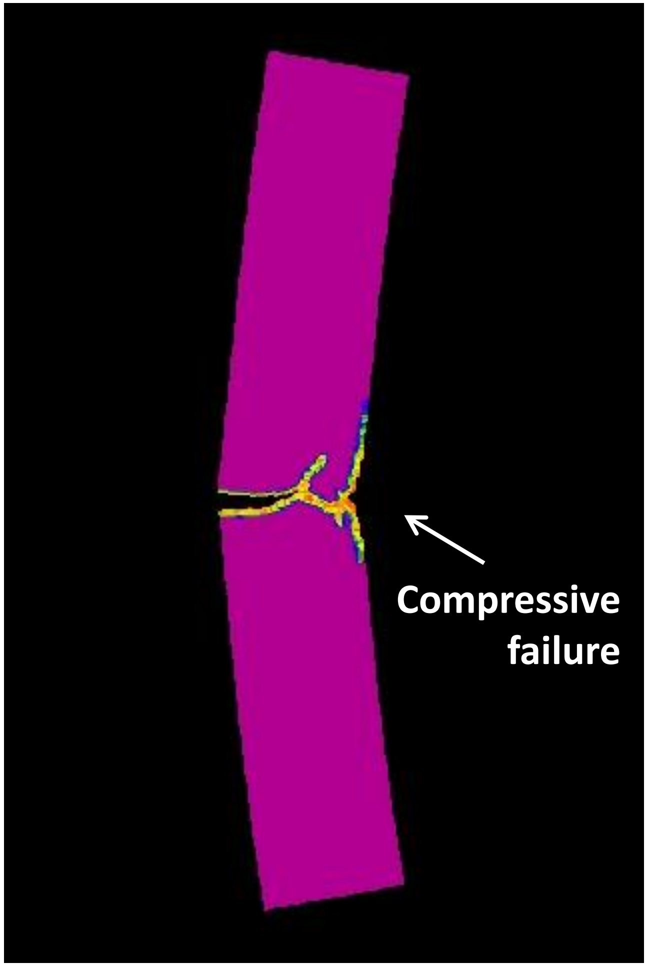
Failure in bending

- Method reproduces the curvature in crack path that is observed as a crack enters the compressive part of the stress field.





Fiber fractured by bending (Image: J. Summerscales, http://www.tech.plym.ac.uk/sme/MATS324/MATS324 A4%20fracture.htm)



Two defects:
Gull wing fractographic pattern

- Glass rod in tension
- 120μm diameter critical defect
- An additional 80μm defect is elevated 33μm out of the plane of the first.
- Crack from the first initializes the second
- Perturbed crack surface shows "gull wing" pattern (similar to Wallner lines)

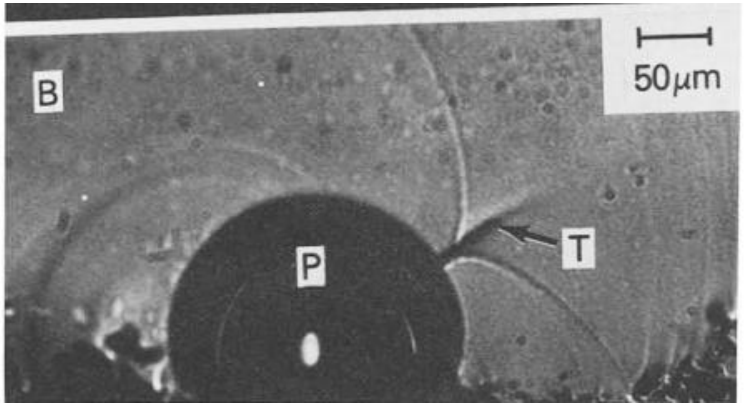
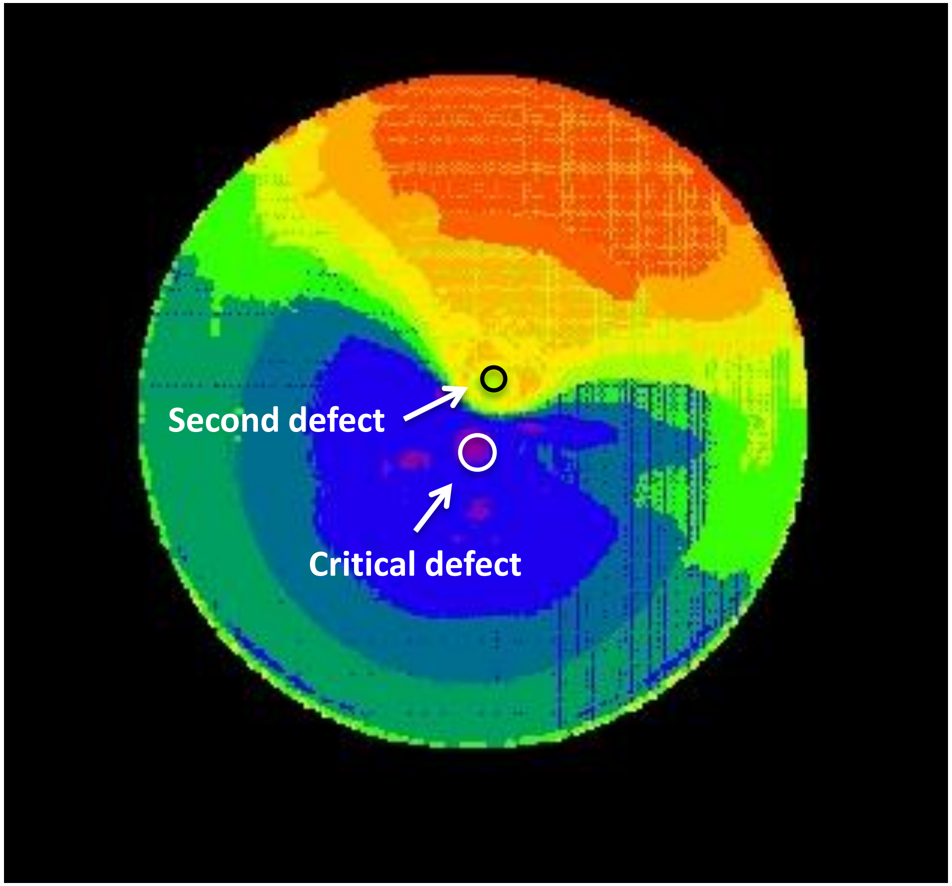


Image: R. W. Rice, in Fractography of ceramic and metal failures, Vol 827 (1984)



Peridynamic model result for the crack surface
Colors show elevation (axial coordinate)

Composite fracture features

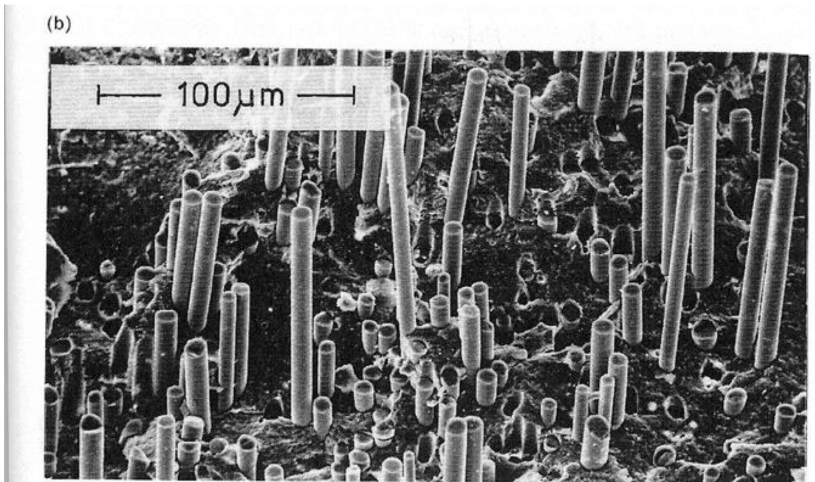
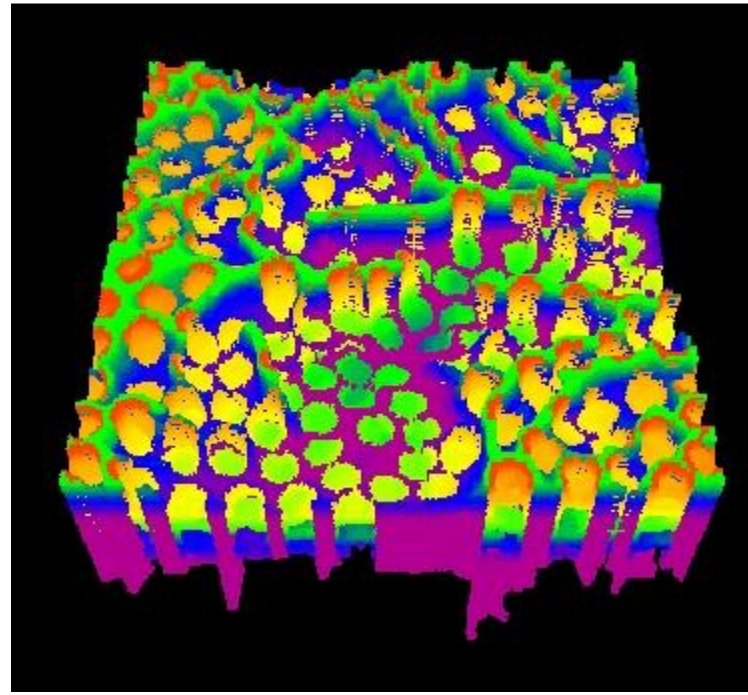


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of 'Silceram' glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

Complex crack path in a composite

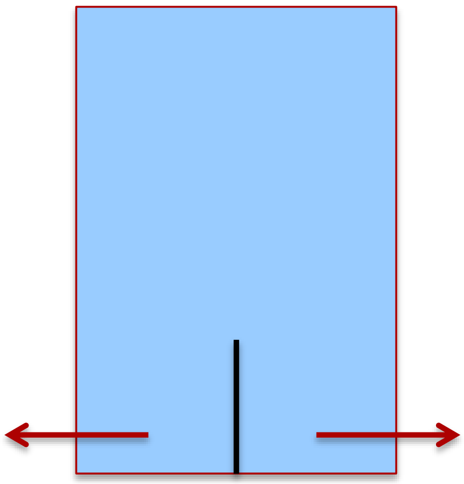


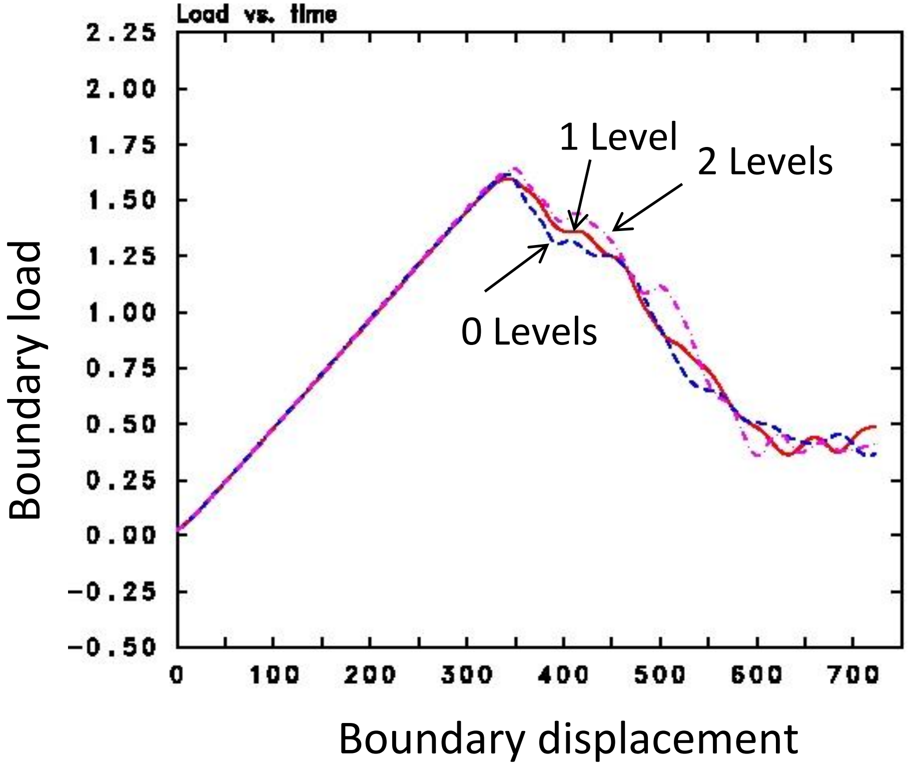
Summary

- Peridynamics is a continuum theory that is compatible with discontinuities.
  - Dynamic fracture is predicted without additional relations.
- Multiscale method adaptively reduces the length scale near a crack front.
- Method appears to reproduce fractographic features such as:
  - Branching, microbranching.
  - Mirror-mist-hackle.
  - Crack curvature under bending loads.
  - Gull wing features near multiple defects.

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