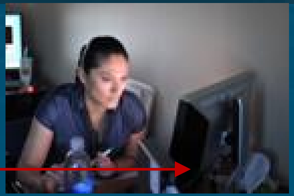
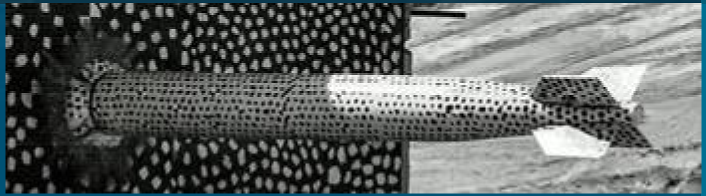
SAND2022-7811C

Some aspects of material stability in peridynamics





Stewart Silling

June 21, 2022
USNCTAM 2022
Austin, TX

SAND2021-0000

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2021

- Working virtually created many challenges.

Dear Boss,
Can't do any work today. Cat on computer.

2022

- But returning to the office is also creating challenges.

Dear Boss,
Can't come to work today. Cat on pants.

Outline

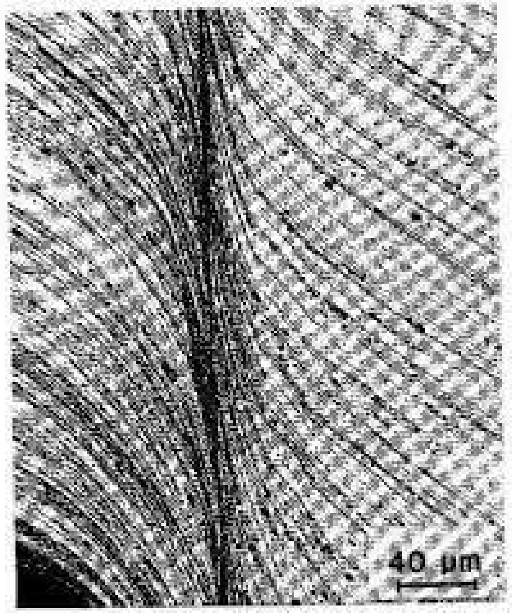
- **The nonlocal length scale affects all aspects of material stability.**
  - Failure kinetics: “Imaginary wave speeds” are useful.
  - Material and structural instability are related, leading to models for:
    - Kink bands in composites.
    - Self-shaping of fibers.
  - Fracture nucleation is a type of material instability.
  - Phase boundaries contain an unstable core.

Some concepts of stability (local theory)

- Real wave speeds (Hadamard stability, strong ellipticity)
- Minimum potential energy
- Bifurcations
- Well-posedness
- Discontinuity in gradient (Ordinary ellipticity)

Material vs. structural stability (local theory)

- Material instability:
  - Happens at a material point, triggered by local conditions
  - Not directly related to the geometry of the body
  - Example: Adiabatic shear band
- Structural instability:
  - Happens to the entire body collectively
  - Example: Buckling of a beam



Adiabatic shear band in aluminum
image: Baxevanis et al.,
www.ima.umn.edu/materials/2008-2009/SP7.13-31.09/8186/ima.pdf

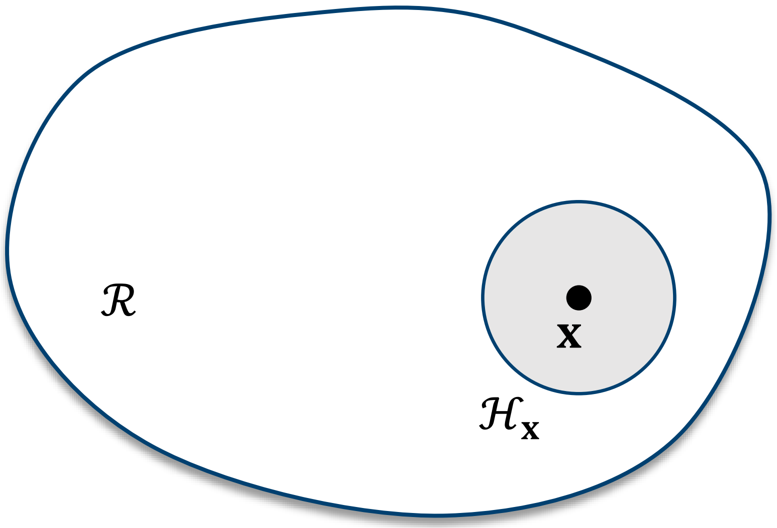
Buckling of a column
image: Klimchik
www.researchgate.net/figure/Examples-of-buckling-in-column-www-civildb-www-highline_fig11_281183936

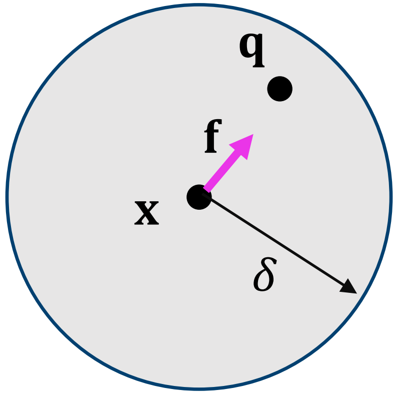
Peridynamics background

- Peridynamic momentum balance in 3D:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\, d\mathbf{q} + \mathbf{b}(\mathbf{x},t) \qquad \forall \mathbf{x} \in \mathcal{R},\ t \geq 0.$$

- $\mathbf{f}$ is the *pairwise bond force density* of the *bond* from $\mathbf{q}$ to $\mathbf{x}$.
- $\mathcal{H}_{\mathbf{x}}$ is the *family* of $\mathbf{x}$, which is a ball centered at $\mathbf{x}$ with radius δ (the *horizon*).





Bond-based materials

- Later we will consider 3D deformations and bending of 1D-like structures.
- But for now, set

$$\mathbf{u} = u\mathbf{e}_1, \qquad \mathbf{M} = \mathbf{e}_1, \qquad \mathbf{f} = C(|q-x|)s\mathbf{e}_1$$

where C is a scalar function of the bond length called the *micromodulus* or *kernel*.

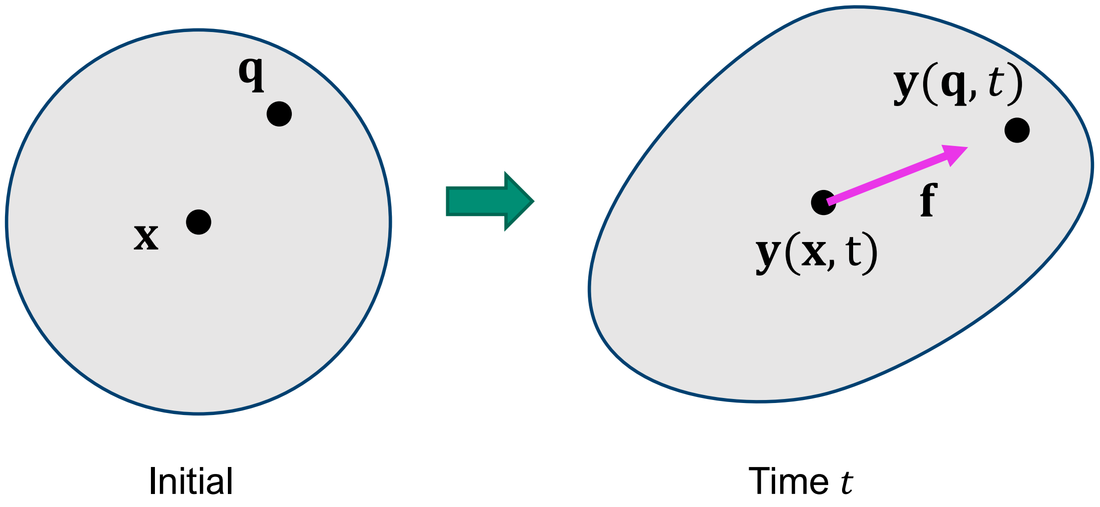
- The momentum balance is now

$$\rho\ddot{u}(x,t) = \int_{-\delta}^{\delta} C(\xi)(u(x+\xi) - u(x))\,\mathrm{d}\xi$$

(similar to Kunin's theory (1983)).

- C must satisfy

$$C(-\xi) = C(\xi) \qquad \forall\xi.$$



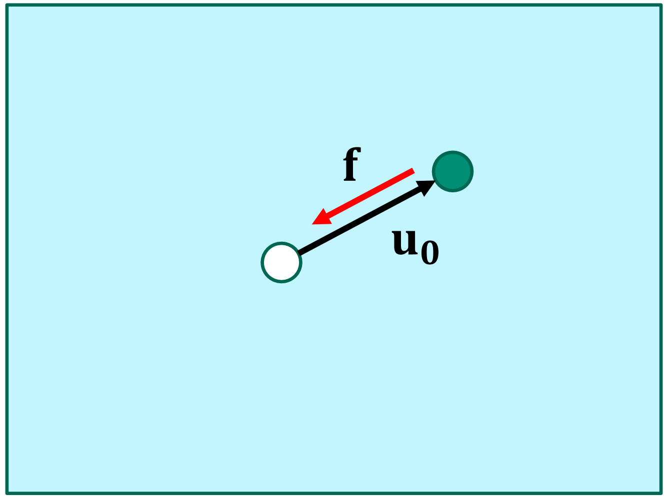
An intuitive notion of stability... and a mysterious tensor

- Equilibrium:

$$\mathbf{L}(\mathbf{x}) + \mathbf{b}(\mathbf{x}) = \mathbf{0}, \qquad \mathbf{L}(\mathbf{x}) = \int_{\mathcal{H}_\mathbf{x}} \mathbf{C}(\boldsymbol{\xi})(\mathbf{u}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{u}(\mathbf{x}))\, d\boldsymbol{\xi}$$

where $\mathbf{L}$ is the force density on $\mathbf{x}$,

- Suppose we "carve out" a small volume surrounding a point $\mathbf{x}$ and displace it by $\mathbf{u}_0$.



- The net force density on the small volume is:

$$\mathbf{L} = -\mathbf{P}\mathbf{u}_0, \qquad \mathbf{P} = \int_{\mathcal{H}_\mathbf{x}} \mathbf{C}(\boldsymbol{\xi})\, d\boldsymbol{\xi}.$$

where $\mathbf{P}$ is the *single point response* tensor.

- *Single point stability*: If

$$\mathbf{u}_0 \cdot (\mathbf{P}\mathbf{u}_0) > 0 \ \ \forall \mathbf{u}_0$$

then the particle always gets pushed back toward where it started. Otherwise $\mathbf{x}$ can fly off to ∞.

Comparable statement in the local theory:

$$c_{ijkl}\epsilon_{ij}\epsilon_{kl} > 0 \quad \forall\ \epsilon$$

Simplify further to 1D, linear microelastic

- Later we will consider 3D deformations and bending of 1D-like structures.
- But for now, set

$$\mathbf{u} = u\mathbf{e}_1, \qquad \mathbf{M} = \mathbf{e}_1, \qquad \mathbf{f} = C(|q-x|)s\mathbf{e}_1$$

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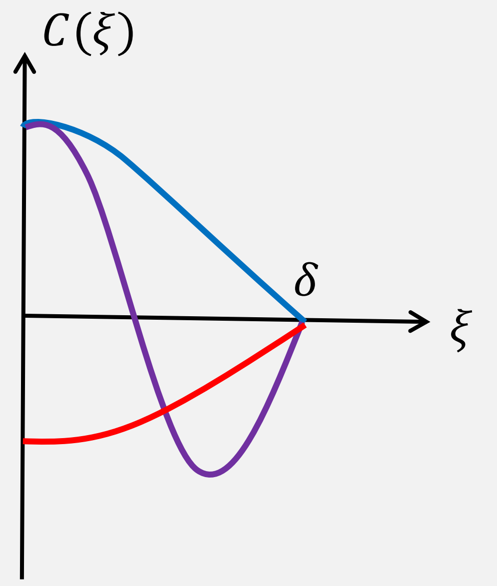


Some possible micromodulus curves

Linear waves: Dispersion curves

- Assume a wave of the form

$$u(x,t) = Ae^{i(kx-\omega t)}$$

where A=amplitude, k=wavenumber, ω=frequency.

- Equation of motion:

$$\rho\ddot{u}(x,t) = \int_{-\delta}^{\delta} C(\xi)\left[u(x+\xi,t) - u(x,t)\right]\, d\xi$$

- leads to

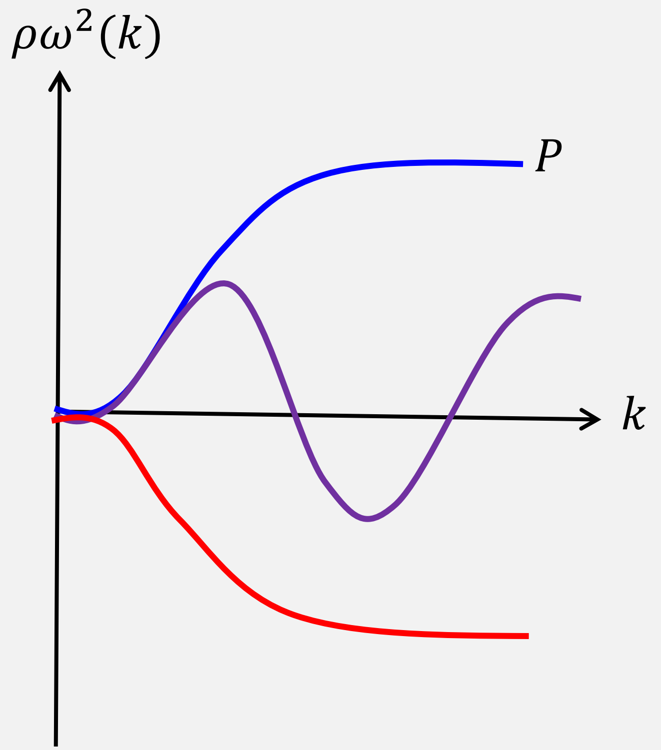
$$-\rho\omega^2 = \int_{-\delta}^{\delta} C(\xi)\left[e^{ik\xi} - 1\right]\, d\xi$$

- Therefore the dispersion relation is

$$\omega(k) = \sqrt{\frac{P - \bar{C}(k)}{\rho}}, \qquad P = \bar{C}(0)$$

We've seen this before!

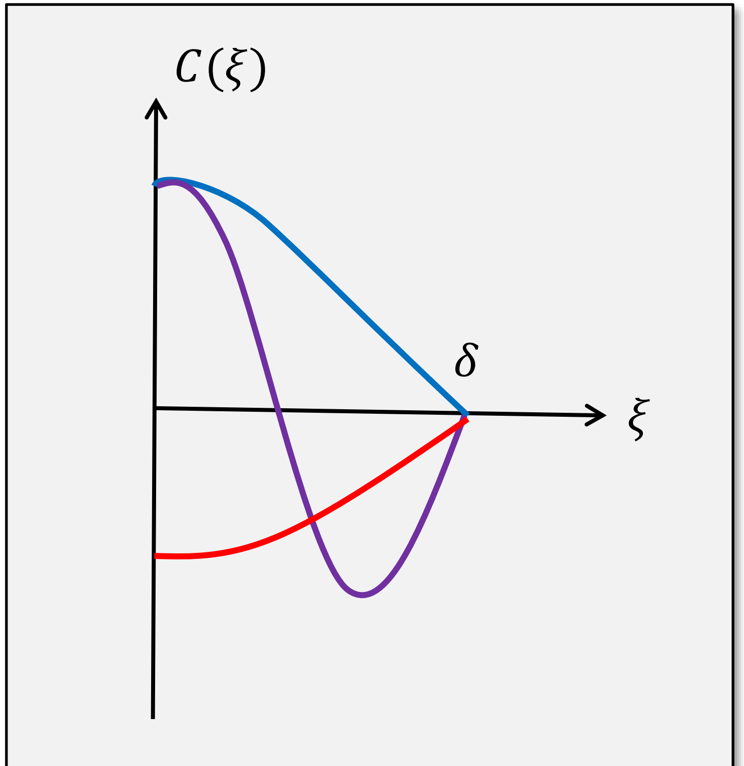
where $\bar{C}(k)$ is the Fourier transform of $C(\xi)$.



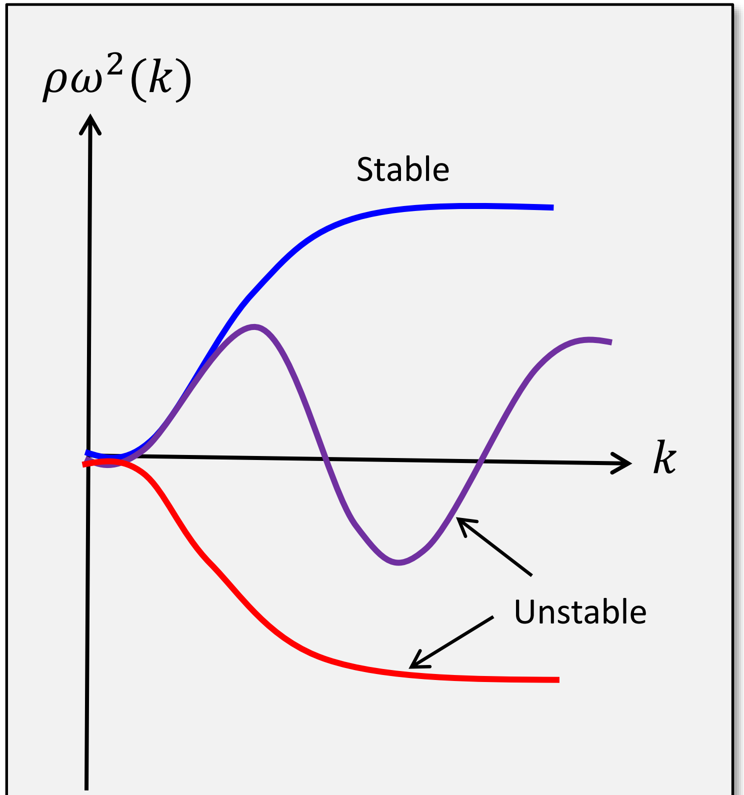
Some possible dispersion curves

Dispersion and material stability

- Purple and red materials have "imaginary wave speeds" $c = \omega/k$.
    - Red: all wavenumbers are unstable.
    - Purple: only some wavenumbers are unstable.

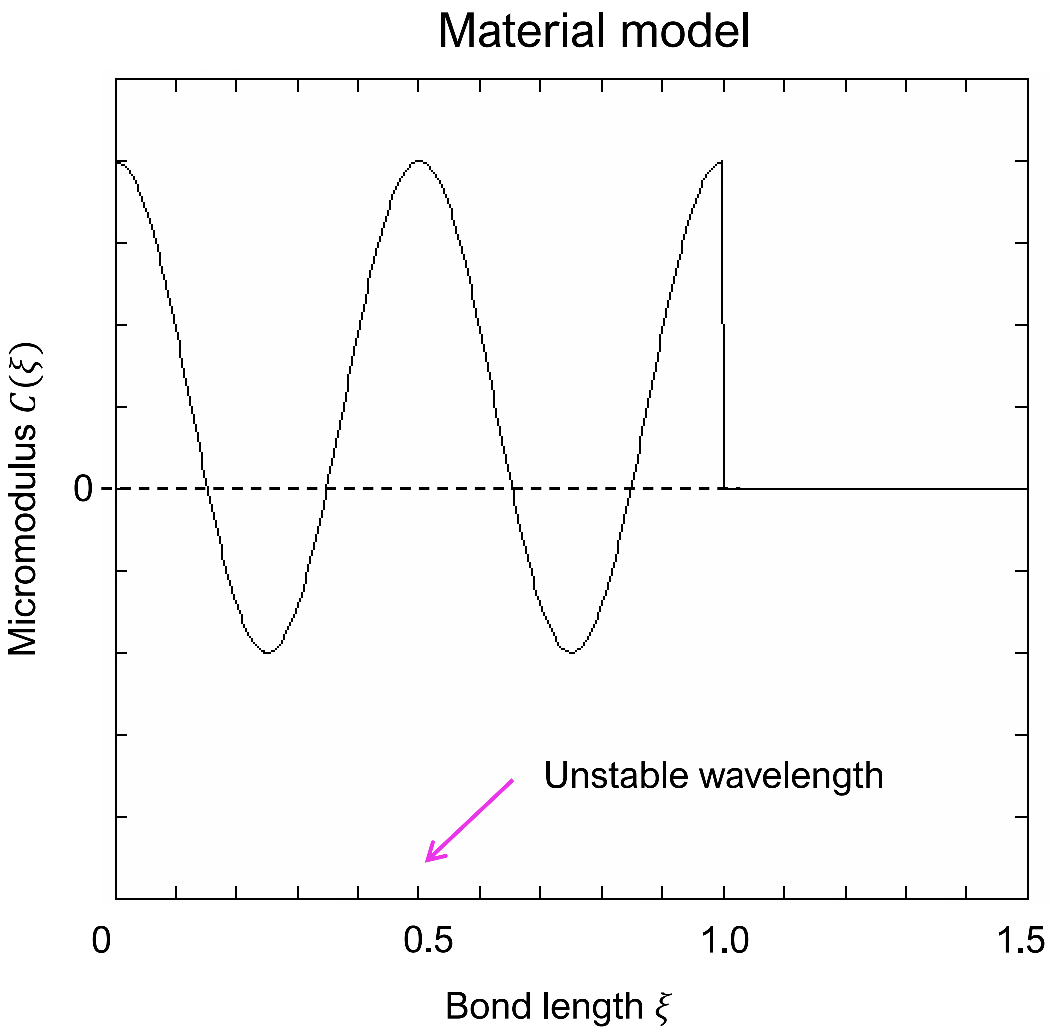


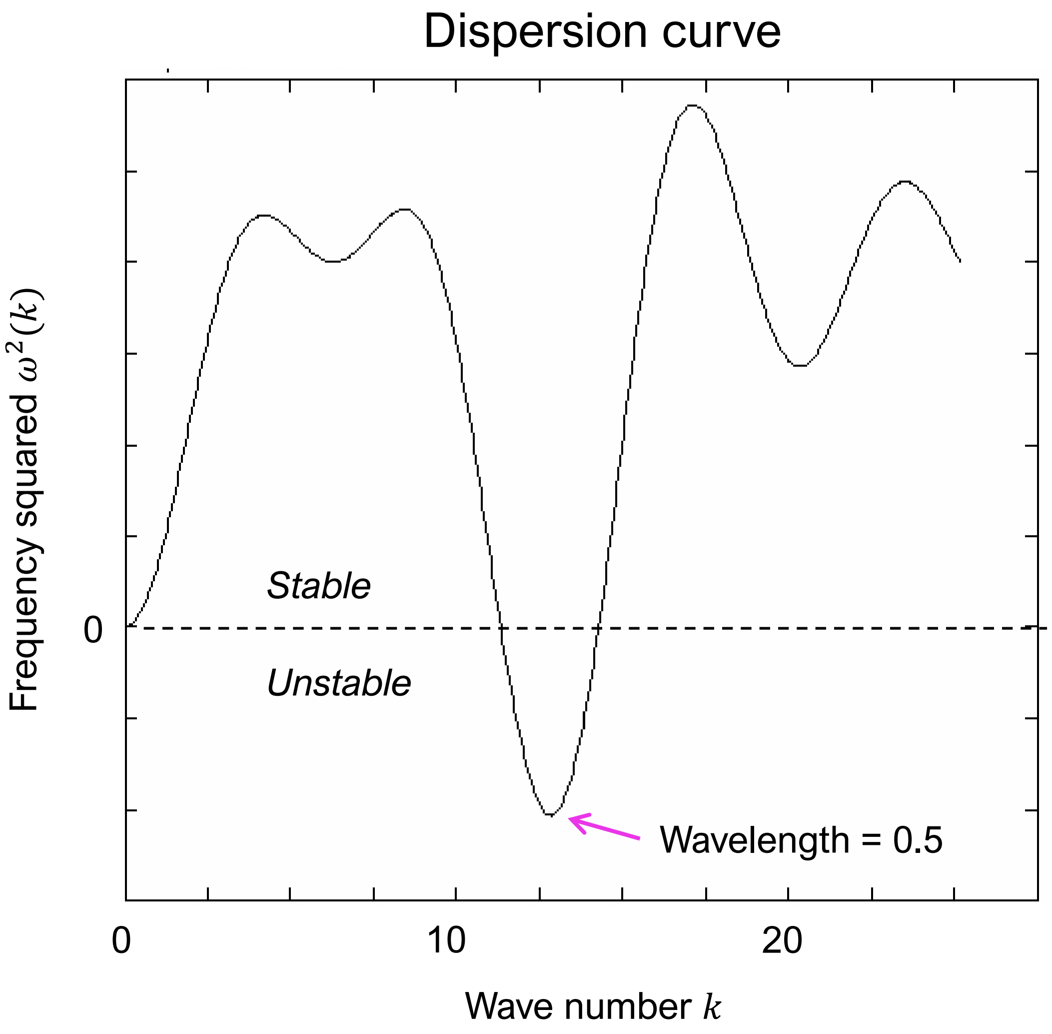
Micromodulus curves



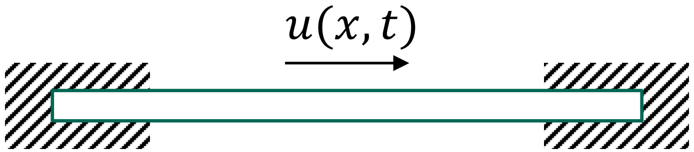
Dispersion curves

Example: A material with a narrow band of unstable wavenumbers

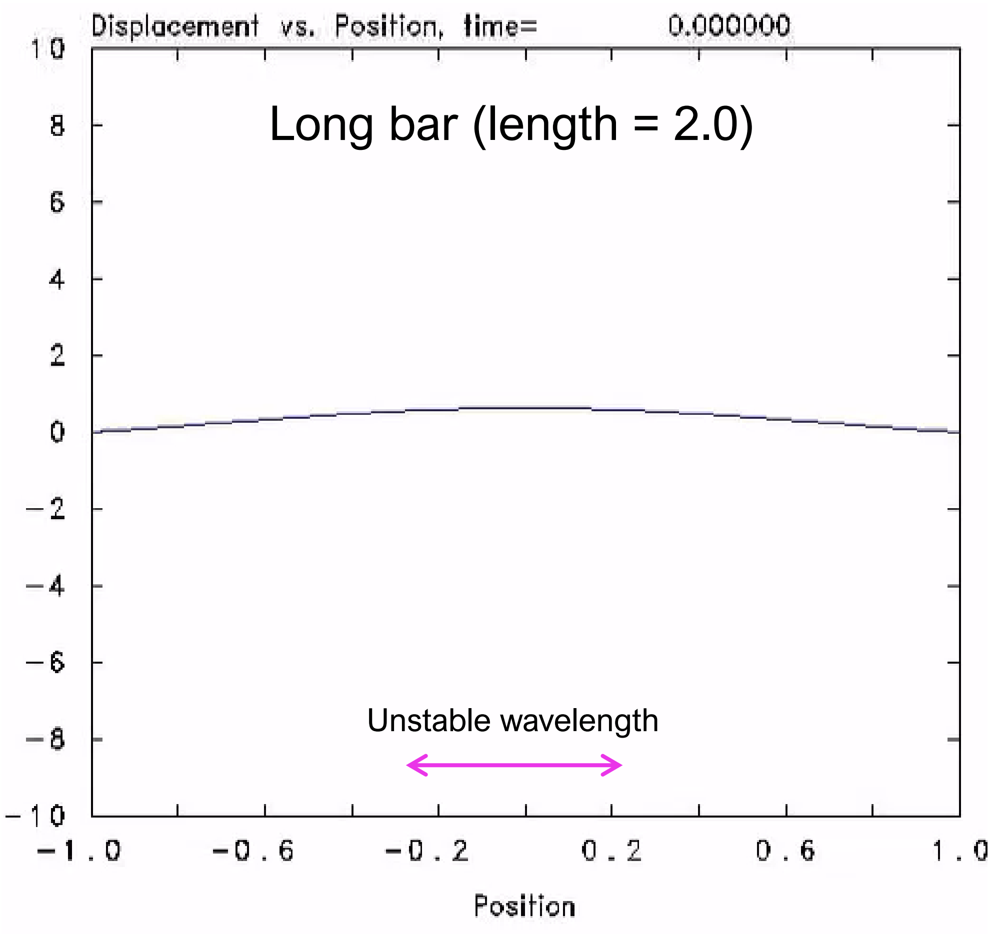


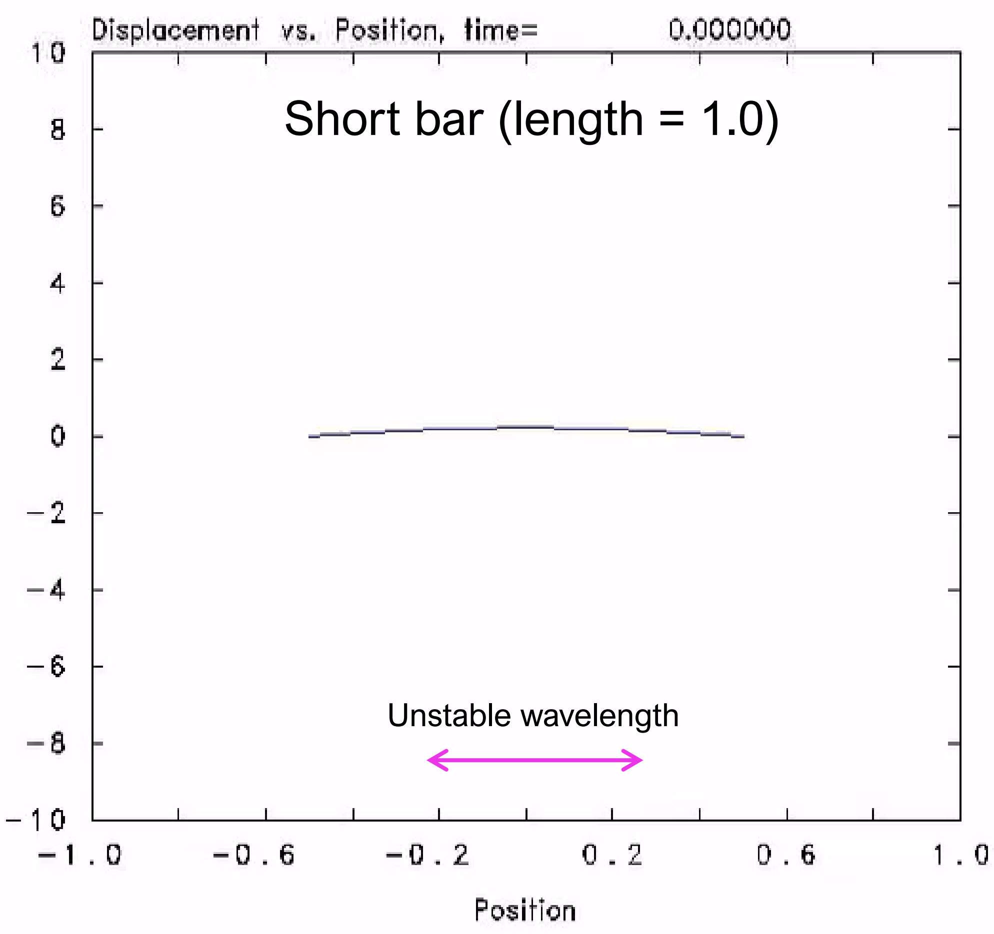


This material is stable in some geometries but unstable in others



VIDEOS





Minimum potential energy is related to wave speed

- Total potential energy in a bounded body:

$$\Phi_{\mathbf{u}} = \frac{1}{2}\int\int w(\mathbf{x}', \mathbf{x})\, d\mathbf{x}'\, d\mathbf{x} + \int \mathbf{b}\cdot\mathbf{u}\, d\mathbf{x}$$

  where w is the bond energy (*micropotential*).

- Consider a set of deformations parameterized by ε:

$$\mathbf{u} = \mathbf{u}_0 + \varepsilon\mathbf{v}$$

  where $\mathbf{v}$ is a vector field.

- Stationary Φ:

$$\frac{d\Phi}{d\varepsilon} = 0 \qquad \forall\mathbf{v}$$

  leads to the equilibrium equation that is satisfied by $\mathbf{u}_0$

$$\int \mathbf{f}(\mathbf{x}', \mathbf{x})\, d\mathbf{x}' + \mathbf{b} = \mathbf{0} \qquad \forall\mathbf{x}.$$

Minimum potential energy is related to wave speed, ctd.

- Now require Φ to be a minimum as well as stationary:

$$\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varepsilon^2} > 0$$

for all $\mathbf{v}$ except rigid motions.

- Leads to

$$\int\int (\mathbf{v}' - \mathbf{v}) \cdot \mathbf{C}(\boldsymbol{\xi})(\mathbf{v}' - \mathbf{v})\,\mathrm{d}\mathbf{x}'\,\mathrm{d}\mathbf{x} > 0 \qquad \forall \mathbf{v}$$

where

$$\mathbf{C} = \frac{\partial \mathbf{f}}{\partial \boldsymbol{\eta}}, \qquad \boldsymbol{\eta} := \mathbf{u}' - \mathbf{u}.$$

Minimum energy implies real wave speeds

- Suppose Φ is minimized by $\mathbf{u}_0$. Let $\mathbf{v}$ be a standing wave (eigenmode, vibrational mode).

$$\int \mathbf{C}(\boldsymbol{\xi})(\mathbf{v}' - \mathbf{v})\ \mathrm{d}\mathbf{x}' + \rho\omega^2\mathbf{v} = \mathbf{0}.$$

- Multiply through by $\mathbf{v}$ and integrate over $\mathbf{x}$:

$$\int\int \mathbf{v}\cdot\mathbf{C}(\boldsymbol{\xi})(\mathbf{v}' - \mathbf{v})\ \mathrm{d}\mathbf{x}'\ \mathrm{d}\mathbf{x} + \rho\omega^2\int \mathbf{v}\cdot\mathbf{v}\ \mathrm{d}\mathbf{x} = \mathbf{0}.$$

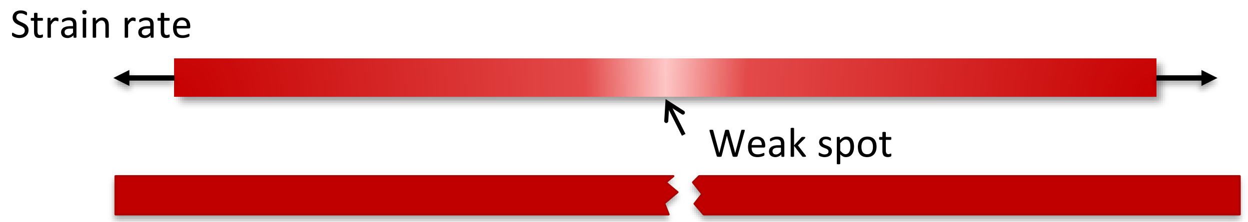
- After some manipulations:

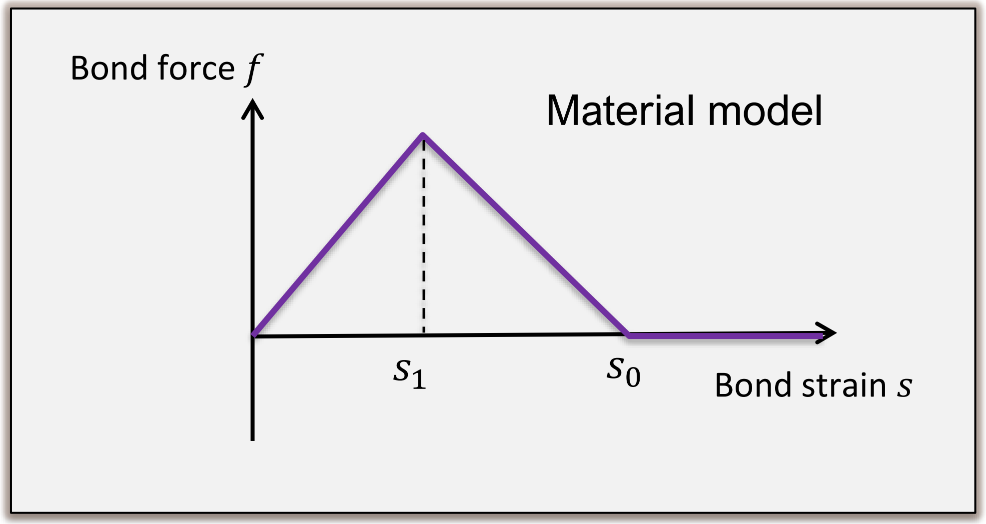
$$\int\int (\mathbf{v}' - \mathbf{v})\cdot\mathbf{C}(\boldsymbol{\xi})(\mathbf{v}' - \mathbf{v})\ \mathrm{d}\mathbf{x}'\ \mathrm{d}\mathbf{x} - 2\rho\omega^2\int \mathbf{v}\cdot\mathbf{v}\ \mathrm{d}\mathbf{x} = \mathbf{0}.$$

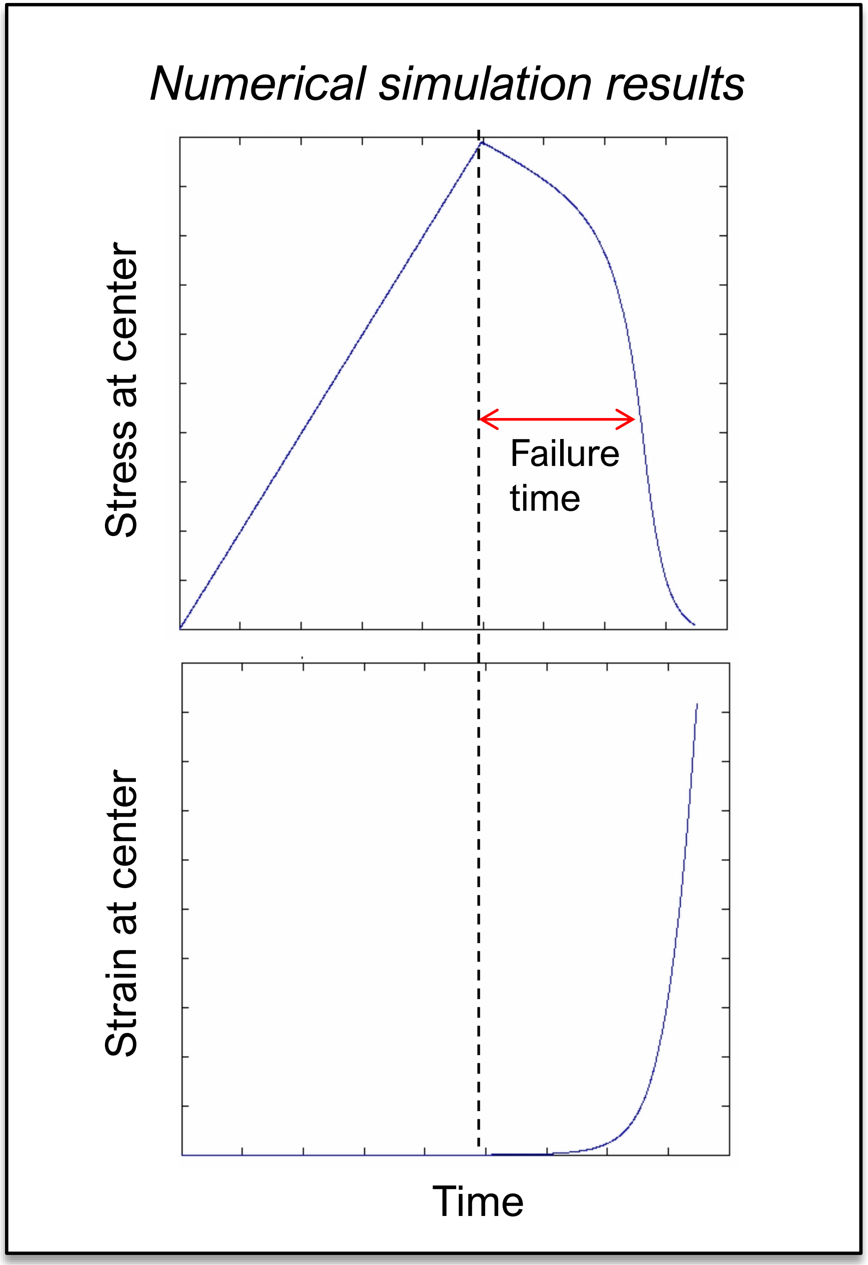
- But we already know that the $\int\int$ is positive.
- Conclude $\omega^2 > 0$. So the wave speeds are real.

Failure kinetics: How much time does it take for material to fail?

- Example: Stretching of a bar with an unstable material model.
  - Bar is stretched from the ends at a constant rate.
  - The bond force vs. strain curve has a descending branch.
  - What happens?







Failure kinetics: Unstable waveforms grow exponentially but at a finite rate

- Initial data in the infinite bar:

$$u(x,0) = A\cos kx, \qquad \dot{u}(x,0) = 0 \qquad \forall x.$$

- If $\omega^2(k) > 0$:

$$u(x,t) = \frac{A}{2}\left[\cos(kx - \omega(k)t) + \cos(kx + \omega(k)t)\right].$$

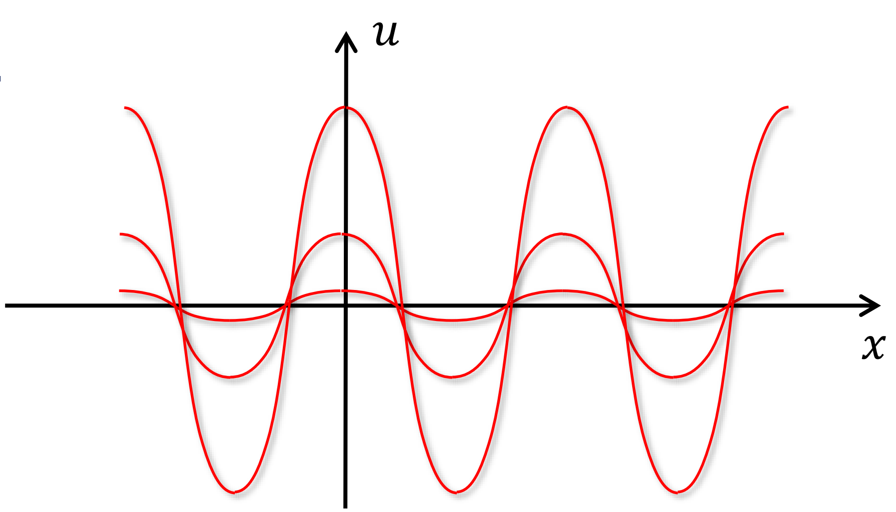
- If $\omega^2(k) < 0$:

$$u(x,t) = A\cos(kx)\cosh(\lambda(k)t)$$

where

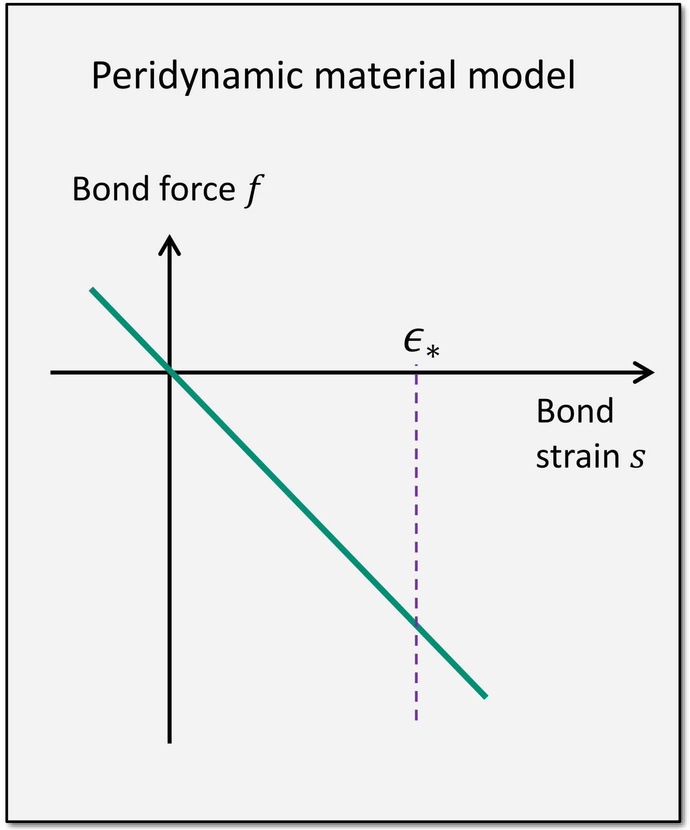
$$\lambda(k) = \sqrt{-\omega^2} \qquad \text{real.}$$

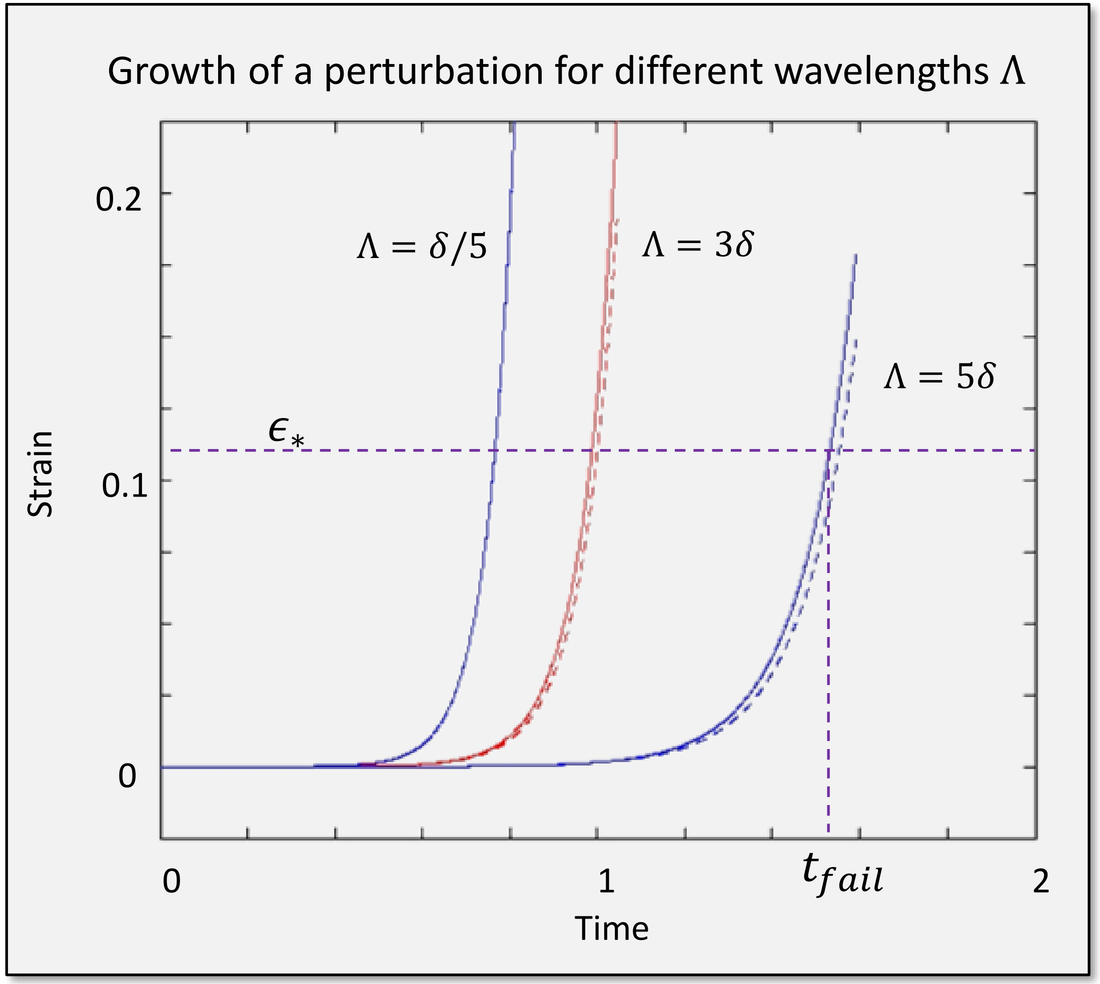
- λ is called the *blow-up rate*.



How much time does it take for an unstable waveform to grow?

- Suppose the material "fails" when the local strain u_x exceeds some given value ϵ_* .

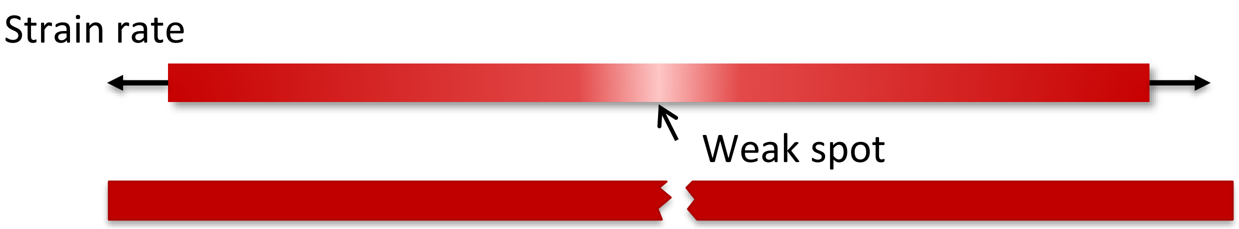


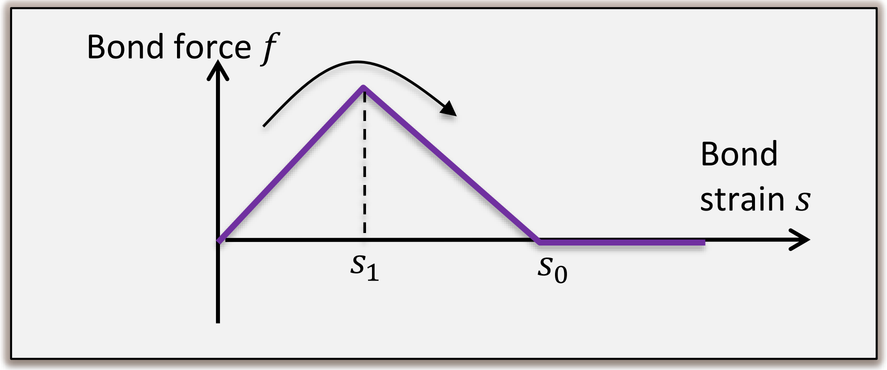


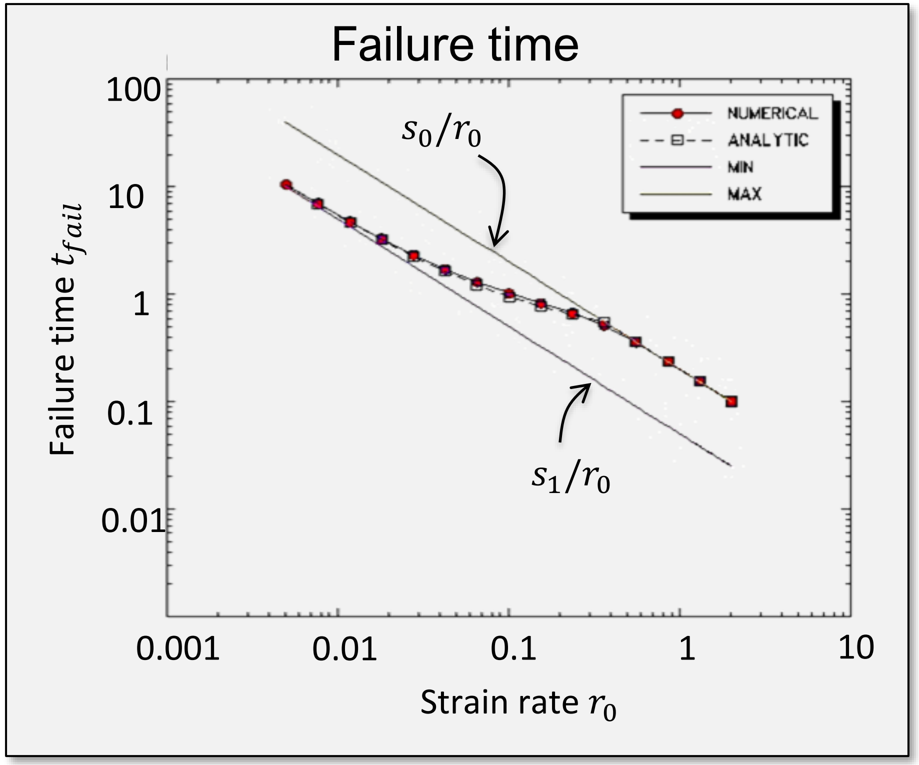
Stretching of a bar: Compute the time to failure

$$t_{fail} \approx \min\left\{\frac{s_0}{r_0}, \left[\frac{s_1}{r_0} + \frac{1}{\lambda_\infty}\log\left(\frac{2(s_0 - s_1)}{h_0(s_1 + r_0/\lambda_\infty)}\right)\right]\right\}$$

$$\lambda_\infty = \sqrt{\frac{-P}{\rho}}$$





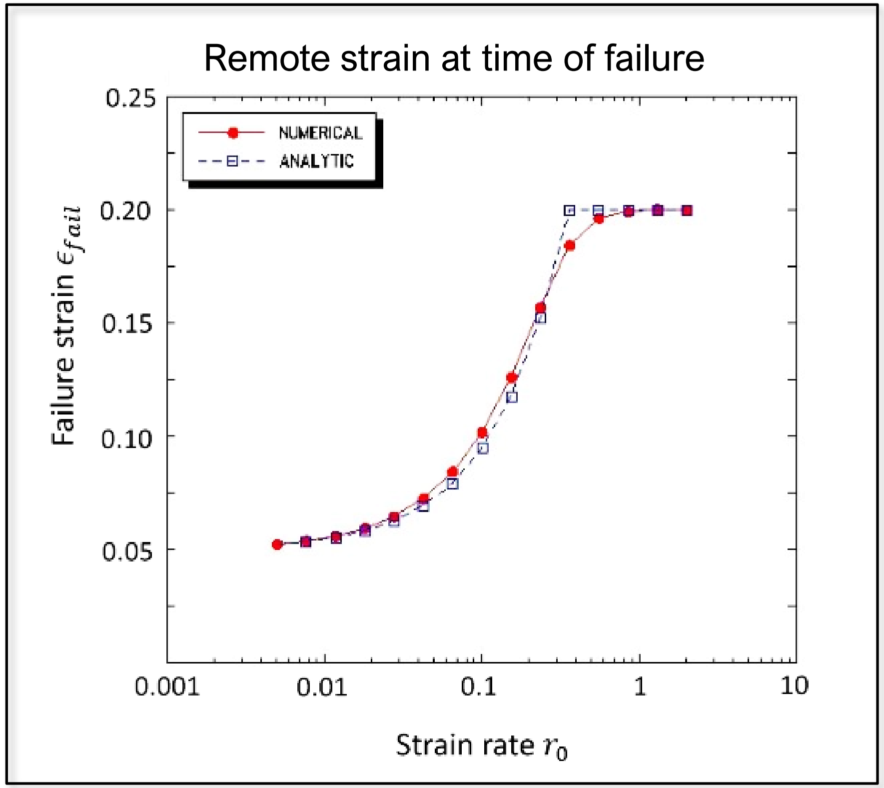


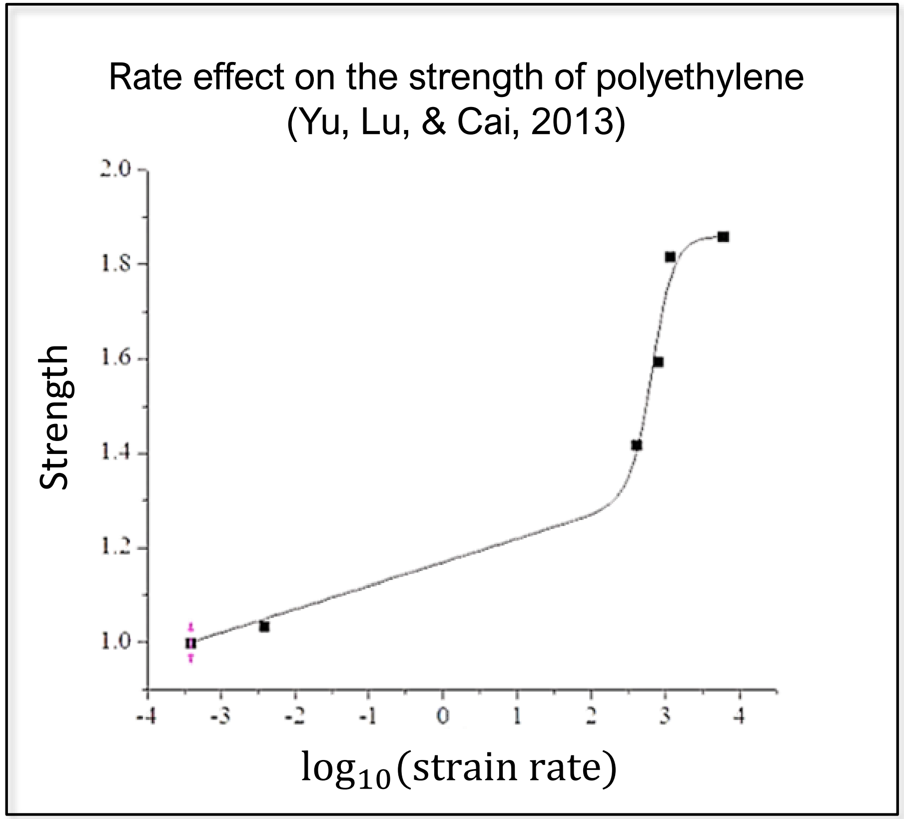
Stretching of a bar: We arrive at a macroscopic rate effect

- It takes time for the bar to fail even after some bonds have crossed the peak.
- Meanwhile, the remote strain is still increasing.
- Result is that higher strain rates lead to higher macroscopic failure strain

$$\epsilon_{fail} = r_0 t_{fail}$$

- Many real materials show a similar trend.

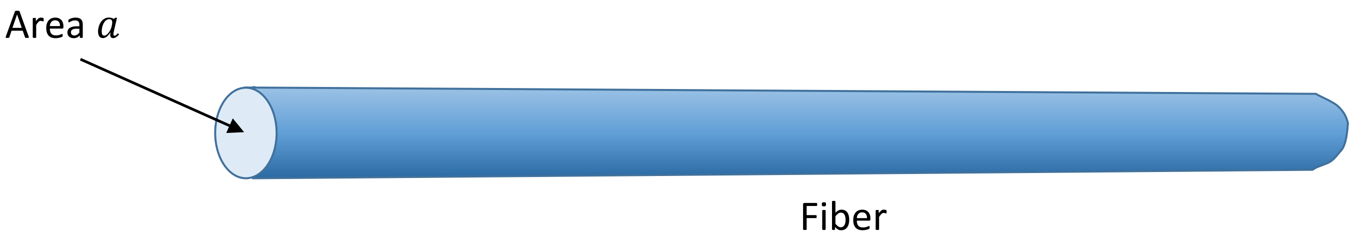


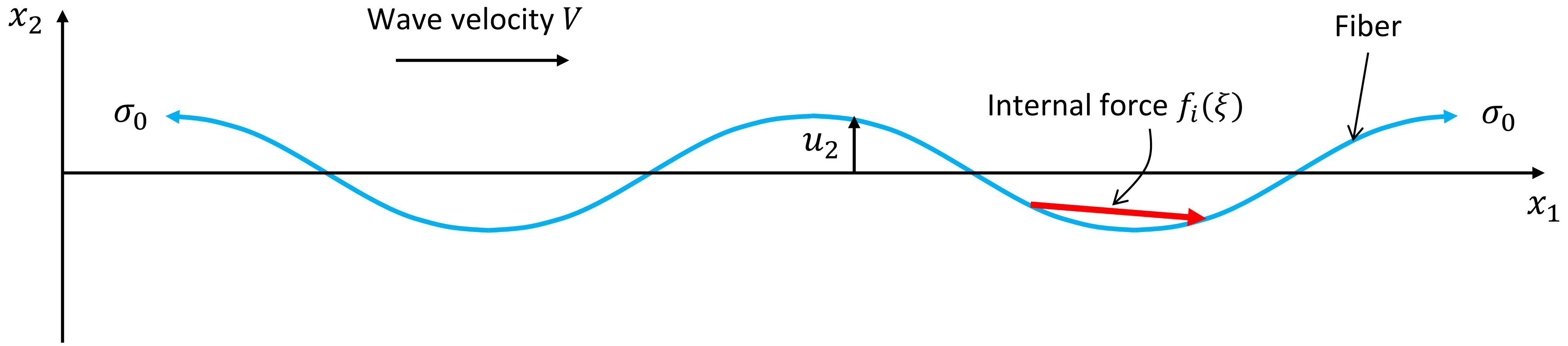


- SS, *Journal of Peridynamics & Nonlocal Modeling* (2021)

Instability due to internal loading in a fiber

- String made of microelastic material
- Constant long-range forces between material points
- Allow rotations (unlike true 1D)
- Study transverse waves and their stability





Internal loading in a fiber accounting for bond rotations

- Recall the 3D momentum balance:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}_\mathbf{x}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\,\mathrm{d}\mathbf{q} + \mathbf{b}(\mathbf{x},t) \qquad \forall \mathbf{x} \in \mathcal{R},\ t \geq 0.$$

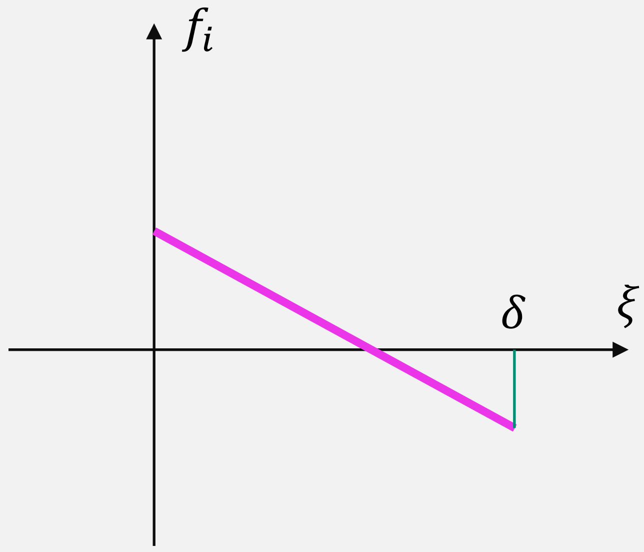
- Allow for bond rotation.

$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = (C(\xi)s + f_i(\xi))\mathbf{M}$$

where s is the bond strain and f_i is the prescibed internal force density in the bond ξ.

- Assume that f_i is self-equilibrated (no net axial stress).

Internal loading as a function of bond length



Transverse waves

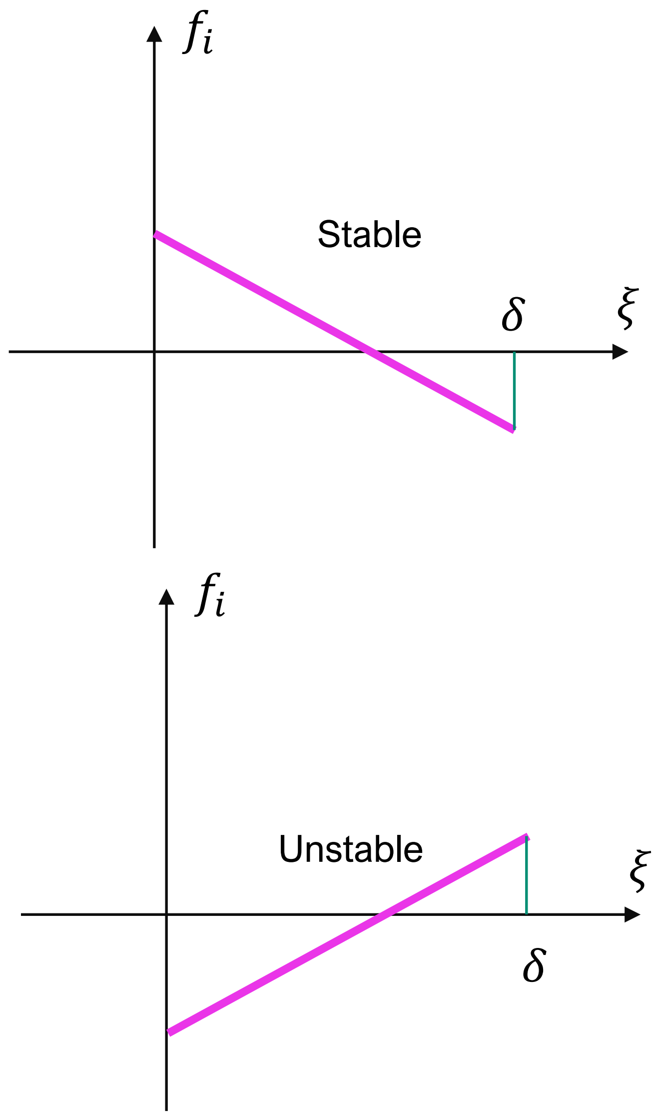
- Assume

$$u_2 = e^{i(kx - \omega t)}.$$

- Repeat derivation of the dispersion curve.

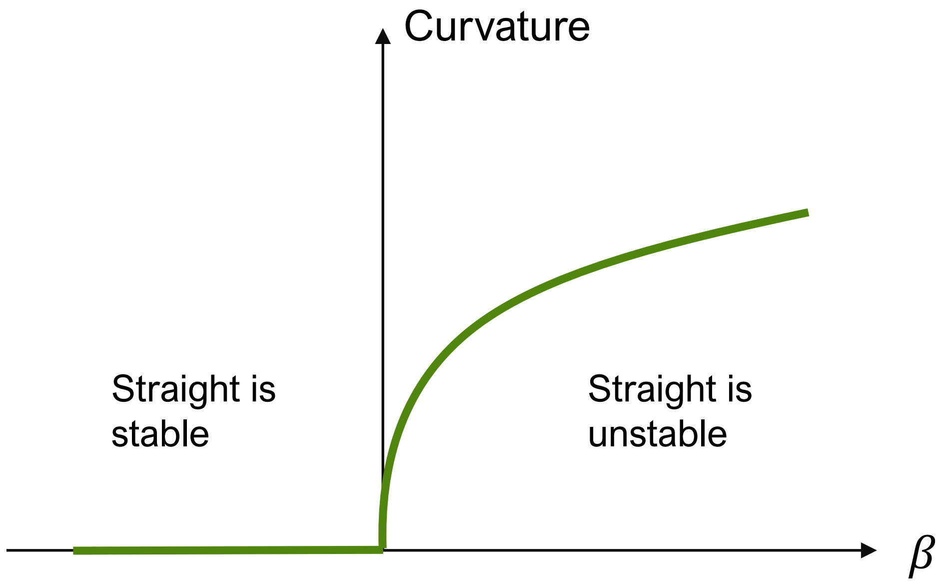
$$\rho\omega^2 = \left[\frac{-a}{12}\int_0^\delta f_i(\xi)\xi^3 \, \mathrm{d}\xi\right] k^4.$$

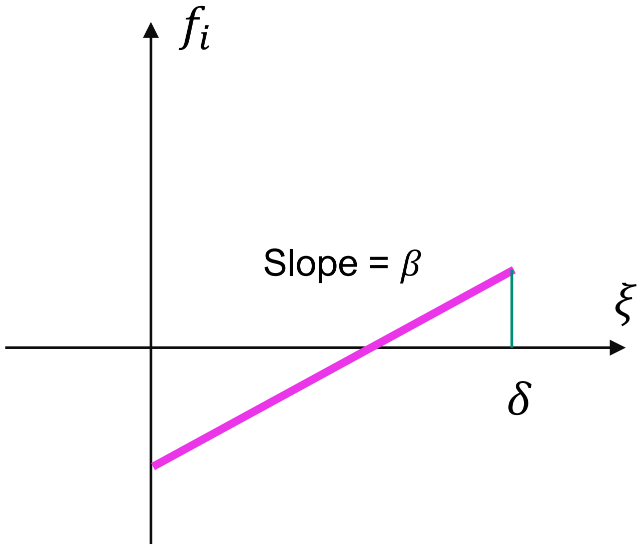
- Long bonds in compression $\implies$ ω is real (stable).
- Long bonds in tension $\implies$ ω is imaginary (unstable).



If a straight fiber is unstable, what does equilibrium look like?

- We can compute* the curvature of a fiber in equilibrium.
- Result:



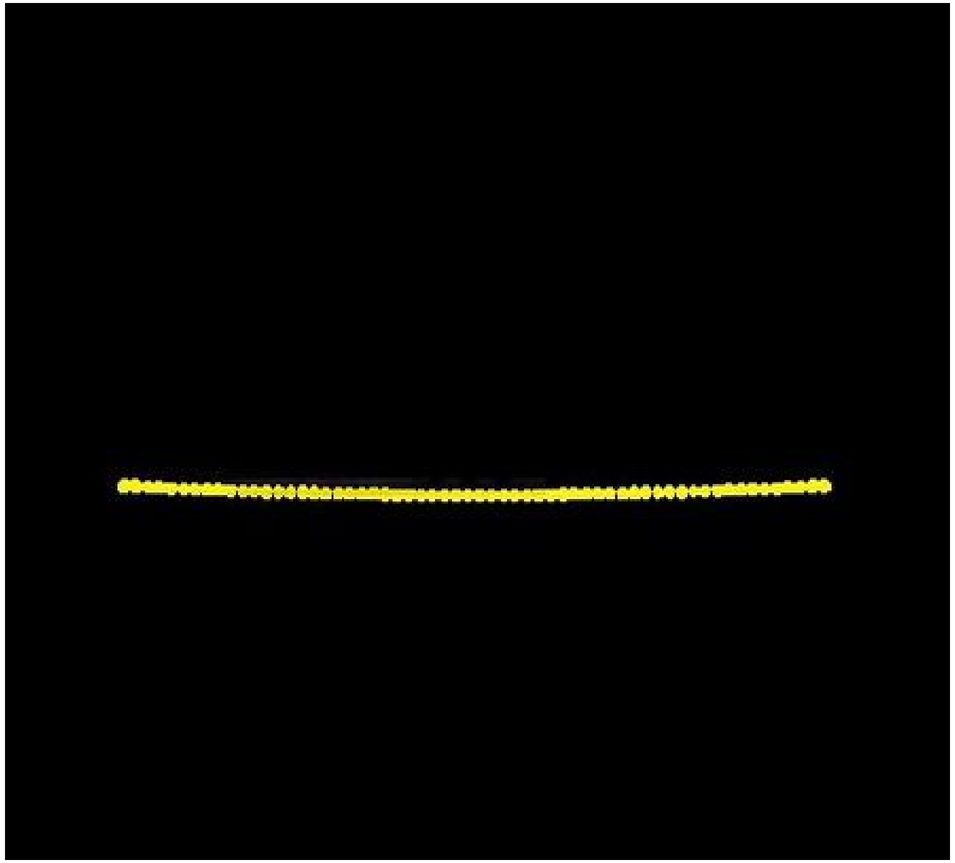


* SS, "Self-induced curvature in an internally loading peridynamic fiber," technical report SAND2022-5539

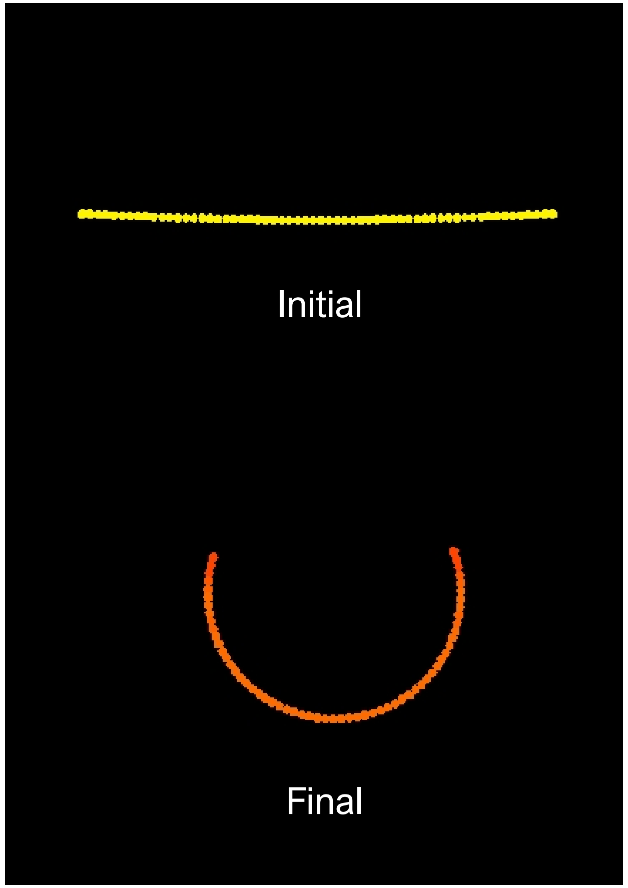
Emu simulation of an internally loaded fiber

- Internal loading is turned on suddenly.

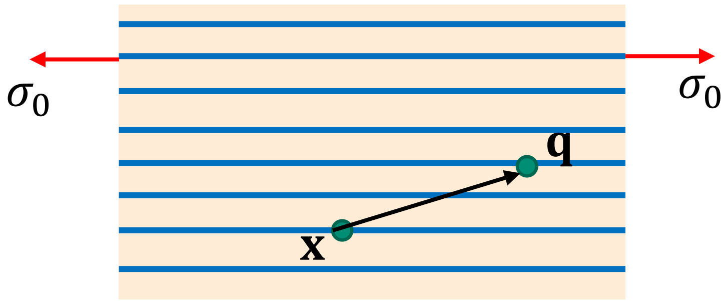
VIDEO



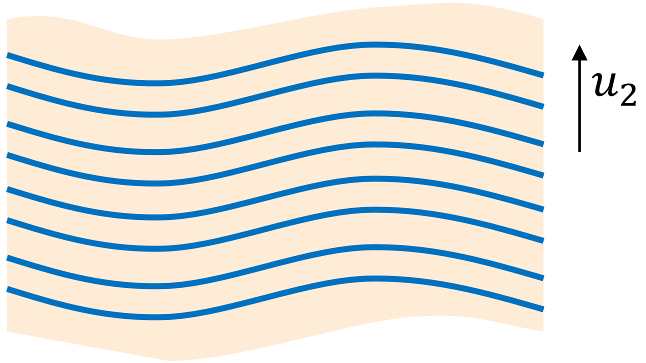
Colors show strain
(red = 0.01)



Homogenized model of many fibers: Kink bands in a fiber-reinforced composite



Fibers in a matrix
Remote loading in fibers is σ_0
Bonds can be either stiff or soft



Transverse wave

- The dispersion relation for transverse waves turns out to be

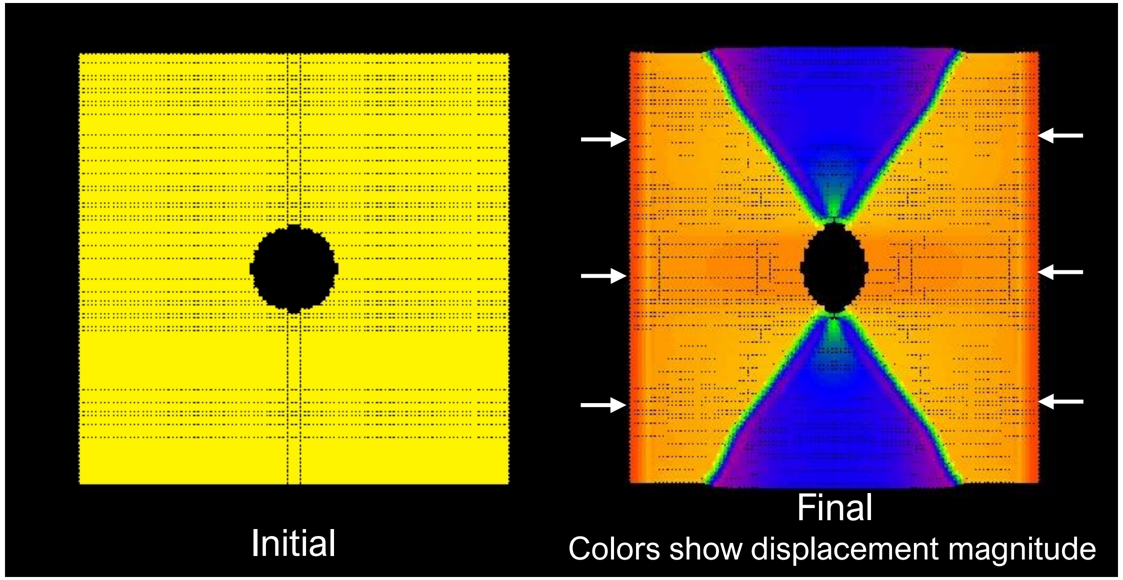
$$\rho\omega^2 = (\sigma_0 + \mu(k))k^2$$

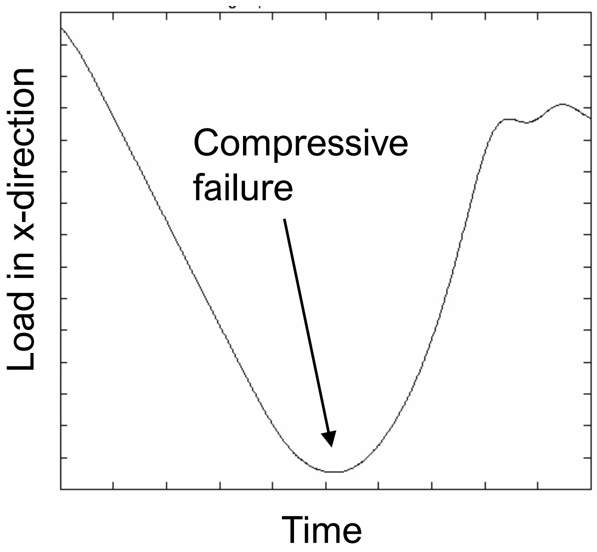
  where $\mu(k)$ characterizes the matrix shear response.

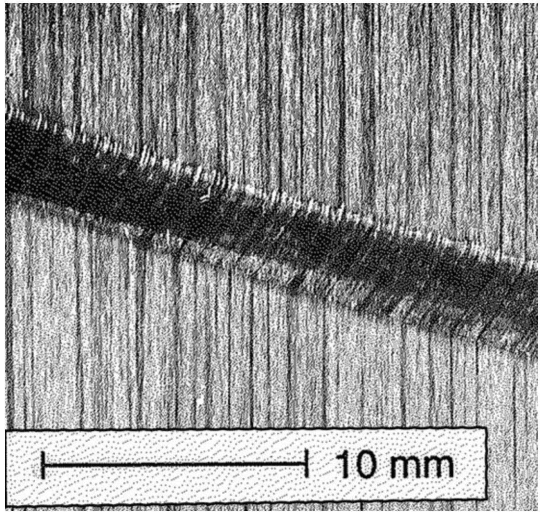
- If the remote loading is compressive ($\sigma_0 < 0$) then ω can be imaginary.

Emu simulation of instability in compression in a composite

- Bonds in the horizontal direction are more stiff than the others.
- Anisotropic, microelastic material model.
- There is no damage (bond breakage) in the peridynamic model.



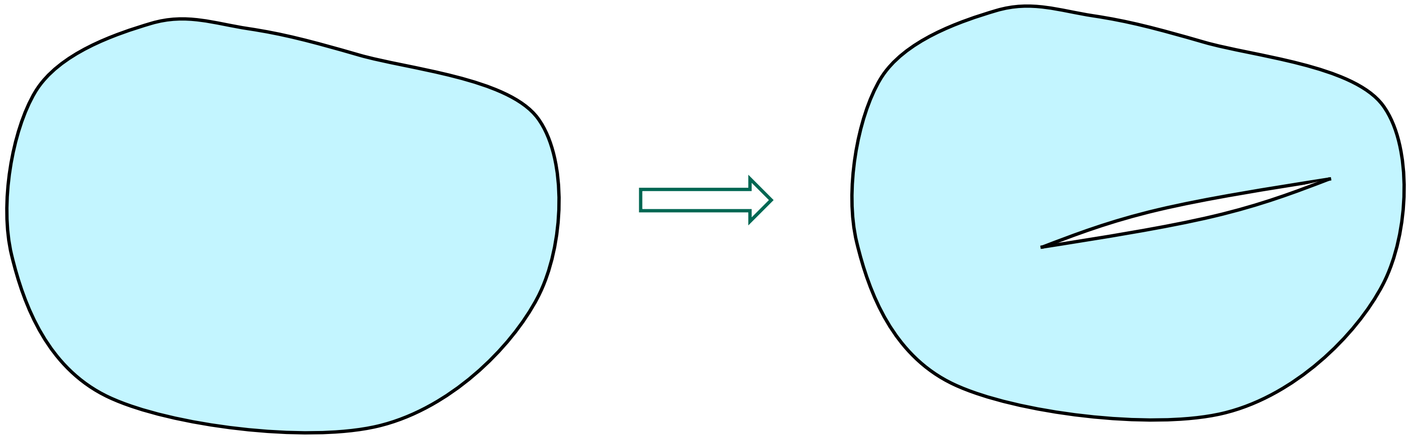




Kink band in a composite
Image: S.P.H. Skovsgard, thesis, 2019

Crack nucleation as a material instability

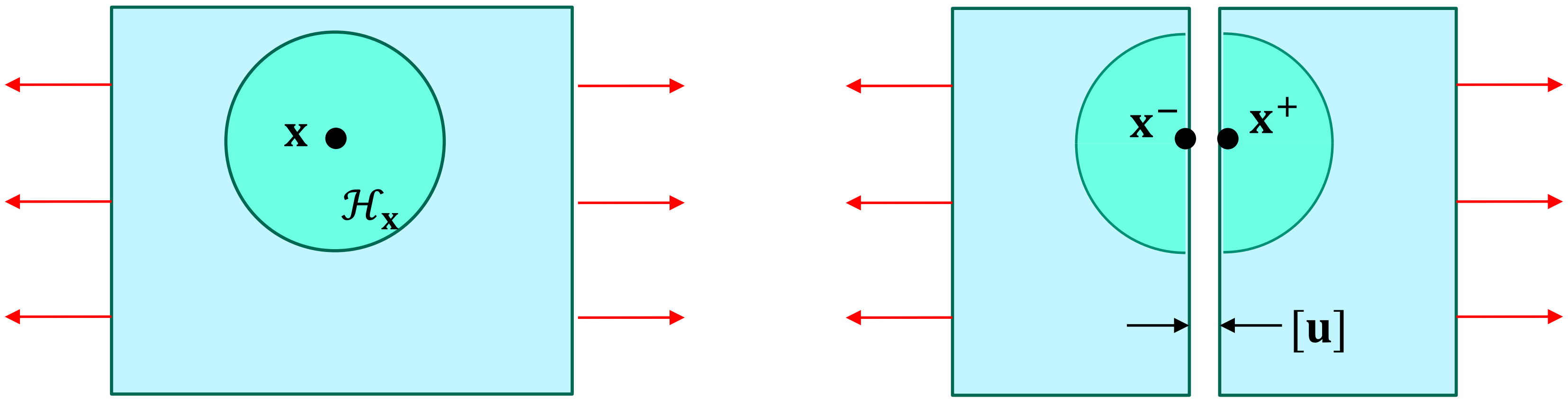
- A body is initially continuous.
- At some later time there is a discontinuity.
- What mathematical conditions need to exist for this to happen?
    - This question is not addressed by fracture mechanics, which assumes a pre-existing defect.



- SS, O. Weckner, E. Askari & F. Bobaru, *Int. J. Fracture* (2010)
- R.P. Lipton, R.B. Lehoucq & P.K. Jha, *J. Peridynamics & Nonlocal Modeling* (2019)

Perturbation by a jump

- Suppose a small virtual discontinuity is inserted into a body under load.
- Does the discontinuity grow or close up?
- Analyze the evolution of the jump $[\mathbf{u}]$.



Perturbation by a jump

- From the momentum balance, find that

$$\rho[\ddot{\mathbf{u}}] = -\left(\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{C}(\boldsymbol{\xi})\ \mathrm{d}\boldsymbol{\xi}\right)[\mathbf{u}] = -\mathbf{P}[\mathbf{u}].$$

- The gap closes up if

$$[\ddot{\mathbf{u}}] \cdot [\mathbf{u}] < 0.$$

- If

$$\mathbf{u}_0 \cdot (\mathbf{P}\mathbf{u}_0) > 0 \qquad \forall \mathbf{u}_0 \neq \mathbf{0}$$

  then a crack cannot form.

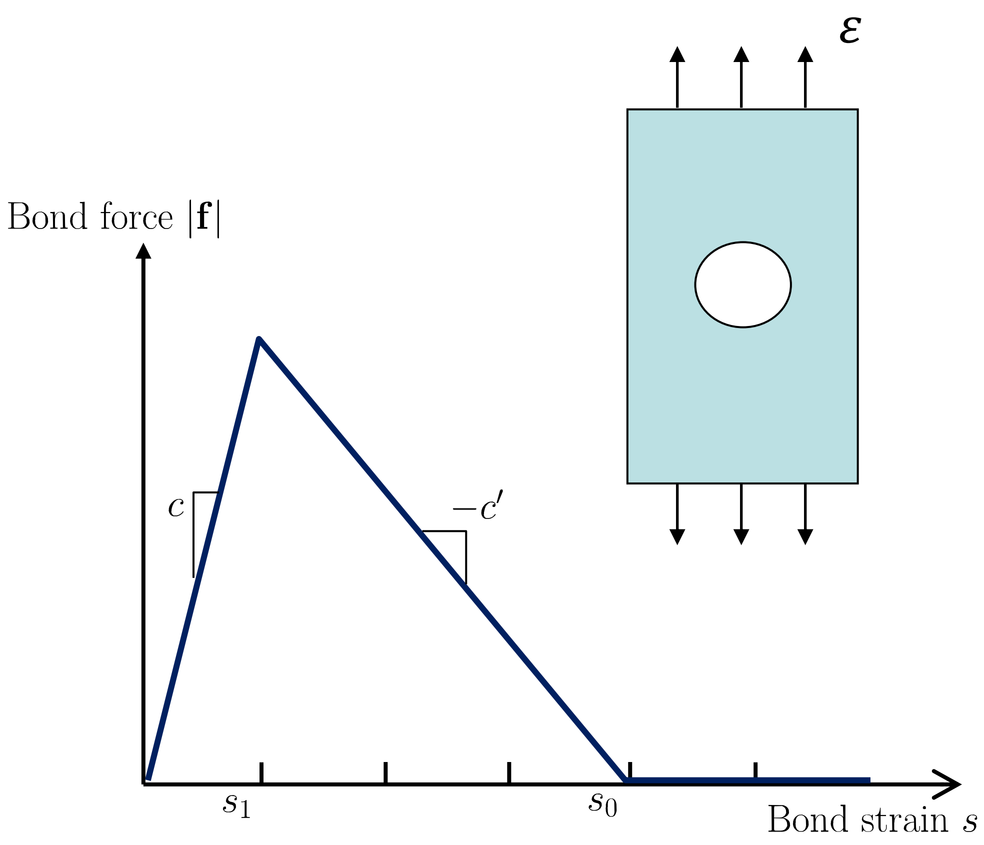
- Let p_1, p_2, p_3 be the eigenvalues of $\mathbf{P}$ (which is symmetric).
- *Stability index*:

$$Z = \min\{p_1, p_2, p_3\}.$$

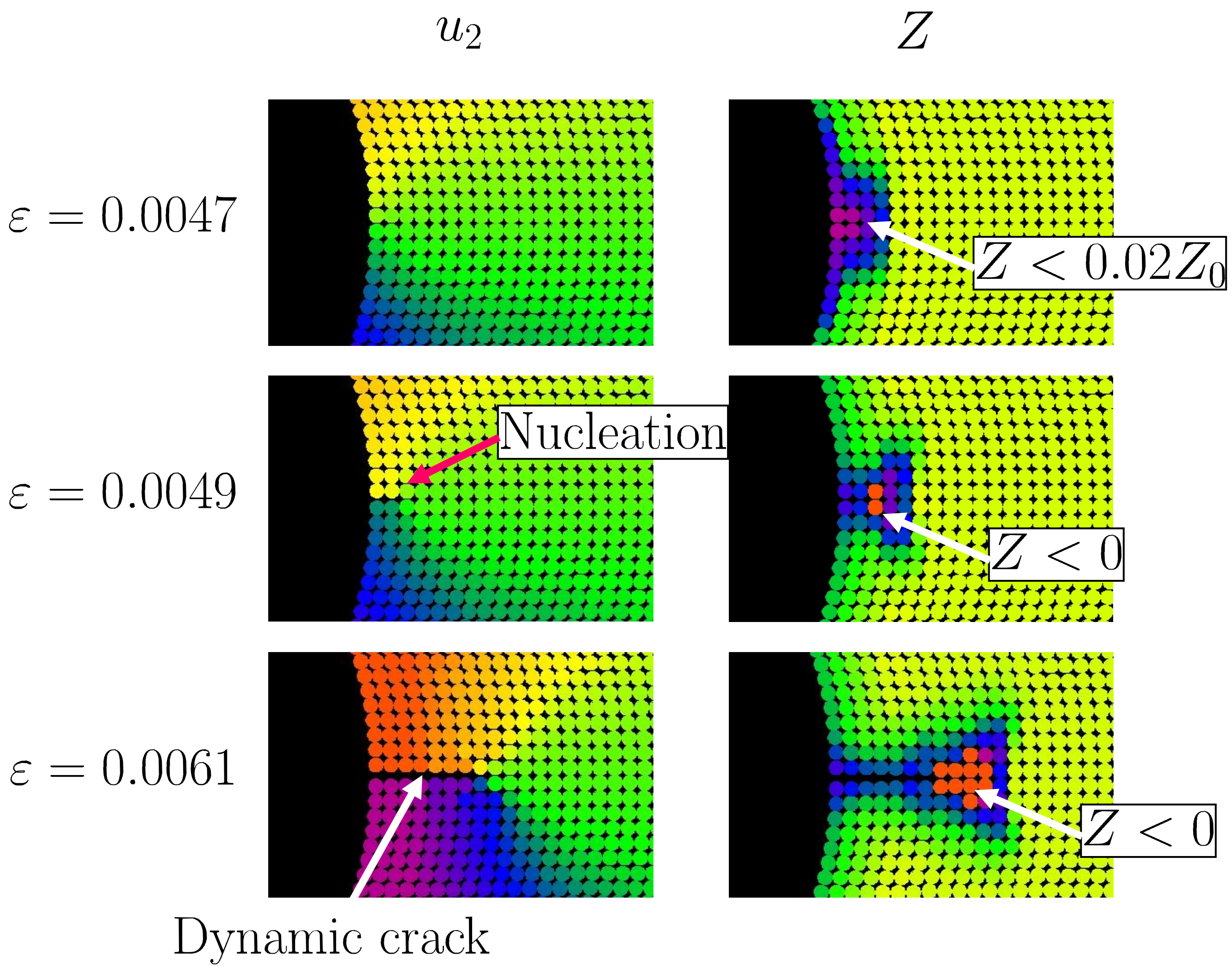
- If $Z \leq 0$, a crack can nucleate. The eigenvector gives the gap displacement.
- The orientation of the crack comes from the underlying stress field.

$Z < 0$ at the crack nucleation site and near a growing crack tip

- There is a process zone near a growing crack tip within which $Z < 0$.

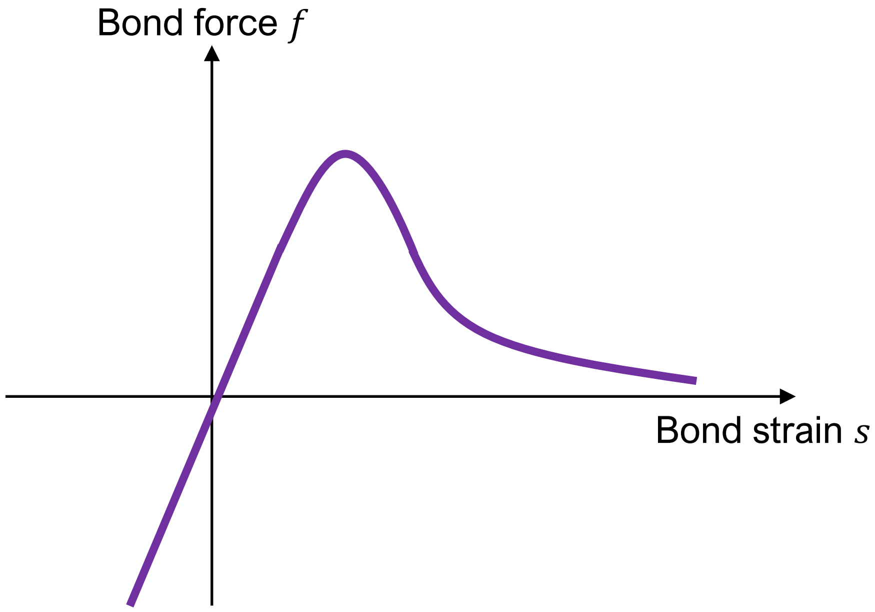


Material model



A nonlocal model of fracture can be well-posed (!)

- Nonconvex elastic peridynamic material.
- Points entering the unstable branch lead to creation of a jump in displacement.
- This discontinuity can grow through the body.
- As it grows, it consumes a definite amount of potential energy per unit crack area (Griffith crack).
- The whole problem can be well-posed.
- These results hold for both static and dynamic cases.



- R.P. Lipton, J. Elasticity (2014)
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- P.K. Jha & R.P. Lipton, SIAM J. Numerical Analysis (2018)
- R. Lipton, E. Said & P.K. Jha - *Handbook of nonlocal continuum mechanics for materials and structures* (2018)
- R.P. Lipton, R.B. Lehoucq & P.K. Jha, *J. Peridynamics & Nonlocal Modeling* (2019)
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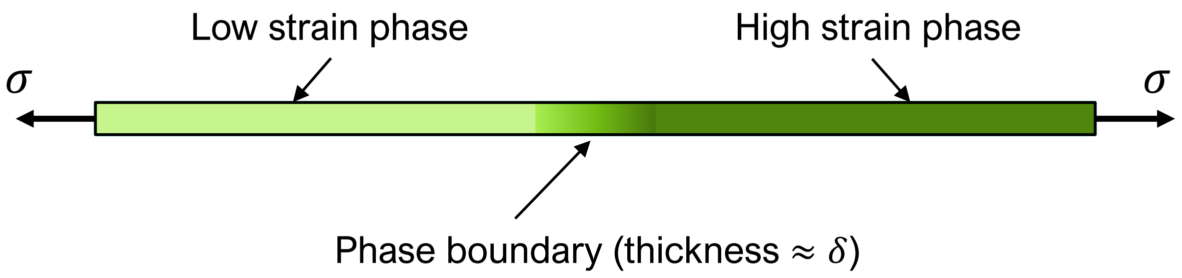
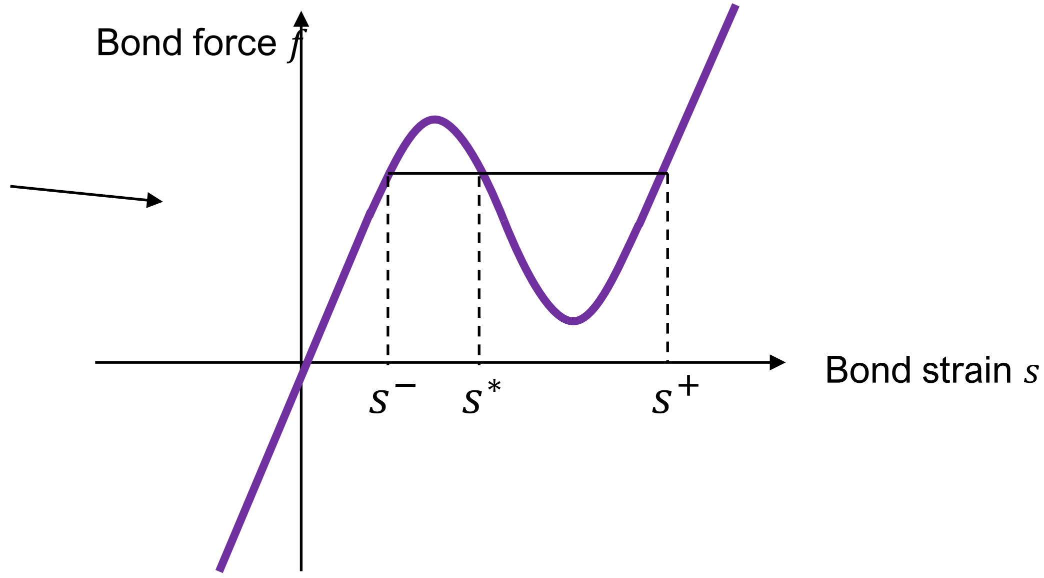
- R.P. Lipton & P.K. Jha, Nonlinear Differential Equations and Applications (2021)

Mechanically induced phase transformation

- Here's another type of nonconvex microelastic material:





- There are multiple bond strains for the same bond force.
- This creates the possibility of multiple phases in a bar in equilibrium.
- Within the phase boundary, there are always some bonds in the unstable part of the material model.

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

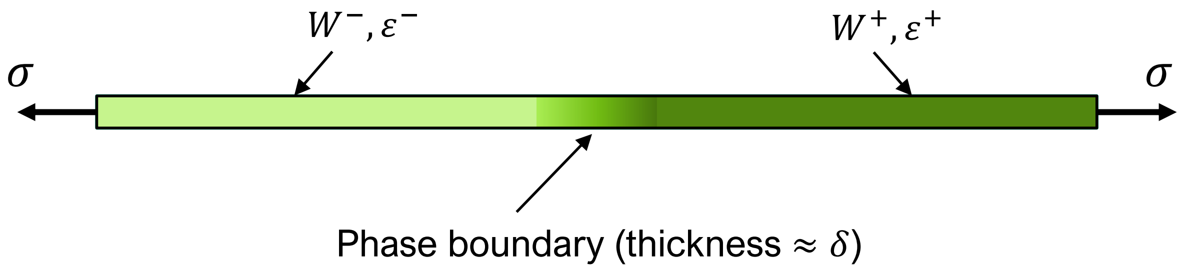
What conditions permit coexistent phases?

- In equilibrium, energy conservation implies

$$W^+ - W^- = (\varepsilon^+ - \varepsilon^-)\sigma$$

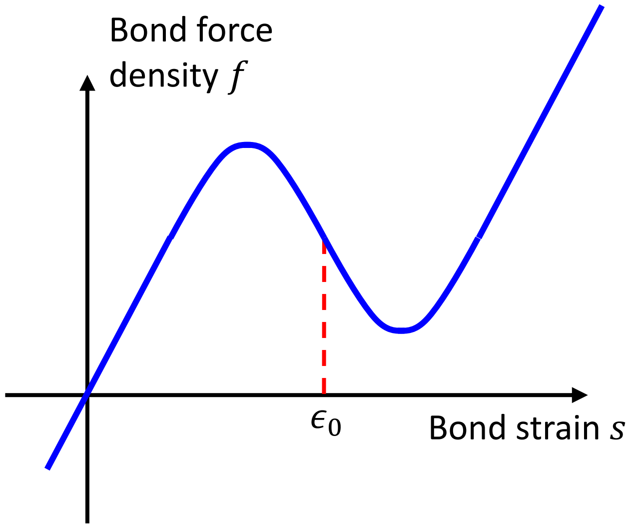
which is formally the same as in the local theory.

- Compare Weierstrass corner condition, Maxwell condition in the calculus of variations.



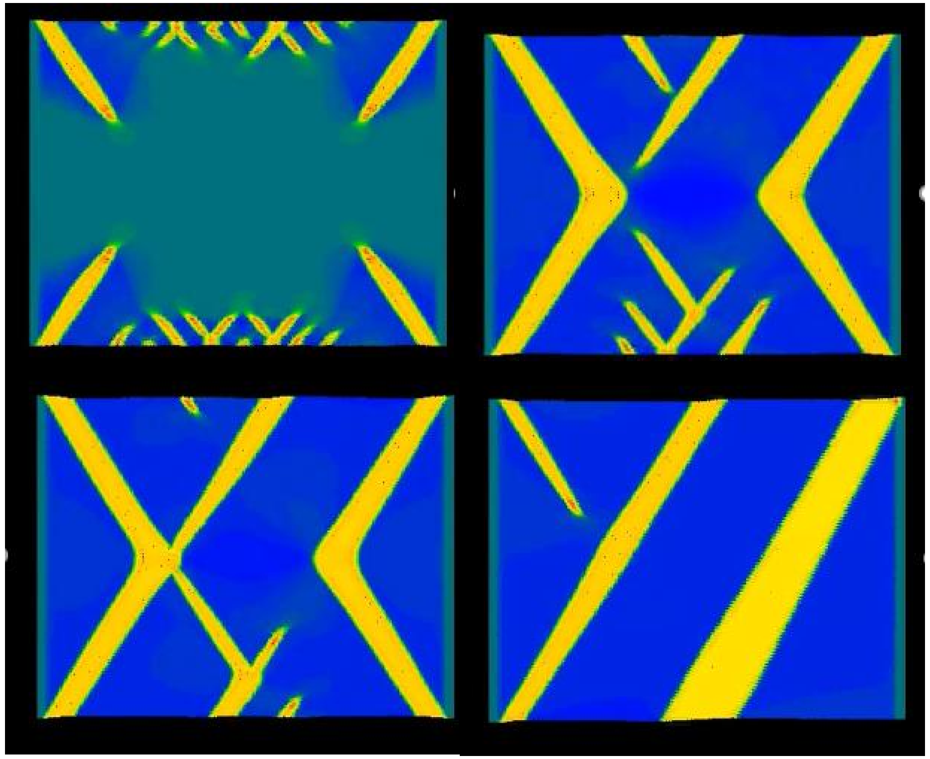
In peridynamics, a phase boundary contains potential energy

- The system evolves over time to reduce the total surface area of phase boundaries.
- We can use this to simulate microstructure evolution.



Microstructure evolution in a plate with initial strain ε_0

Colors show bond strain



Microstructure evolution over time

VIDEO

Microstructure evolution in a plate with initial strain ε_0

Colors show bond strain

Summary

- Nonlocality changes everything about material stability.
- We can do meaningful continuum mechanics within an unstable material.
- We can use this to simulate real phenomena:
  - Rate effect on bulk material strength
  - Fracture nucleation, Griffith criterion
  - Compressive failure modes in composites
  - Microstructure evolution