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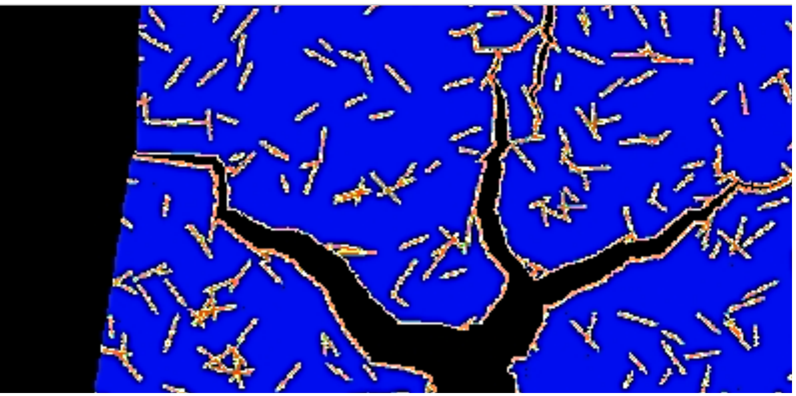
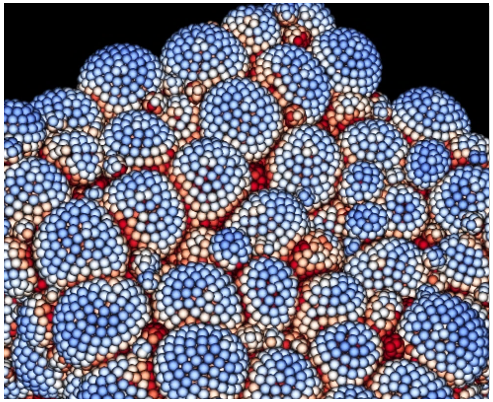
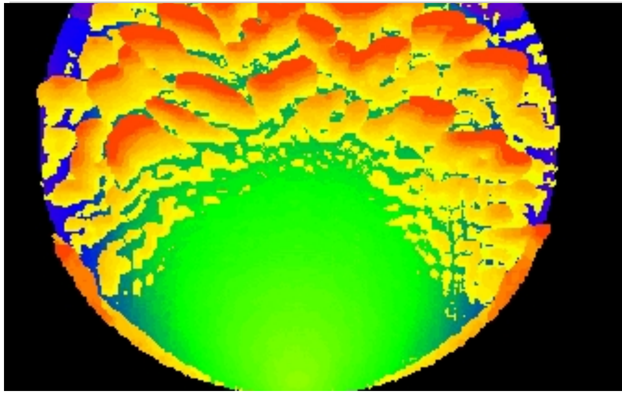

Modeling microstructure and defects with peridynamics

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Sandia National Laboratories
Albuquerque, New Mexico

SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, July 11, 2018

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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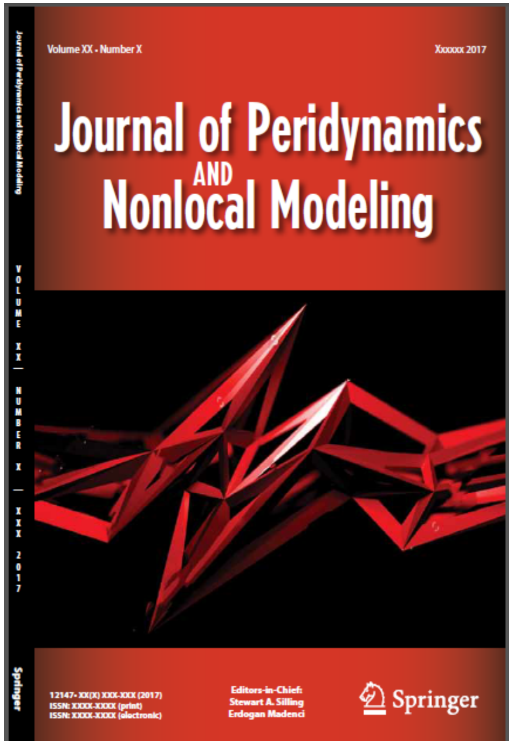
Outline

- Peridynamic theory summary
- Defects and material failure
- Phase changes and microstructure

New journal from Springer Nature
First issue Jan 2019



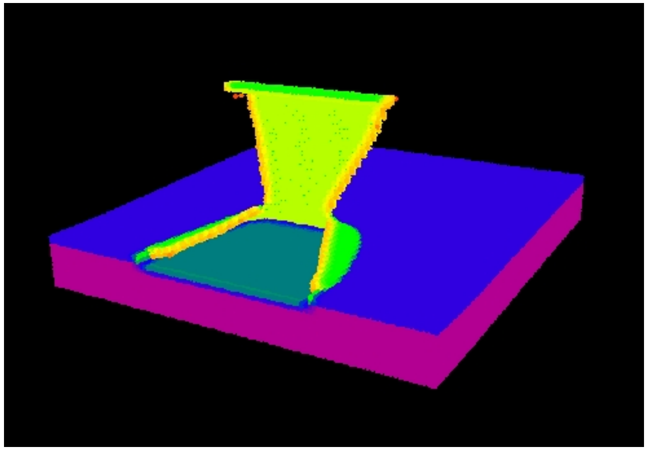
Gaps in classical continuum mechanics

- Momentum balance, 1D:

$$\rho u_{tt} = (\sigma(u_x))_x + b$$

where u=displacement, σ=stress, b=external body force.

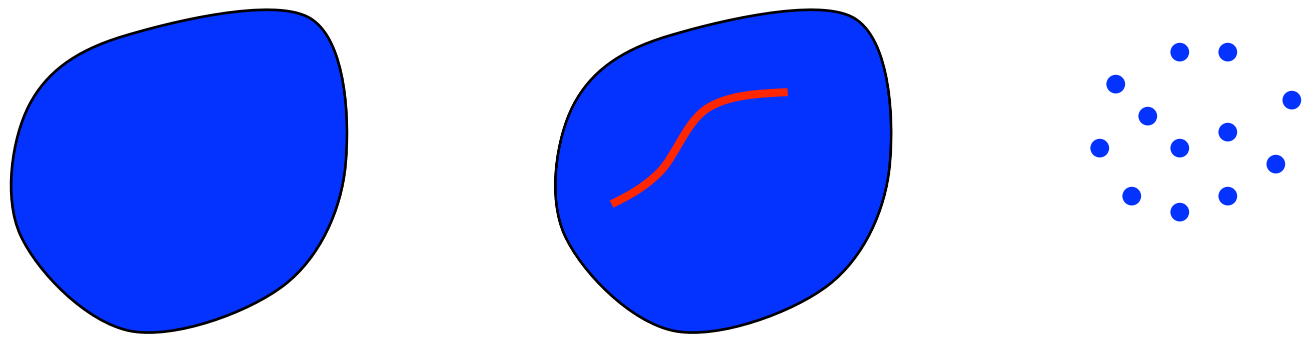
- Requires u to be twice continuously differentiable.
- Doesn't apply on cracks or growing discontinuities.
- Predicts infinite stress near defects.
- Can't include nanoscale forces.



Humble Scotch® tape

Peridynamics:* What it is

- It's an extension of continuum mechanics to media with cracks and long-range forces.
- It unifies the mechanics of continuous and discontinuous media within a single, consistent set of equations.



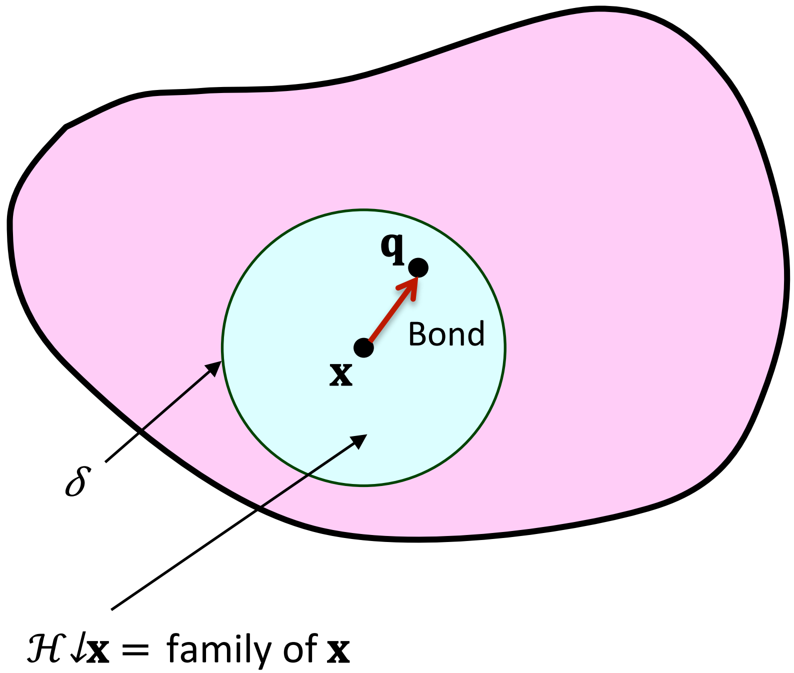
Continuous body | Continuous body with a defect | Discrete particles

- Our goals
  - Nucleate cracks and seamlessly transition to growth.
  - Model complex fracture patterns.
  - Communicate across length scales.

* Peri (near) + dyn (force)

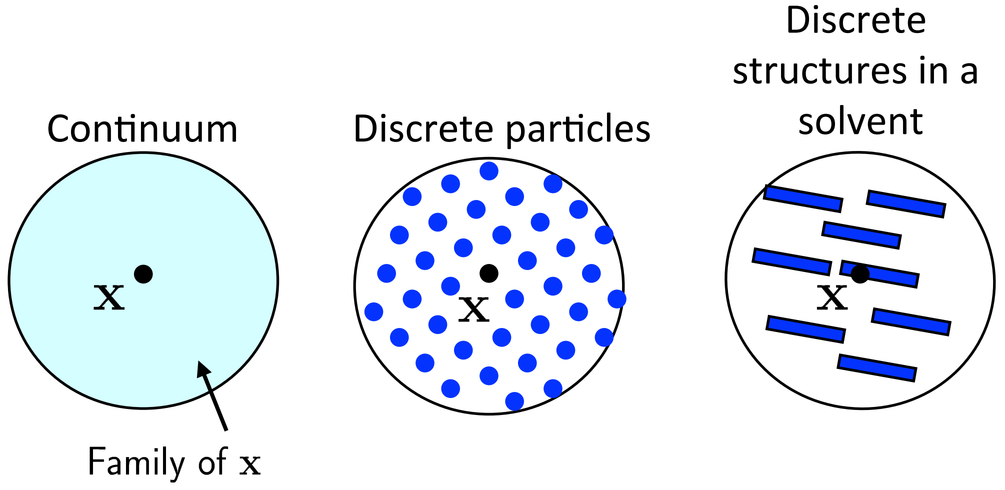
Peridynamics concepts: Horizon and family

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

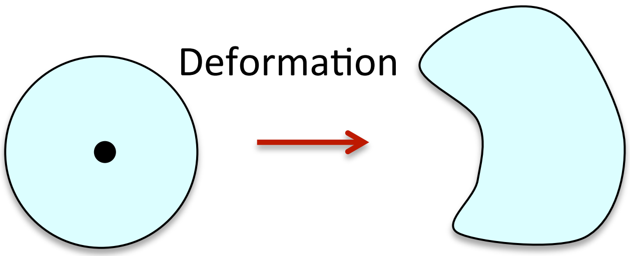


- SS, *J. Mechanics and Physics of Solids* (2000)
- SS & Lehoucq, *Advances in Applied Mechanics* (2010)

Peridynamic concept of strain energy density at a point

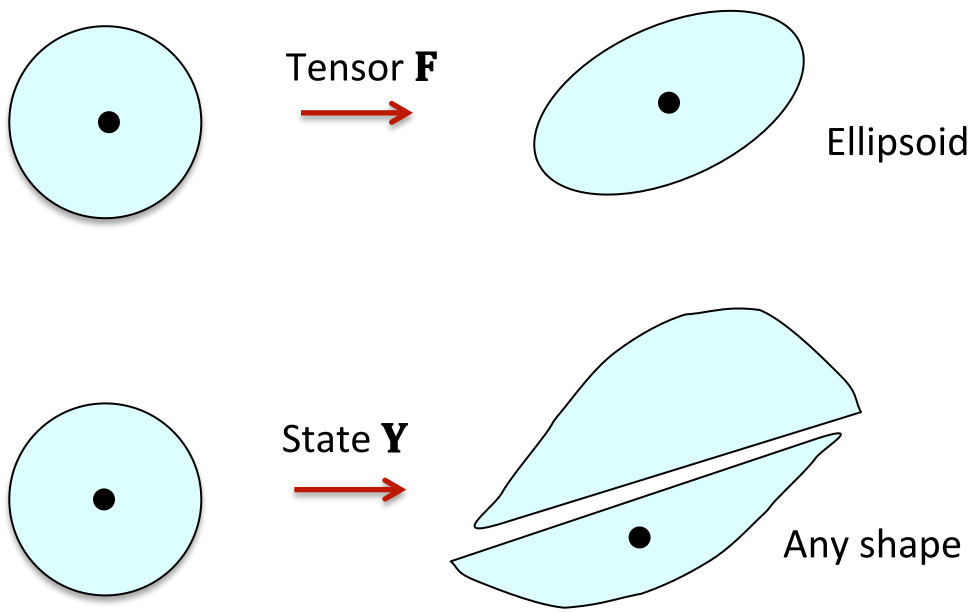


- The strain energy density $W(\mathbf{x})$ is determined by the deformation of the entire family of $\mathbf{x}$.
- How to describe this dependence? **States**



States: Nonlinear analogues of second order tensors

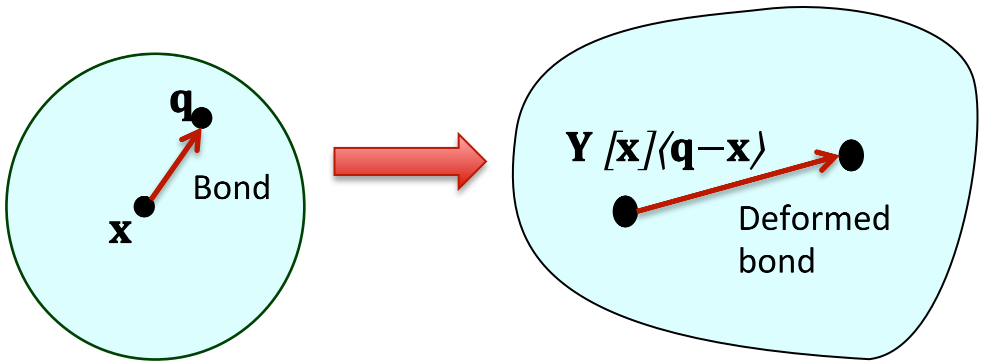
- Classical theory uses tensors (linear mappings from vectors to vectors).
- Peridynamics uses states (nonlinear mappings from vectors to vectors).



States

- A *state* is a mapping whose domain is all the bonds ξ in a family.

$$\underline{\mathbf{A}}\langle\xi\rangle = \text{something} \qquad \forall\xi \in \mathcal{H}.$$



- Deformation state...

$$\underline{\mathbf{Y}}[\mathrm{x}]\langle\mathbf{q} - \mathbf{x}\rangle = \mathbf{y}(\mathbf{q}) - \mathbf{y}(\mathbf{x}) = \text{deformed image of the bond}$$

Strain energy density: $W(\mathbf{Y})$

Operations with states

- Two operators on states are defined by

$$\underline{\mathbf{A}} \bullet \underline{\mathbf{B}} = \int_{\mathcal{H}} \underline{\mathbf{A}}\langle \xi \rangle \cdot \underline{\mathbf{B}}\langle \xi \rangle \, dV_{\boldsymbol{\xi}} \qquad \text{...dot product (a scalar)}$$

$$\underline{\mathbf{A}} \star \underline{\mathbf{B}} = \int_{\mathcal{H}} \underline{\mathbf{A}}\langle \xi \rangle \otimes \underline{\mathbf{B}}\langle \xi \rangle \, dV_{\boldsymbol{\xi}} \qquad \text{...tensor product (a 2nd order tensor)}$$

- Two more useful states...

$$\underline{\mathbf{1}}\langle \xi \rangle = 1 \qquad \forall \xi \in \mathcal{H} \qquad \text{...unity state,}$$

$$\underline{\mathbf{X}}\langle \xi \rangle = \xi \qquad \forall \xi \in \mathcal{H} \qquad \text{...identity state.}$$

Functions of states

- Let $\Psi(\underline{\mathbf{A}})$ be a scalar-valued function of a state.
- Suppose there is a state $\Psi_{\underline{\mathbf{A}}}(\underline{\mathbf{A}})$ such that for any small increment $d\underline{\mathbf{A}}$,

$$\Psi(\underline{\mathbf{A}} + d\underline{\mathbf{A}}) - \Psi(\underline{\mathbf{A}}) = \Psi_{\underline{\mathbf{A}}}(\underline{\mathbf{A}}) \bullet d\underline{\mathbf{A}}.$$

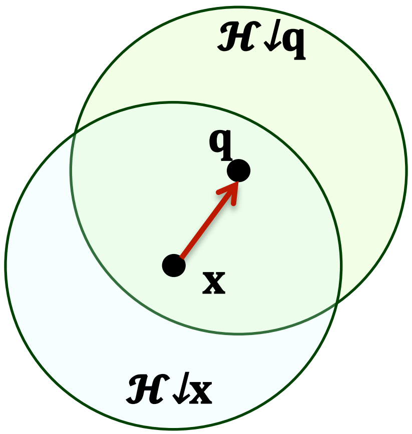
- Then $\Psi_{\underline{\mathbf{A}}}(\underline{\mathbf{A}})$ is the *Fréchet derivative* of Ψ at $\underline{\mathbf{A}}$.

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:

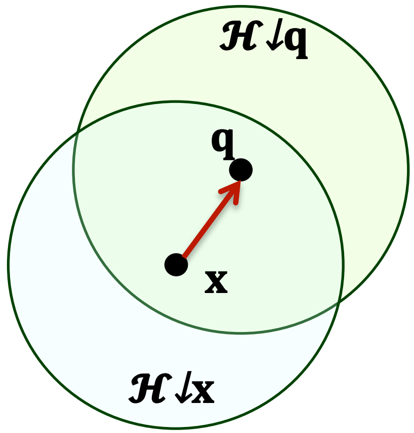
$$\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q}, \mathbf{x})\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}) = 0$$

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

- f is found from the Fréchet derivatives of W at $\mathbf{x}$ and each $\mathbf{q}$:

$$\mathbf{f}(\mathbf{q}, \mathbf{x}) = W_{\underline{\mathbf{Y}}}[\mathbf{x}]\langle \mathbf{q} - \mathbf{x} \rangle - W_{\underline{\mathbf{Y}}}[\mathbf{q}]\langle \mathbf{x} - \mathbf{q} \rangle.$$

Material models



- Recall the equilibrium equation:

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

where (from the first variation of Φ)

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

- $\underline{\mathbf{T}}[\mathbf{x}]$ is the *force state* obtained from the material model $\hat{\underline{\mathbf{T}}}$ applied to the family of $\mathbf{x}$:

$$\underline{\mathbf{T}}[\mathbf{x}] = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}[\mathbf{x}]).$$

- SS, Epton, Weckner, Xu, & Askari, *J. Elasticity* (2007)

Examples of material models

- Bond-based (each bond responds independently of the others):

$$\underline{\mathbf{T}}\langle\xi\rangle = f(s,\xi)\frac{\underline{\mathbf{Y}}\langle\xi\rangle}{|\underline{\mathbf{Y}}\langle\xi\rangle|}, \qquad s = \frac{|\underline{\mathbf{Y}}\langle\xi\rangle| - |\xi|}{|\xi|}$$

where s=bond strain.

Direction of the deformed bond $\boldsymbol{\xi}$

- Isotropic solid:

$$\underline{\mathbf{T}}\langle\xi\rangle = \alpha s + \beta\vartheta, \qquad \vartheta = \underline{\mathbf{U}} \bullet \underline{\mathbf{X}}, \qquad \underline{\mathbf{U}} = \underline{\mathbf{Y}} - \underline{\mathbf{X}}$$

where α, β are constants and ϑ is a measure of the volume change in the family, and $\underline{\mathbf{U}}$=displacement state.

- Linearized:

$$\underline{\mathbf{T}} = \underline{\mathbb{K}} \bullet \underline{\mathbf{U}}, \qquad \underline{\mathbb{K}} = W_{\underline{\mathbf{YY}}}$$

where $\underline{\mathbb{K}}$ is the micromodulus double state (second Fréchet derivative).

$$\underline{\mathbf{T}}\langle\xi\rangle = \int_{\mathcal{H}} \underline{\mathbb{K}}\langle\xi,\zeta\rangle \cdot \underline{\mathbf{U}}\langle\zeta\rangle \, dV_\zeta.$$

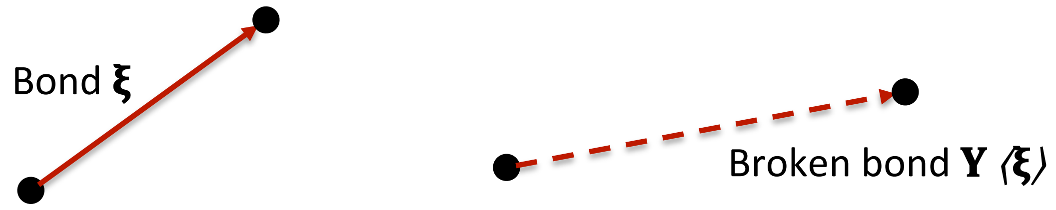
Damage

- Damage is usually treated through *bond breakage*.
- After a bond ξ *breaks* according to some criterion, it no longer carries any force.
- Typical breakage criterion: prescribed *critical bond strain* s_0:

$$s = \frac{|\underline{\mathbf{Y}}\langle\xi\rangle| - |\xi|}{|\xi|} \qquad \text{bond strain.}$$

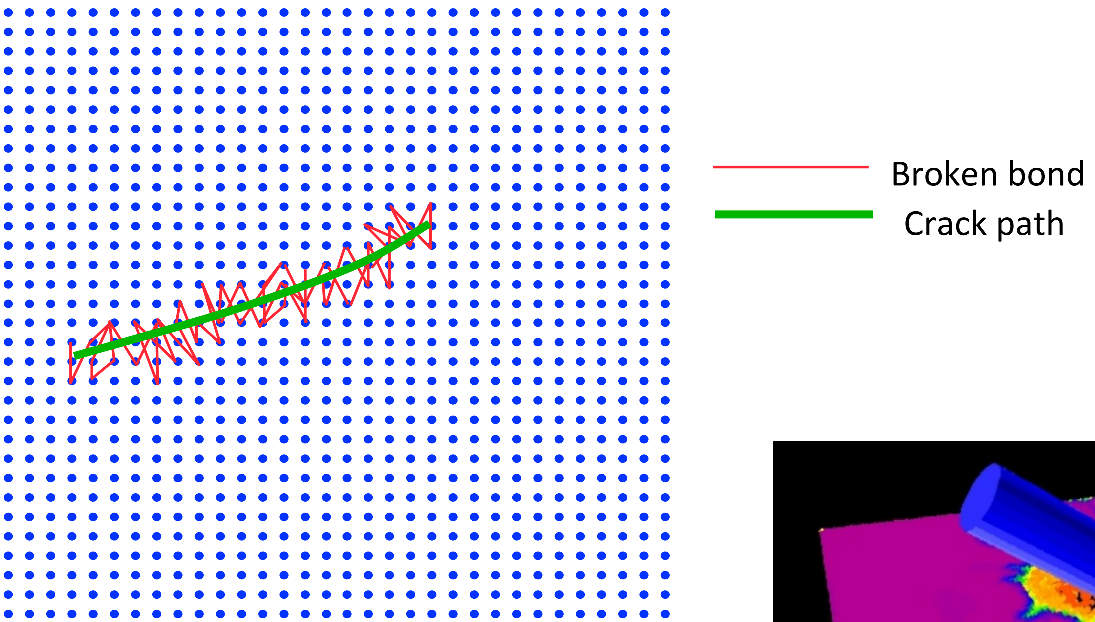
$$s >= s_0 \text{ at some time } t_0$$

means the bond remains broken for all $t \geq t_0$.

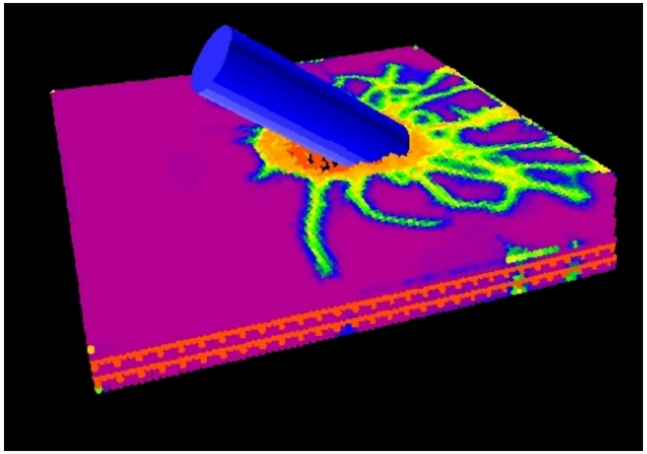


Discontinuities are treated within the basic field equations

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



Cracking in a composite lamina



Impact against reinforced concrete

Emu numerical method

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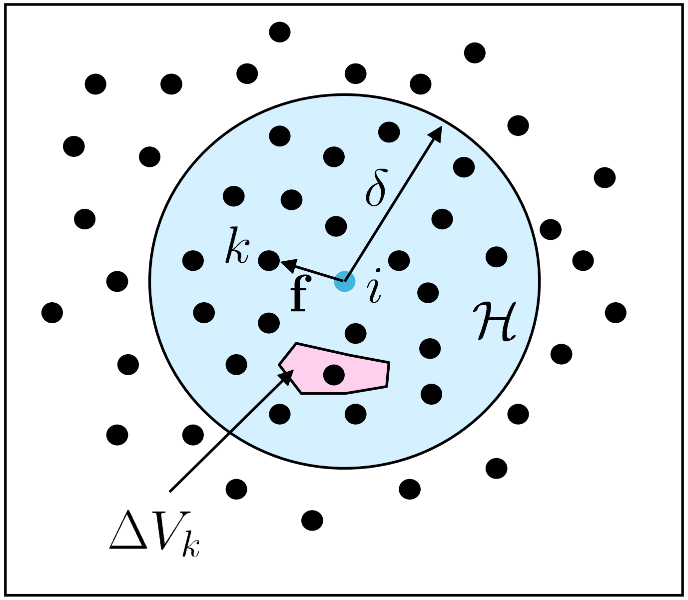
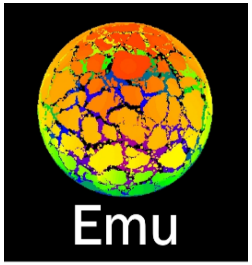
- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

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





- SS & Askari, *Computers & Structures* (2005)
- *Tian & Du, SIAM Journal on Numerical Analysis* (2014)

Force states and stress

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- For a homogeneous deformation of a homogeneous body,

$$\boldsymbol{\sigma} = \underline{\mathbf{T}} \star \underline{\mathbf{X}} \qquad \text{or} \qquad \boldsymbol{\sigma} = \int_{\mathcal{H}} \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \otimes \boldsymbol{\xi} \, dV_{\boldsymbol{\xi}}.$$

- This $\boldsymbol{\sigma}$ is called the *partial stress*.
- It has the usual mechanical interpretation (force/area).
- For non-homogeneous deformations, in general for this $\boldsymbol{\sigma}$

$$\nabla \cdot \boldsymbol{\sigma} + \mathrm{b} \neq \mathbf{0}.$$

- But there is a more general peridynamic stress tensor for which equality holds.

- Lehoucq & SS, *J. Mechanics and Physics of Solids (2008)*
- SS, Littlewood & Seleson, *J. Mechanics of Materials & Structures* (2014)

Peridynamic form of thermodynamics

- First law:

$$\dot{e} = \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + h + r$$

where e=internal energy density, h=energy transport rate, r=energy source rate.

- h is usually given by a nonlocal diffusion law such as

$$h(\mathbf{x}) = \int_{\mathcal{H}_\mathbf{x}} k(\mathbf{q}, \mathbf{x})(\theta(\mathbf{q}) - \theta(\mathbf{x}))\, dV_\mathbf{q}$$

where k is a conductivity, θ=temperature.

- Second law:

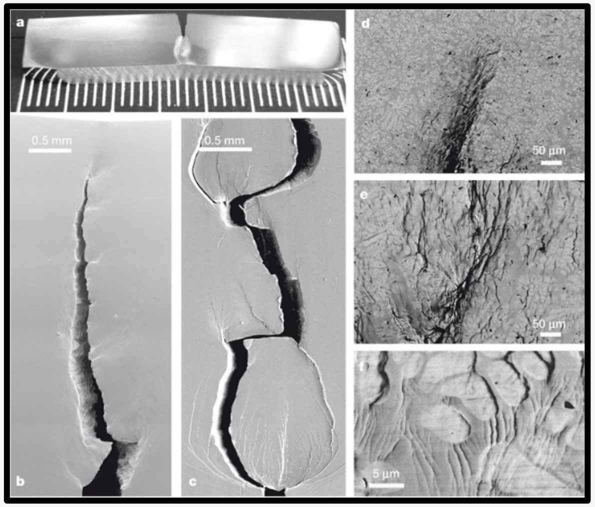
$$\theta \dot{\eta} >= h + r$$

where η=entropy density.

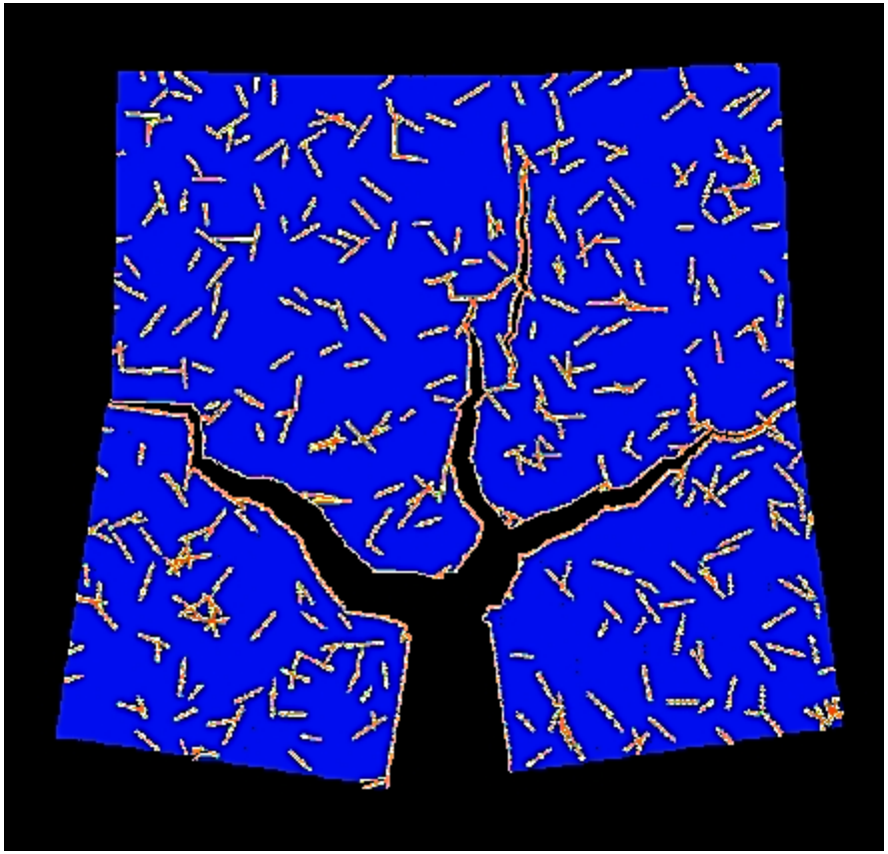
- SS & Lehoucq, *Advances in Applied Mechanics* (2010)
- Bobaru, & Duangpanya, *J. Computational Physics* (2012)
- Oterkus, Madenci, & Agwai, *J. Mechanics & Physics of Solids* (2014)

Fracture in a brittle plate with a lot of defects

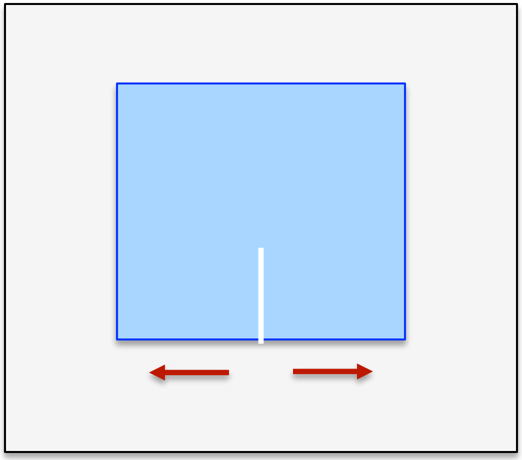
- How do defects join up to form a macroscopic crack?



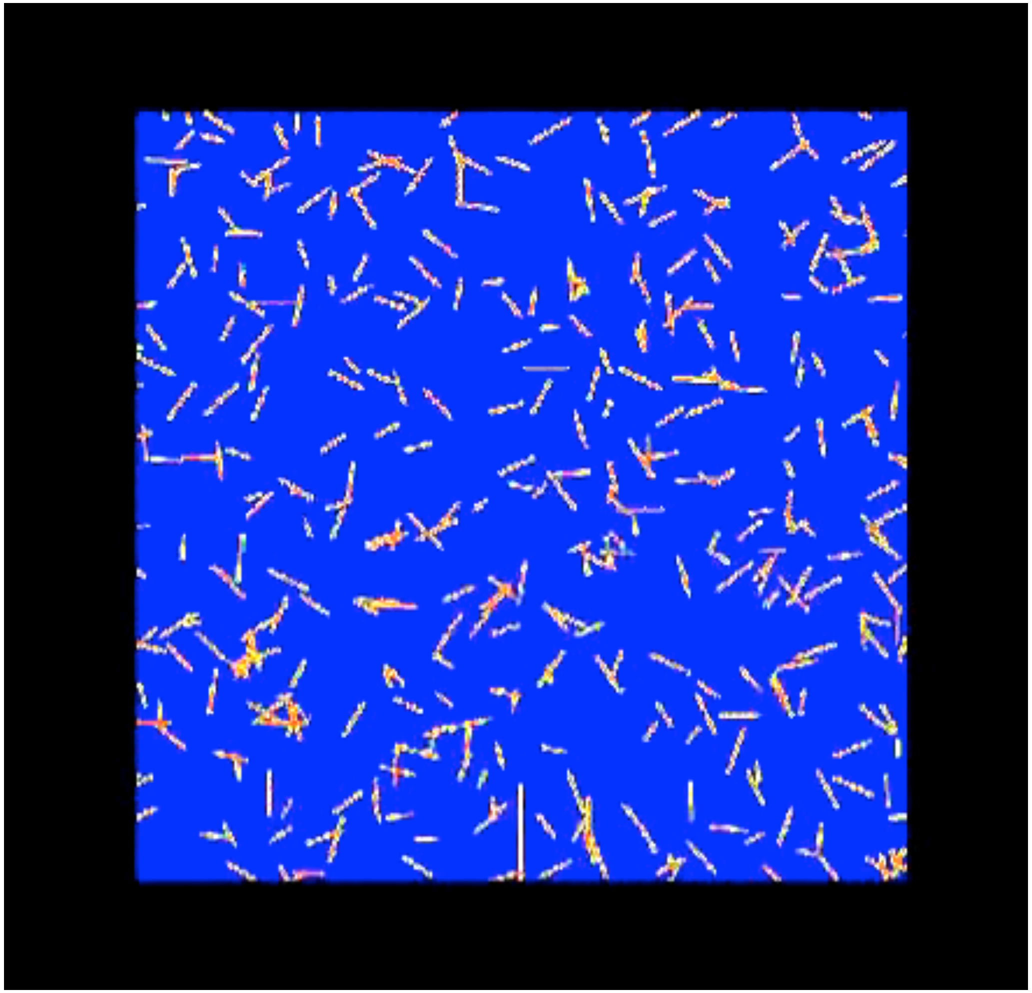
Metallic glass fracture (Hofmann et al, Nature 2008)



Fracture in a brittle plate with a lot of defects



VIDEO

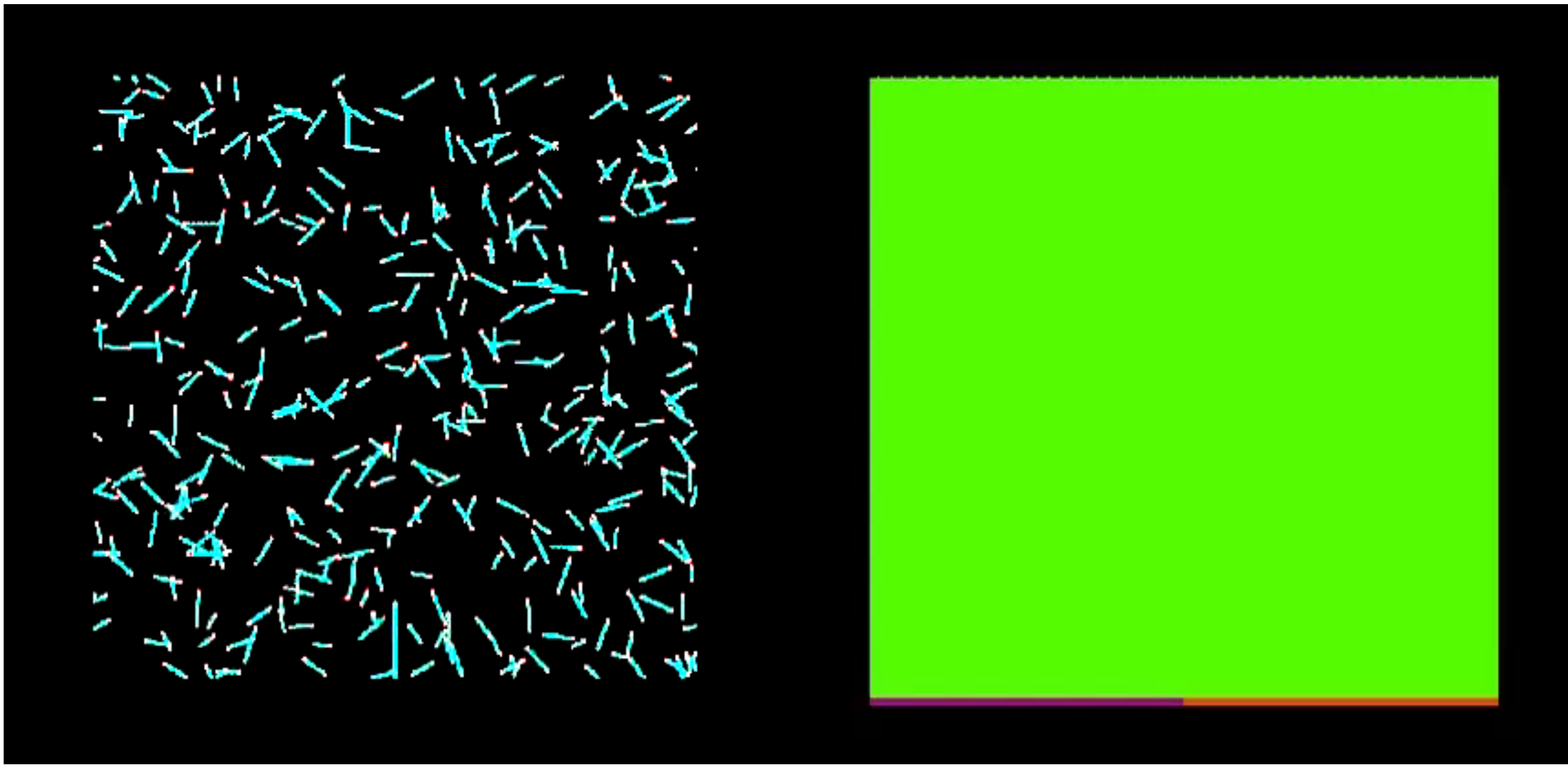


Fracture in an elastic-plastic plate with a lot of defects

VIDEOS

Defects

Displacement



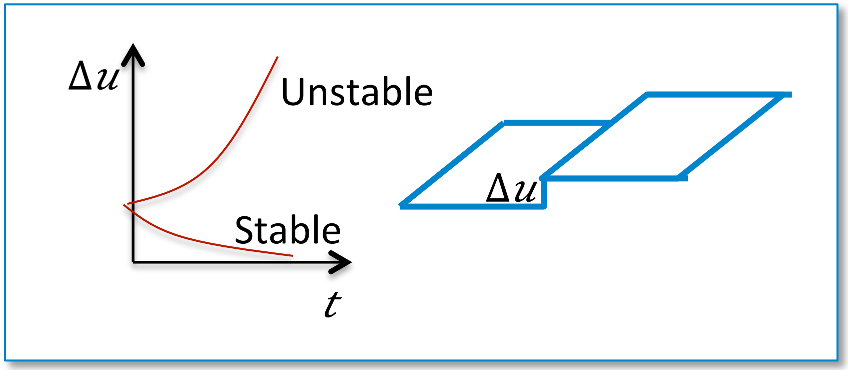
Cracks nucleate due to a material instability

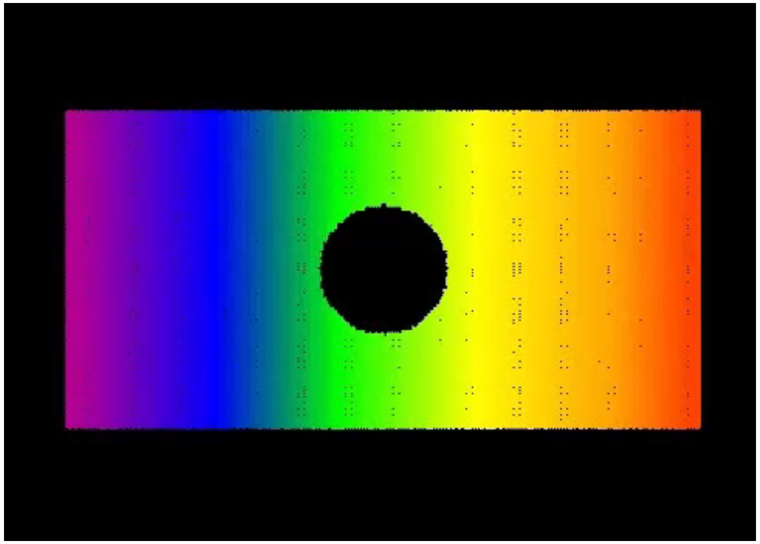
- Condition for growth of a discontinuity in displacement:

$$\det(\underline{1} \bullet \underline{\mathbb{K}} \bullet \underline{1}) = 0$$

where $\underline{\mathbb{K}}$ is a tensor-valued state obtained from the second Fréchet derivatives of the strain energy density:

$$\underline{\mathbb{K}} = W_{\underline{\mathbf{YY}}}.$$

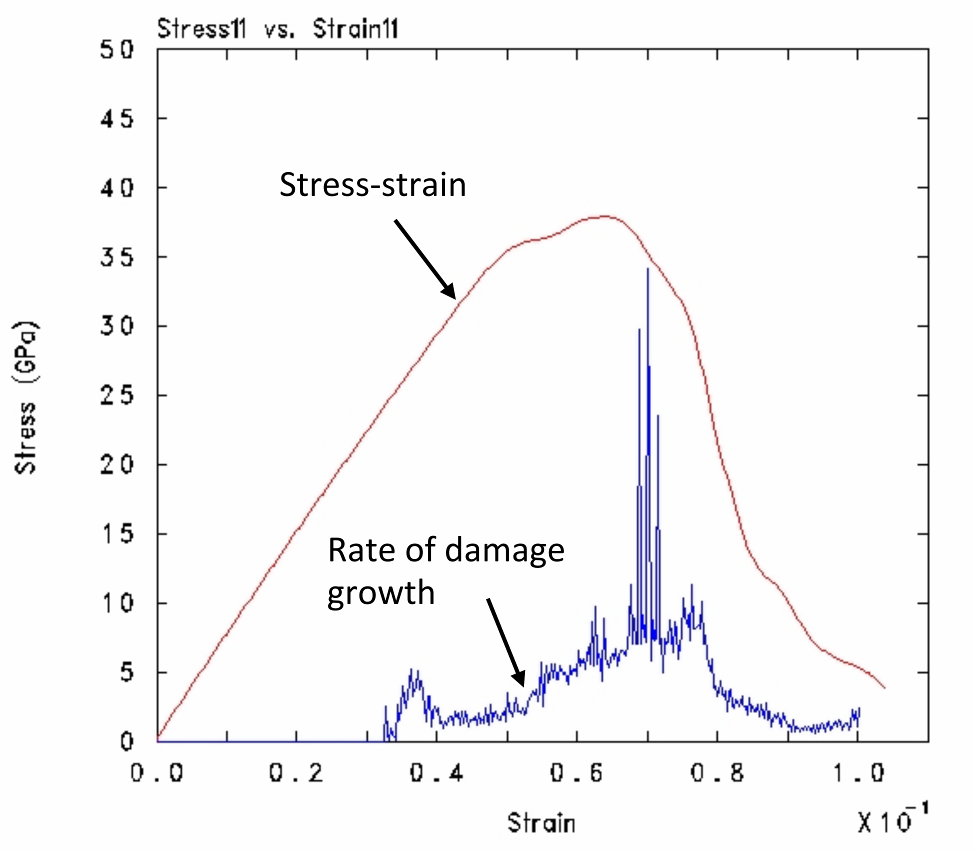


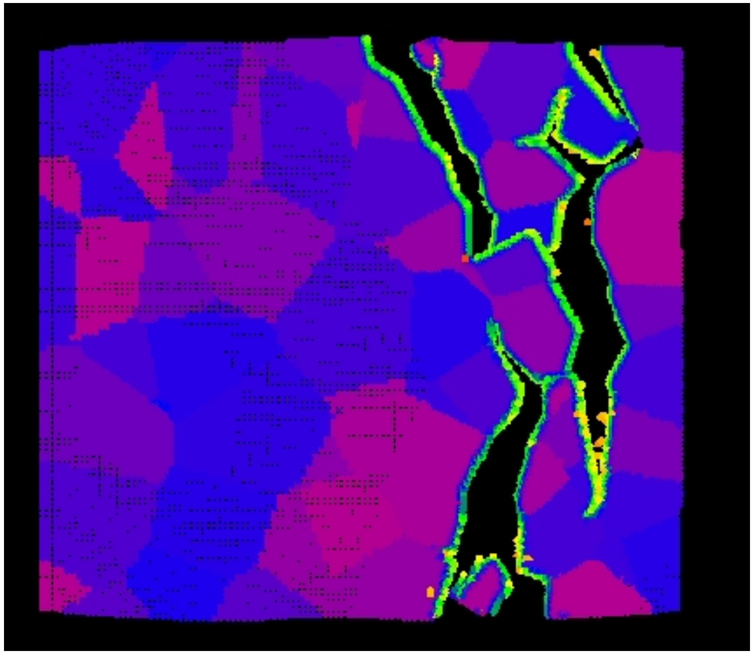


- SS, Weckner, Askari, & Bobaru, *Int. J. Fracture* (2010)
- Lipton, *J. Elast.* (2014)
- Lipton, *J. Elast*. (2015)

Multiscale model of a graphene sheet

- Assign strength randomly to grain boundaries.
- This one realization fails at some stress under uniaxial tension.
- Repeating with more realizations leads to statistical distribution of strength of the polycrystal.





Cracks are mostly along grain boundaries

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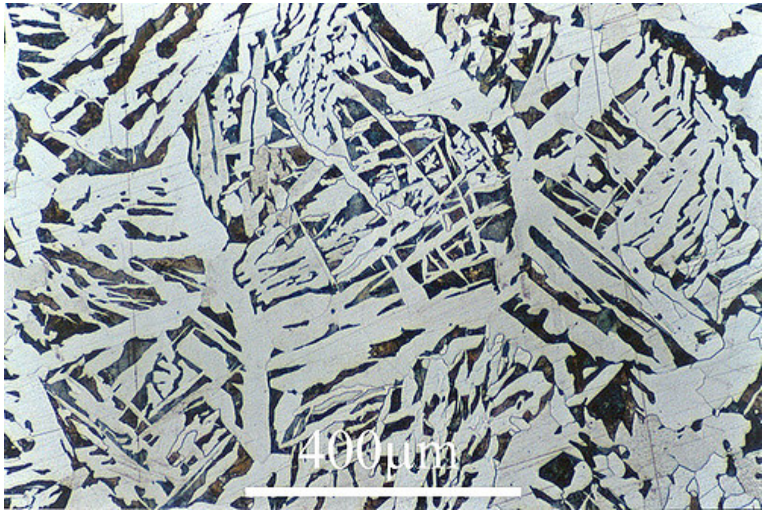
Microstructure

- Properties of metals are strongly influenced by their microstructure (sizes and shapes of grains).
- Microstructure evolution is largely about the energetics of grain boundaries.
- Will demonstrate:
  - Phase boundaries in peridynamics contain finite energy.
  - They dissipate energy as they move.
  - They move in the direction of lower total potential energy of the system.



Steel microstructure
Image: R F Cochrane, University of Leeds

Bond-based model for coexistent phases*

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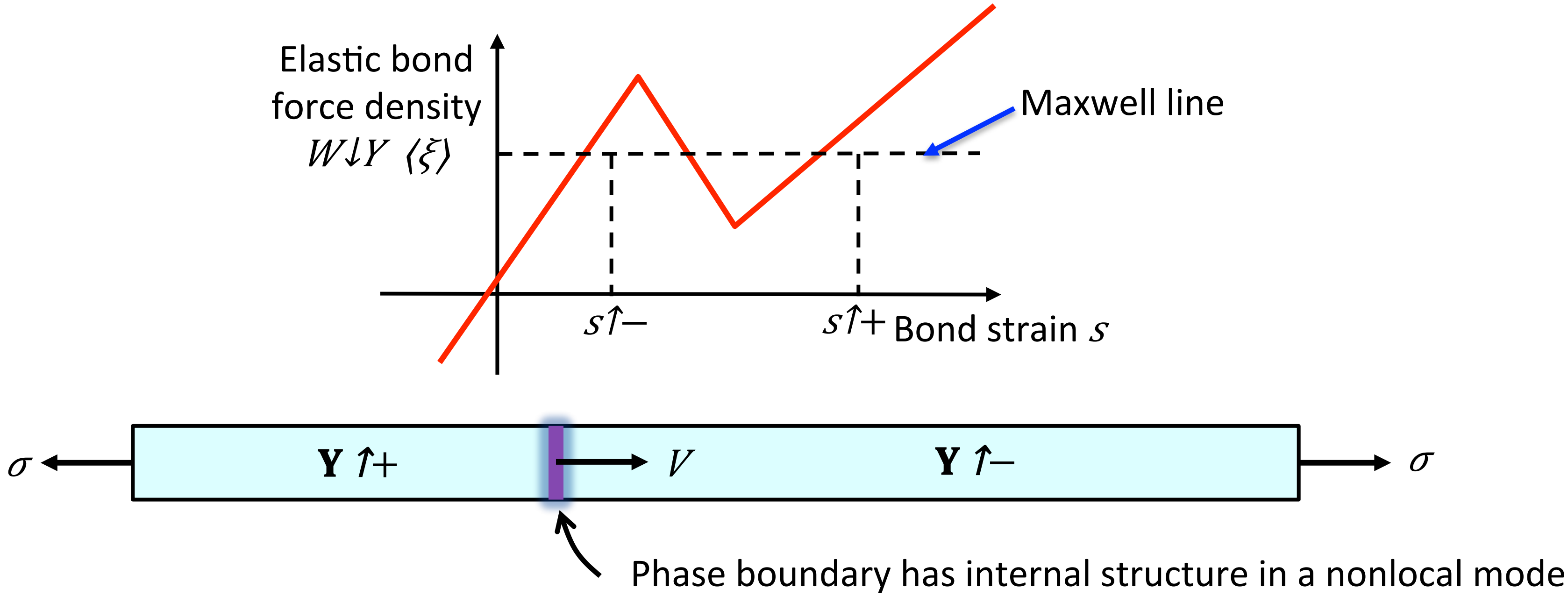
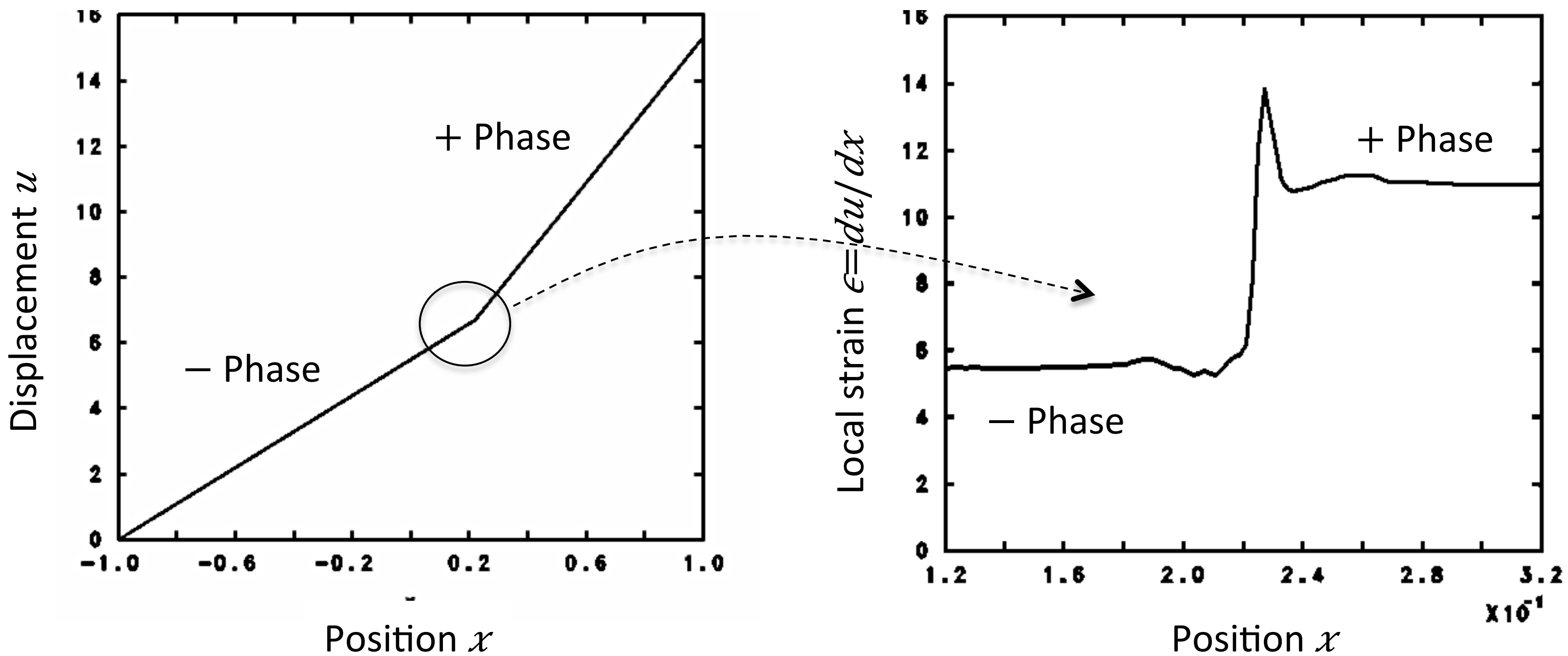


*Dayal & Bhattacharya, *J. Mechanics & Physics of Solids* (2006)

- Elastic bars: Ericksen, *J. Elast.* (1975)
- Crystals: James, *Archive for Rational Mechanics & Analysis* (1981)
- Strings: Purohit & Bhattacharya, *J. Mechanics & Physics of Solids* (2003)
- Lattices: Truskinovsky & Vainchtein, *SIAM J. Applied Math*. (2005)
- Inelastic continuum: Levitas, *Int. J. Solids & Structures* (1998)
- 3D elasticity: Abeyaratne & Knowles, *Archive for Rational Mechanics & Analysis* (1991)

Structure of the phase boundary in a peridynamic model

- Hard load problem in a bar.
- The phase boundary contains internal structure, finite width and energy.

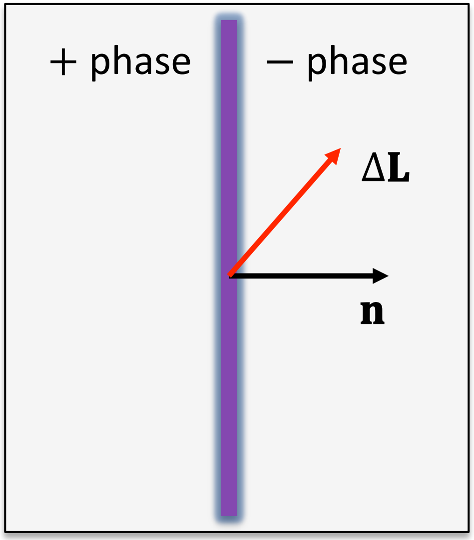


- Dayal & Bhattacharya, *J. Mechanics & Physics of Solids* (2006)..

Condition for nucleation of a phase boundary

- Momentum balance across the phase boundary:

$$\left(\int_{\mathcal{H}} \Delta\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \otimes \boldsymbol{\xi}\, dV_{\boldsymbol{\xi}}\right)\mathbf{n} = 0 \qquad \text{or} \qquad (\Delta\underline{\mathbf{T}} \star \underline{\mathbf{X}})\mathbf{n} = 0.$$



- Continuity of displacement in the plane of the phase boundary:

$$\Delta\underline{\mathbf{U}} = (\mathbf{n} \otimes \Delta\mathbf{L})\underline{\mathbf{X}} \qquad \text{for some vector } \Delta\mathbf{L} \neq 0.$$

- Linear material model: $\underline{\mathbf{T}} = \underline{\mathbb{K}} \bullet \underline{\mathbf{U}}$.

- The above lead to the following condition:

$$\left[\mathsf{C}(\mathbf{n} \otimes \mathbf{n})\right]\Delta\mathbf{L} = 0.$$

where C is the fourth order elasticity tensor, $\mathsf{C} = \underline{\mathbf{X}} \bullet (\underline{\mathbb{K}} \bullet \underline{\mathbf{X}})$.

- This condition holds if and only if $\det\left[\mathsf{C}(\mathbf{n} \otimes \mathbf{n})\right] = 0$. This is formally the same as loss of *ordinary ellipticity* in the local theory.

Condition for energy minimization with multiple phases

- Stationary potential energy for 2-phase equilibrium implies

$$\mathbf{n} \cdot (\Delta \mathbf{P} \mathbf{n}) = 0 \qquad (1)$$

where $\mathbf{P}$ is the Eshelby energy-momentum tensor, defined by

$$\mathbf{P} = W\mathbf{1} - \underline{\mathbf{T}} \star \underline{\mathbf{Y}} \qquad \text{or} \qquad \mathbf{P} = W\mathbf{1} - \int_{\mathcal{H}} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \otimes \underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle \, dV_{\boldsymbol{\xi}}.$$

- (Compare classical version: $\mathbf{P} = W\mathbf{1} - \boldsymbol{\sigma}\mathbf{F}^T$.)
- (1) leads to

$$\Delta\{W - (\underline{\mathbf{T}} \cdot \mathbf{n}) \bullet (\underline{\mathbf{Y}} \cdot \mathbf{n})\} = 0$$

which is the 3D peridynamic version of the 1D Maxwell condition for phase equilibrium

$$\Delta W - \sigma \Delta \epsilon = 0.$$

Energy dissipation model for a bond

- A moving phase boundary must dissipate energy.
- Introduce a dissipative term into the material model:

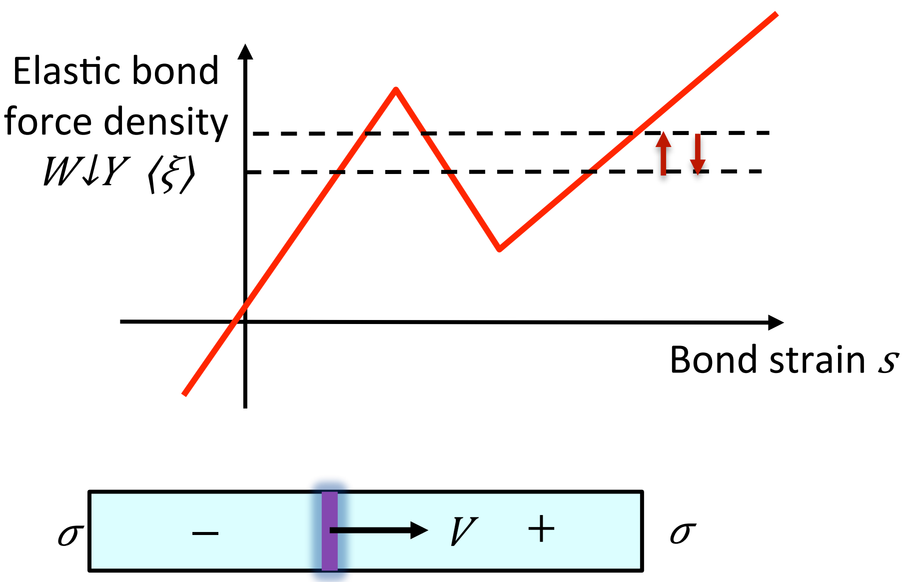
$$\begin{aligned}\underline{\mathbf{T}}\langle\xi\rangle &= W_{\underline{\mathbf{Y}}}\langle\xi\rangle + \gamma(\dot{\underline{\mathbf{Y}}}\langle\xi\rangle + \dot{\underline{\mathbf{Y}}}\langle -\xi\rangle) \\ &= W_{\underline{\mathbf{Y}}}\langle\xi\rangle + \gamma(\dot{\mathbf{y}}(\mathbf{x}+\xi) - 2\dot{\mathbf{y}}(\mathbf{x}) + \dot{\mathbf{y}}(\mathbf{x}-\xi)),\end{aligned}$$

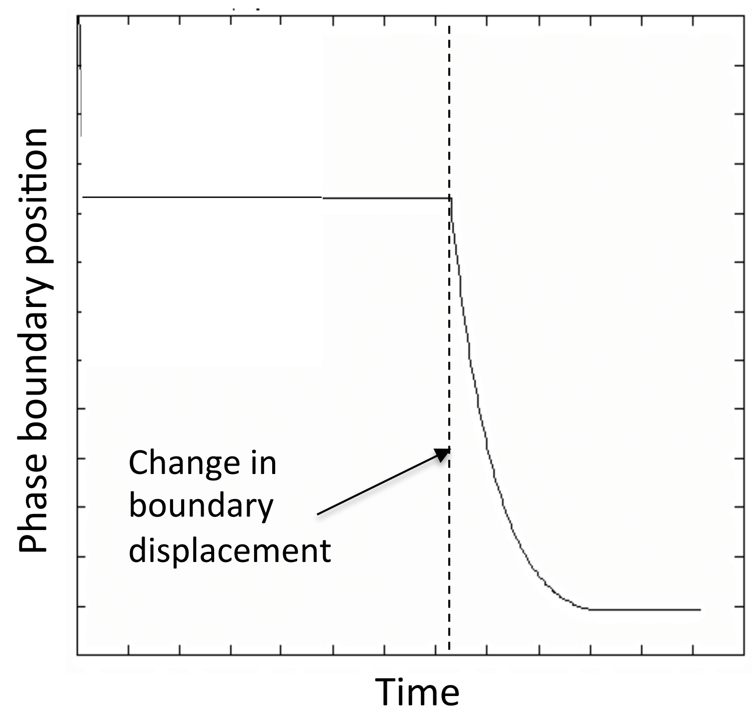
  where $\gamma > 0$ is a constant.
- Can show the new term satisfies the dissipation inequality.
- Observe the dependence on the "curvature" of the velocity field – expect it to be significant only *within* a phase boundary.

- Abeyaratne & Knowles, *Archive for Rational Mechanics & Analysis* (1991).

Phase boundary seeks out the Maxwell line asymptotically

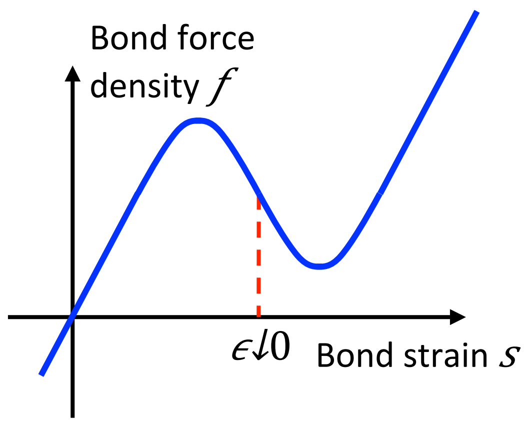
- Peridynamic simulation of a bar using the dissipation model discussed above.
- Perturb the boundary conditions and watch the phase boundary motion.
- The phase boundary moves so the system lowers its energy.

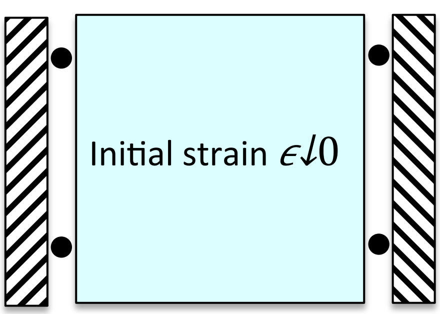




Deformation gradually reduces the area of a phase boundary in 2D

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



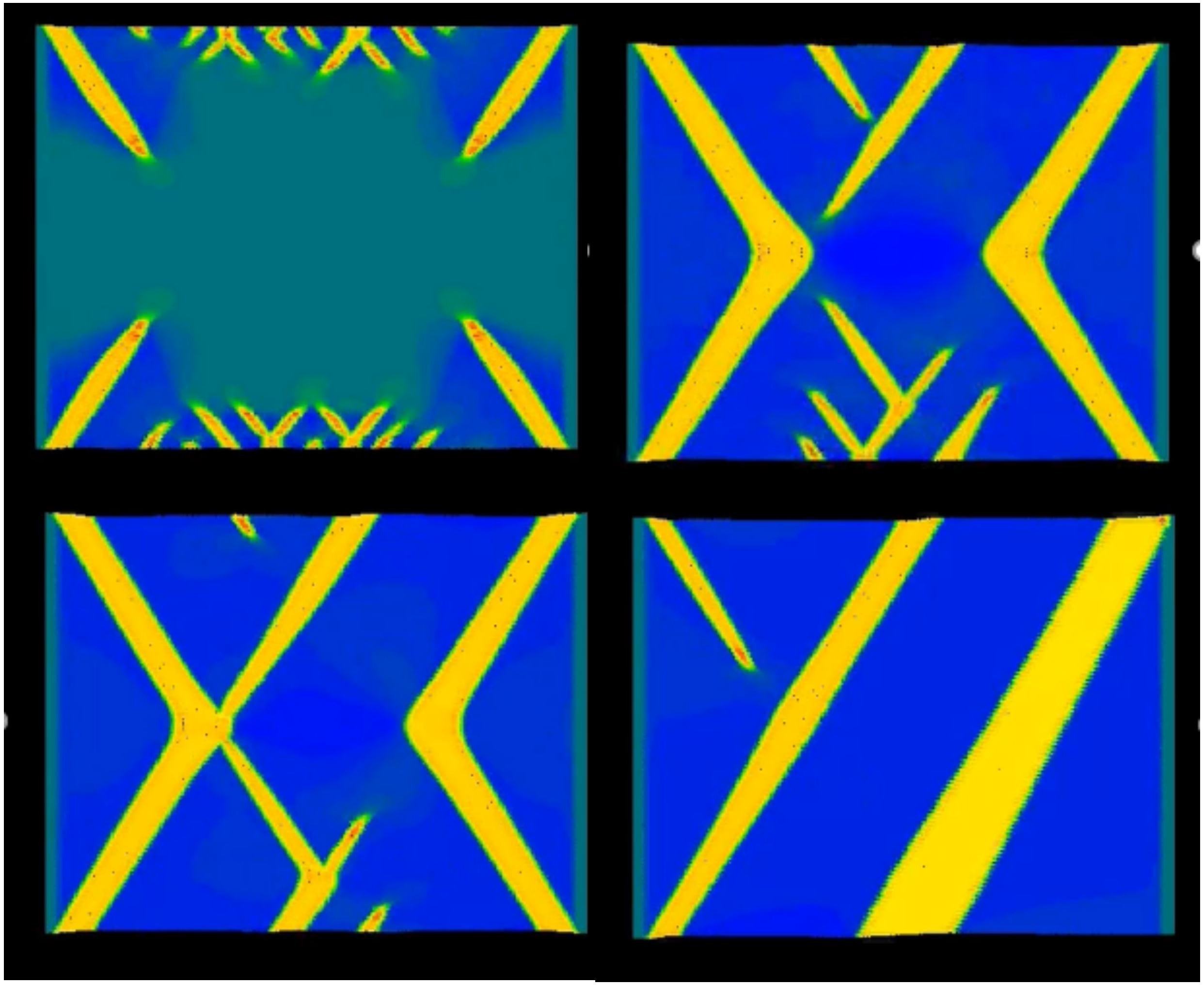


VIDEO

Colors show bond strain

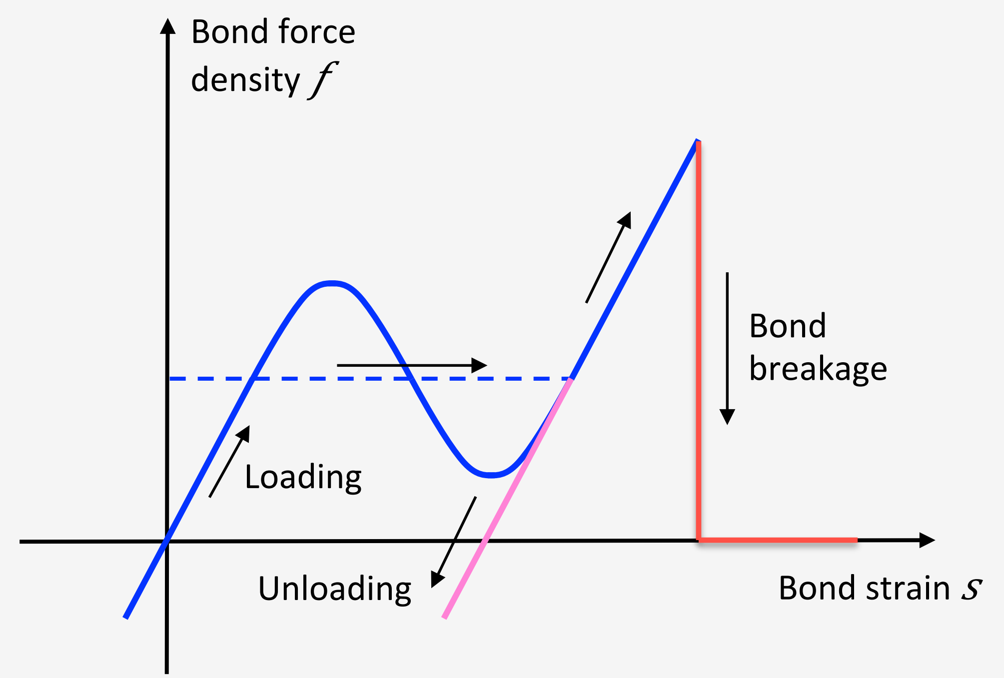
Deformation gradually reduces the area of a phase boundary in 2D

Colors show bond strain

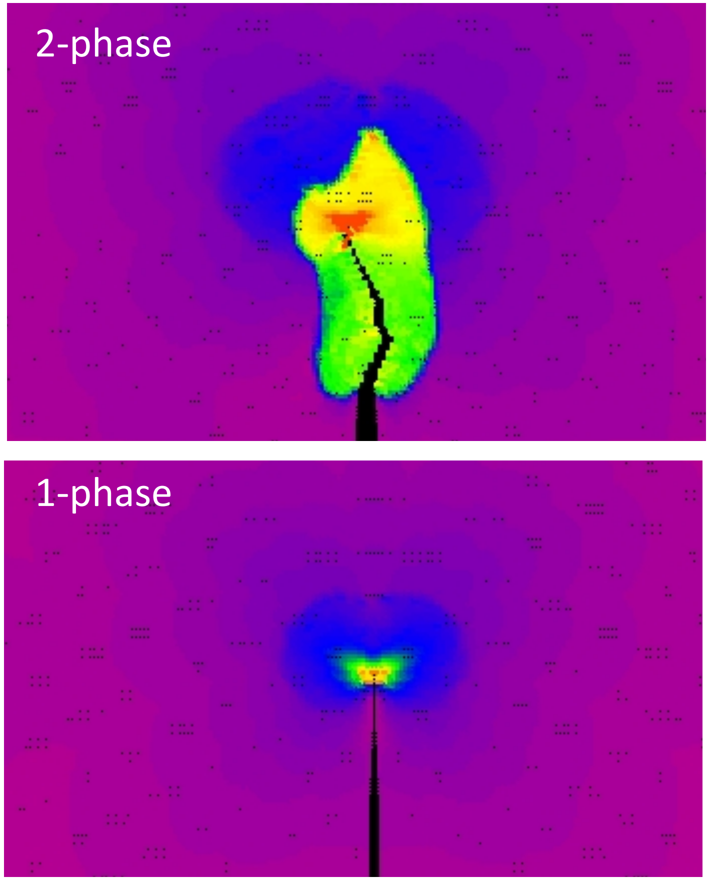


Transformation toughening (isothermal)

- Can a phase transformation make a crack try to stay closed?
- Permanent transformation in each bond.



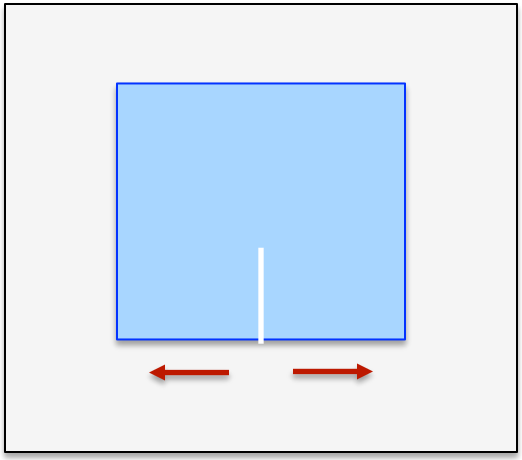
2-phase peridynamic material model with permanent transformation



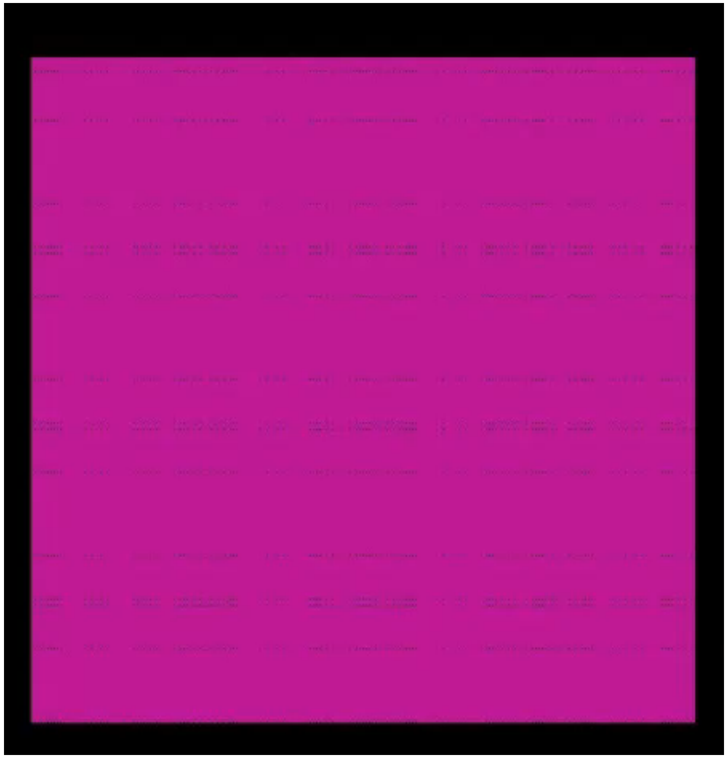
Colors show bond strain

Transformation toughening, ctd.

- Crack path deviates to avoid the toughened material in front of it.



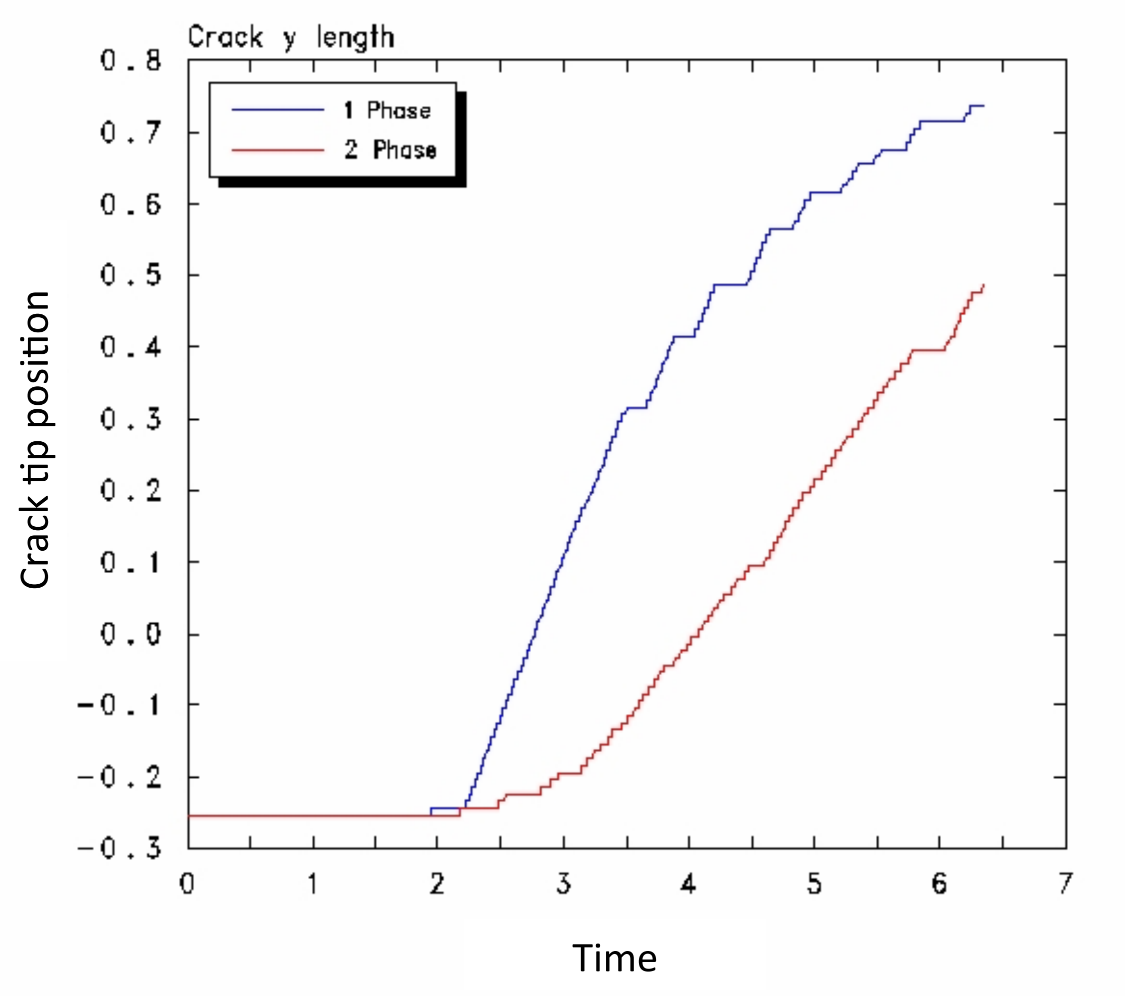
VIDEO



Colors show bond strain

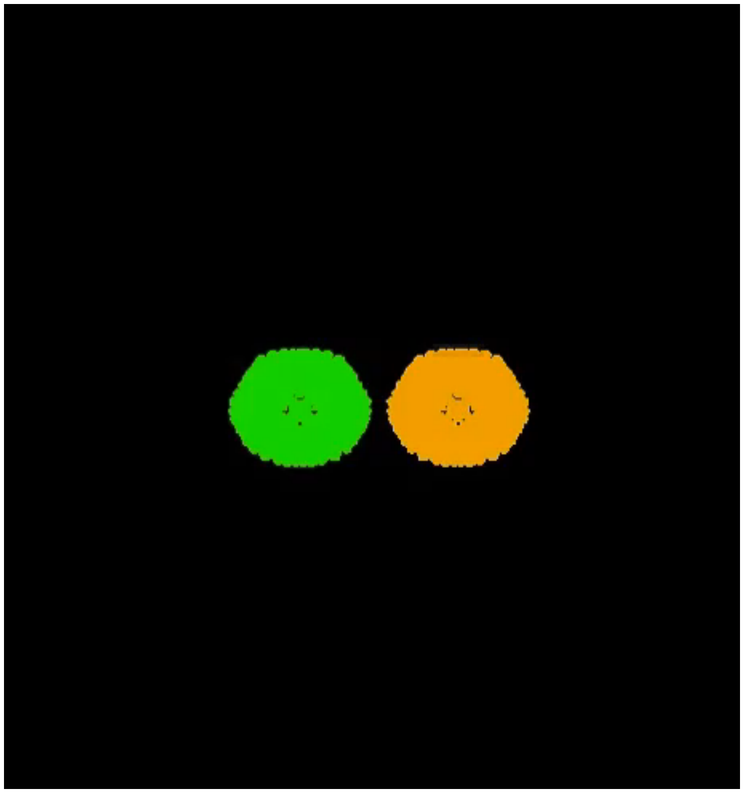
Transformation toughening, ctd.

- Crack grows slower in the 2-phase material.

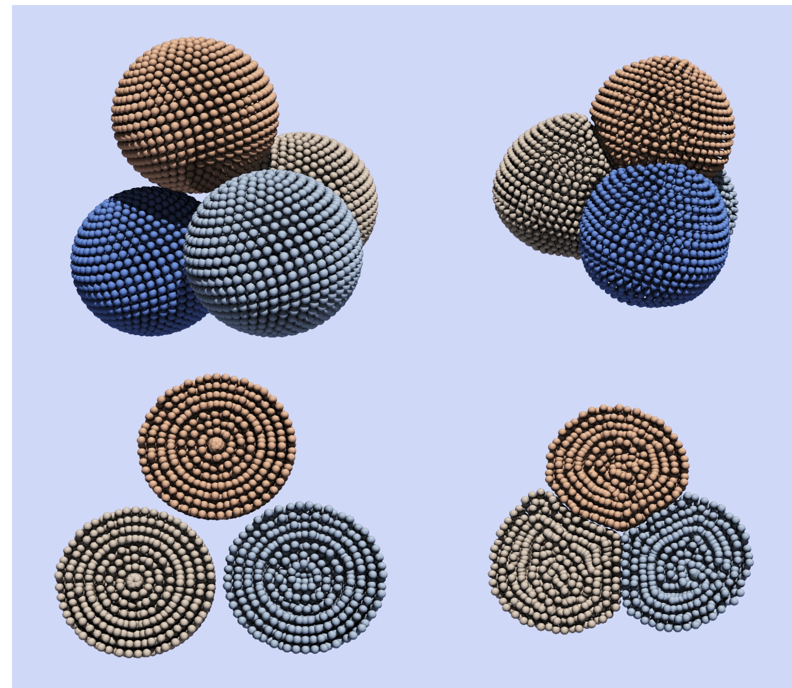


Free surfaces and material boundaries can have energy too

VIDEO



Droplet motion driven by surface tension



Sintering of 4 copper grains

Summary

- By treating discontinuous and continuous deformation within the same field equations we gain a lot in modeling some aspects of materials science.
  - Autonomous nucleation and growth of defects.
  - Phase boundaries evolve according to driving force.
  - Defects “do what they want.”
  - We avoid the need for supplemental equations that govern defect evolution.