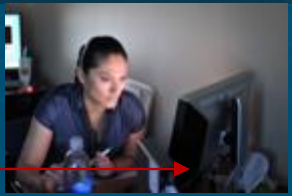
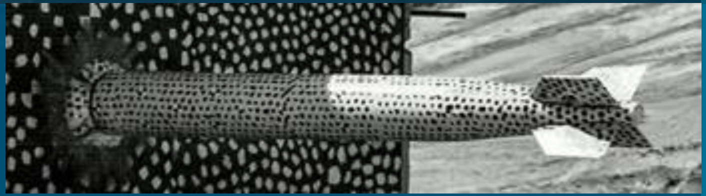
Sandia National Laboratories

Peridynamic modeling of self-shaping in fibers





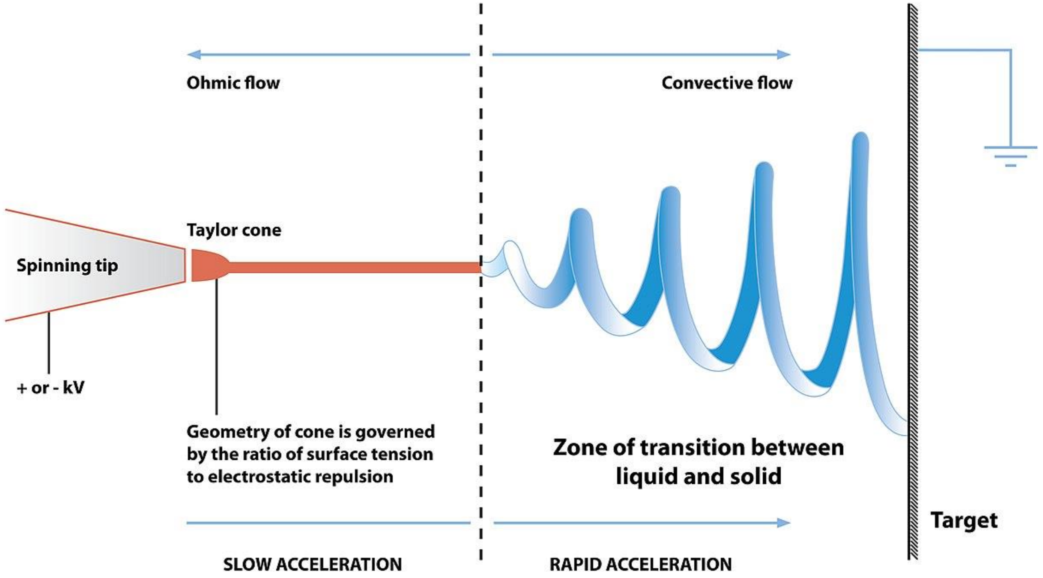
Stewart Silling

January 4, 2023
Joint Mathematics Meetings
Boston, Mass.

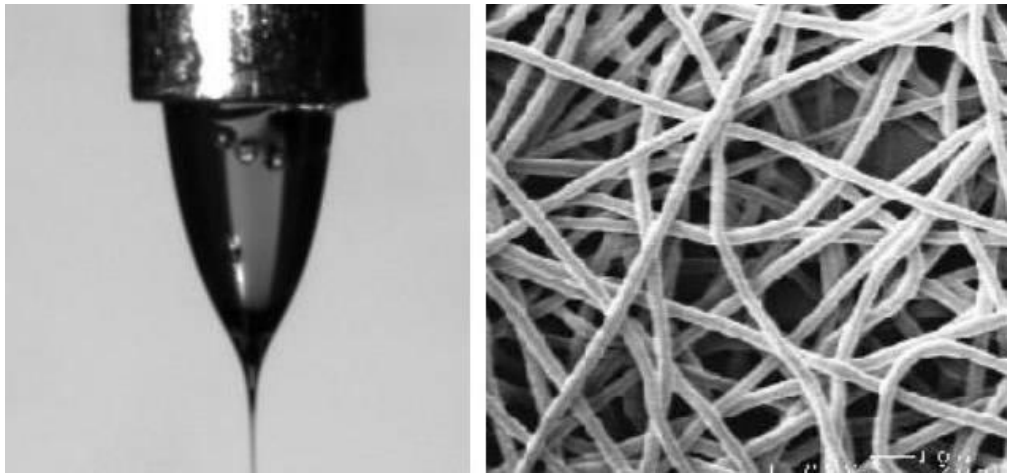
SAND2022-xxxx

Electrospinning

- Method for turning a liquid (such as a polymer) into a solid fiber.
- Applied electrostatic charge makes the liquid want to elongate.
- Process is used a lot to make nanofibers.
- How to model this?



Electrospinning schematic*

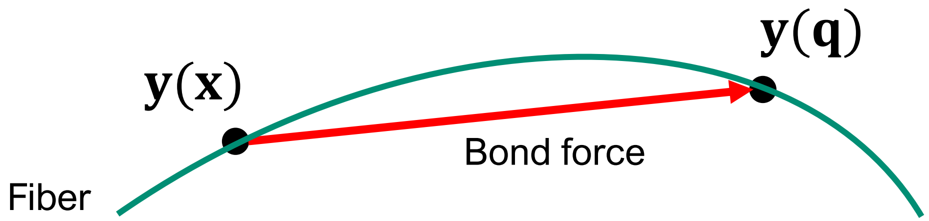


Nanofiber fabrication**

*Joanna Gatford - The New Zealand Institute for Plant and Food Research Ltd, CC BY 3.0, https://commons.wikimedia.org/w/index.php?curid=5521755
** Rutledge Research Group (MIT) https://rutledgegroup.mit.edu/electrospinning-fundamentals/

Outline

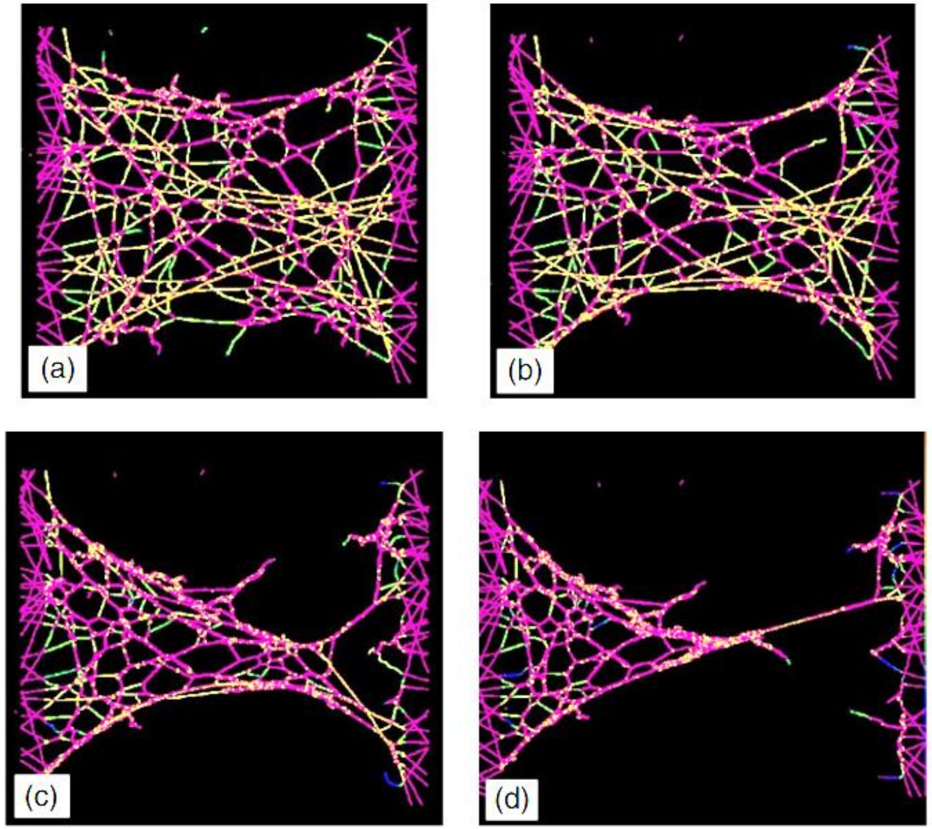
- We'll consider a peridynamic model of a long, thin structure.
  - The structure includes force interactions between points independent of the deformation.
  - These "internal forces" can be included in a nonlocal material model.
  - The equilibrium of the structure is affected by material stability.
  - The minimum energy configuration may or may not be straight.



Long-range forces

- Long-range forces are inherently nonlocal, for example:
  - Electrostatic
  - Van der Waals
  - Surface forces
  - Interatomic and intermolecular forces
- Molecular dynamics: All forces are explicitly nonlocal.

- **This talk: Long-range forces within a single structure.**



Fracture of nanofiber network held together by Van der Waals forces*.

*F. Bobaru, *Modelling and Simulation in Materials Science and Engineering* (2007).

Some concepts of stability (local theory)

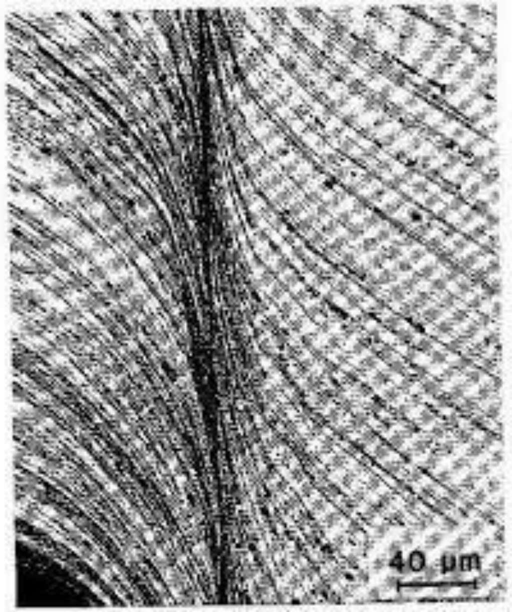
- Real wave speeds (Hadamard stability, strong ellipticity)
- Minimum potential energy
- Bifurcations
- Well-posedness*
- Discontinuity in gradient (Ordinary ellipticity)

*Summary of well-posedness result for nonlocal theories: see:

- Qiang Du, "Nonlocal calculus of variations and well-posedness of peridynamics." *Handbook of peridynamic modeling*. (2016)
- R. Lipton's papers on nonconvex strain energy in crack nucleation.

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
- We'll see that this distinction becomes less useful in a nonlocal model.



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

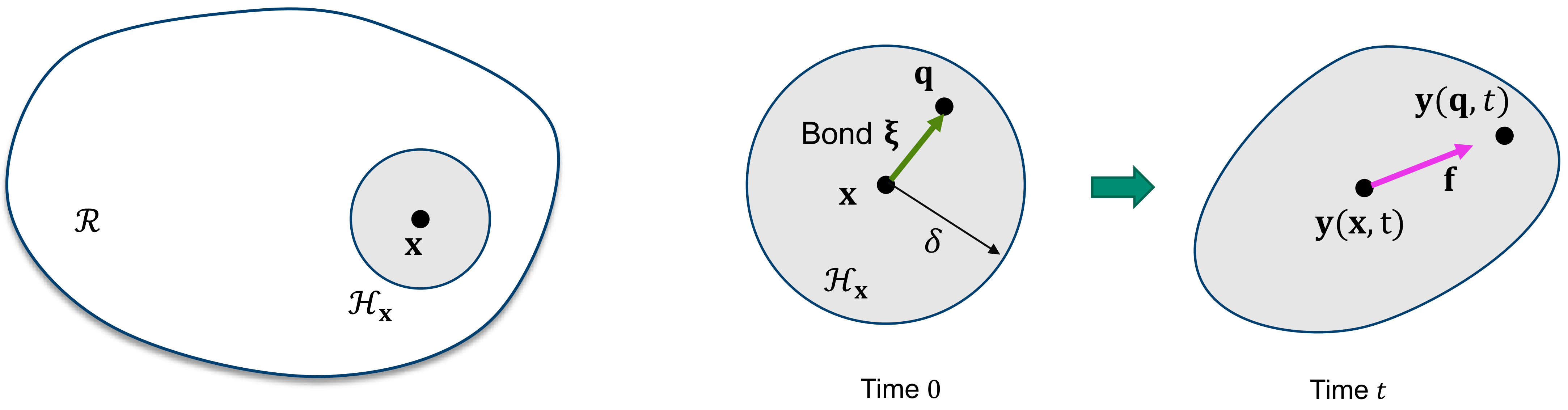
Buckling of a column
image: Klimchik
www.researchgate.net/figure/Examples-of-buckling-in-column-www-civildb-www-highline_fig11_281183936

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 deformation and rotation

- $\mathbf{y}$ = deformation map, $\mathbf{u}$ = displacement vector,

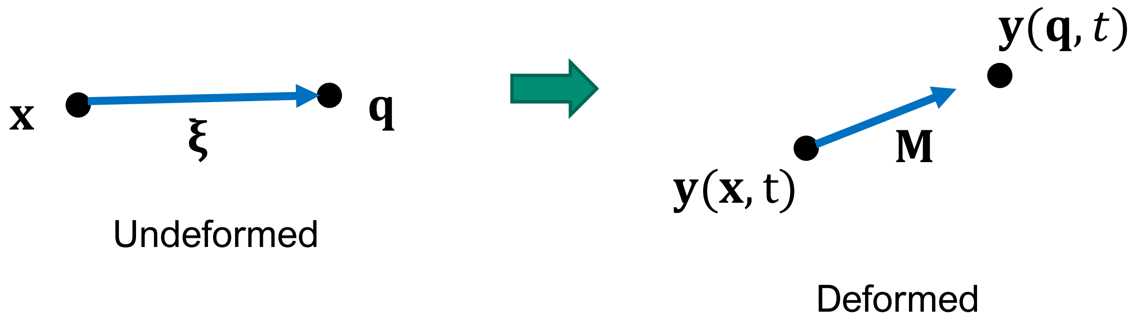
$$\mathbf{y}(\mathbf{x},t)=\mathbf{x}+\mathbf{u}(\mathbf{x},t).$$

- $\boldsymbol{\xi}$ = bond, p = deformed bond length, s = bond strain:

$$p=|\mathbf{y}(\mathbf{x}+\boldsymbol{\xi},t)-\mathbf{y}(\mathbf{x},t)|, \qquad s=\frac{p}{|\boldsymbol{\xi}|}-1.$$

- $\mathbf{M}$ = deformed bond direction vector:

$$\mathbf{M}=\frac{\mathbf{y}(\mathbf{x}+\boldsymbol{\xi},t)-\mathbf{y}(\mathbf{x},t)}{p}.$$



Linear bond force model

- Each bond has a *micropotential*:

$$w(s, \boldsymbol{\xi}) = \frac{c(\boldsymbol{\xi})}{2} |\boldsymbol{\xi}| s^2$$

where $c(\boldsymbol{\xi})$ is the bond micromodulus.

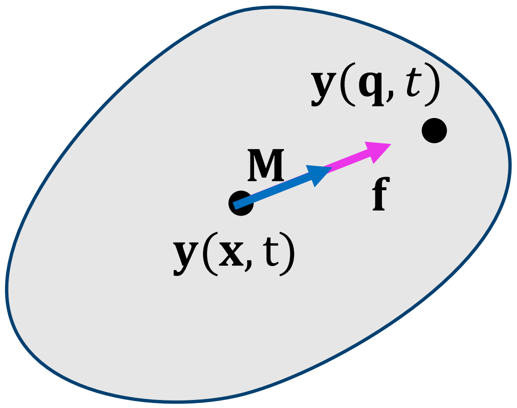
- The strain energy density at $\mathbf{x}$ is

$$W(\mathbf{x}) = \frac{1}{2} \int_{\mathcal{H}} w(s, \boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}.$$

- The bond force for this material is

$$\mathbf{f}(\mathbf{q}, \mathbf{x}) = c(\boldsymbol{\xi}) s \mathrm{M}.$$

- The model is linear in strain but accounts for large rotations.



Deformed

Linear bond force model with internal force

- Quadratic micropotential led to a bond force that was linear in strain.
- Now a term that is linear in bond strain:

$$w(s, \boldsymbol{\xi}) = \frac{c(\boldsymbol{\xi})}{2}|\boldsymbol{\xi}|s^2 + f_i(\boldsymbol{\xi})|\boldsymbol{\xi}|s.$$

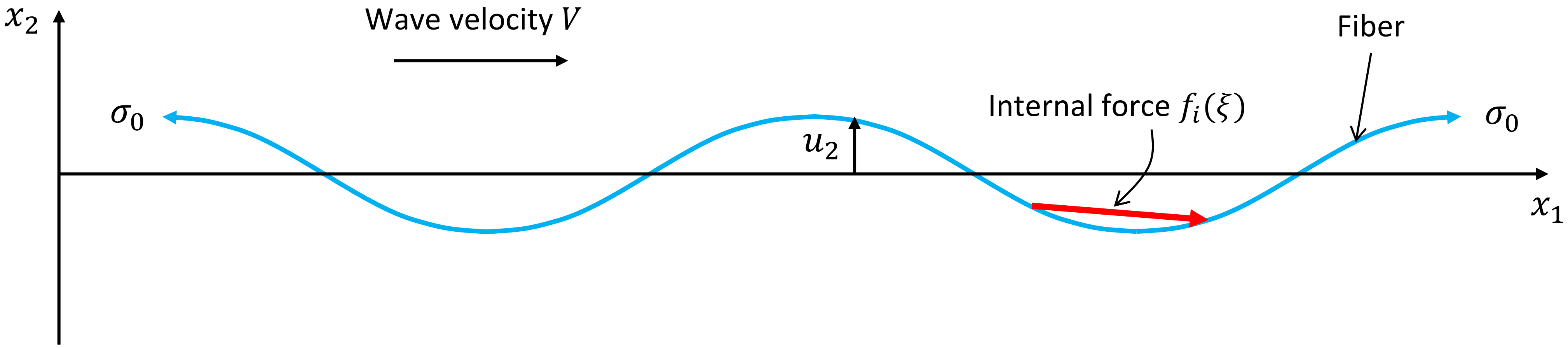
  where $f_i(\boldsymbol{\xi})$ is independent of the deformation.
- The new term leads to

$$\mathbf{f}(\mathbf{q}, \mathbf{x}) = \big(c(\boldsymbol{\xi})s + f_i\big)\mathbf{M}.$$

- So the new force is independent of bond strain but rotates with the bond.

Fiber with internal forces

- Fiber is initially along the x_1 axis.
- It can have both u_1 and u_2 displacement components.
- It can have a remotely applied axial stress σ.
- Study transverse waves and their stability.



Transverse waves in the fiber

- Assume a wave of the form

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

where k is the wavenumber and ω is the (angular) frequency.

- The deflection leads to bond rotations:

$$M_2 = \frac{u_2(x_1+\xi, t) - u_2(x_1, t)}{|\xi|}.$$

- The balance of momentum in the transverse direction becomes

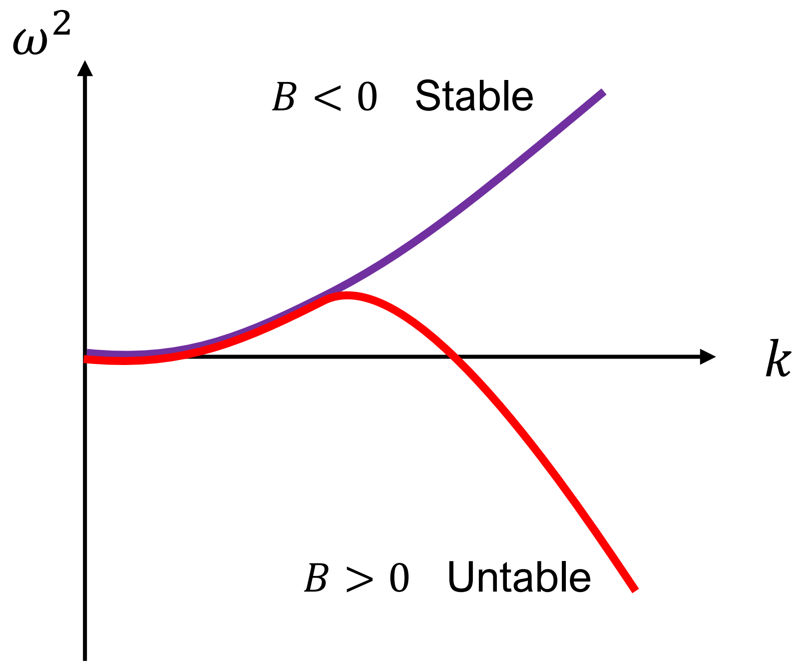
$$\rho \ddot{u}_2(\mathrm{x}, t) = a \int_{-\delta}^{\delta} f_2(x_1+\xi, x_1, t)\, \mathrm{d}\xi.$$

- The dispersion relation for long waves turns out to be

$$\rho\omega^2(k) = \sigma_0 k^2 - Bk^4$$

where

$$B = \frac{a}{12} \int_0^{\delta} (c(\xi)\varepsilon_0 + f_i(\xi))\xi^3\, \mathrm{d}\xi.$$



Dispersion curves

The forms of $c(\xi)$ and $f_i(\xi)$ determine the stability of the fiber

- Example: Assume a material in which c is constant but f_i varies linearly with bond length ξ as shown.

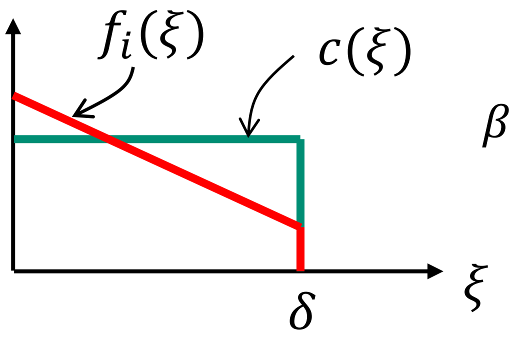
$$c(\xi) = 1, \qquad f_i(\xi) = \eta + \beta\left(\frac{\xi}{\delta} - \frac{2}{3}\right)$$

where η and β are constants.

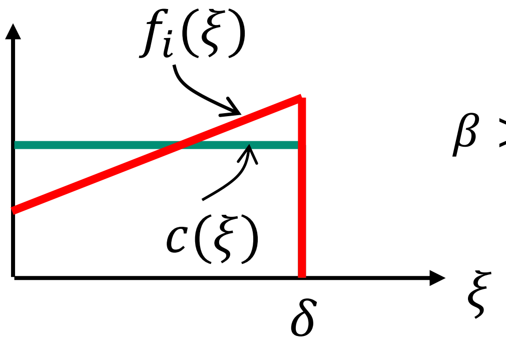
- Set $\sigma_0 = 0$ (fiber is floating in space). Then

$$\rho\omega^2(k) = \frac{a\delta^4}{360}\beta k^4.$$

- $\beta < 0 \implies$ stable (f_i more compressive for long bonds).
- $\beta > 0 \implies$ unstable (f_i more tensile for long bonds).



$\beta < 0$ Stable



$\beta > 0$ Untable

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

- Suppose the fiber is unstable. Try to find the equilibrium curvature. Define

$$\kappa = \frac{1}{r^2}$$

  where r is any radius of curvature.

- Let ε_0 be the axial strain in the *straight* fiber (known).
- Let ε be the axial strain in the *curved* fiber.
- Both ε and κ are unknown.
- Compute the strain energy at any point in terms of these unknowns:

$$W = W_0 + \sigma_0\varepsilon - A_1\kappa + A_2\varepsilon^2 + A_3\kappa^2 - A_4\varepsilon\kappa$$

  where

$$W_0 = a\varepsilon_0 \int_0^\delta \left[\frac{c(\xi)}{2}\varepsilon_0 + f_i(\xi)\right] \xi \, \mathrm{d}\xi, \qquad A_1 = \frac{a\lambda_0^3}{24}\int_0^\delta \left[c(\xi)\varepsilon_0 + f_i(\xi)\right] \xi^3 \, \mathrm{d}\xi,$$

$$A_2 = \frac{a}{2}\int_0^\delta c(\xi)\xi \, \mathrm{d}\xi = \frac{E}{2}, \qquad A_3 = \frac{a\lambda_0^5}{1920}\int_0^\delta \left[c(\xi)\left(\frac{5\lambda_0}{3} + \varepsilon_0\right) + f_i(\xi)\right] \xi^5 \, \mathrm{d}\xi,$$

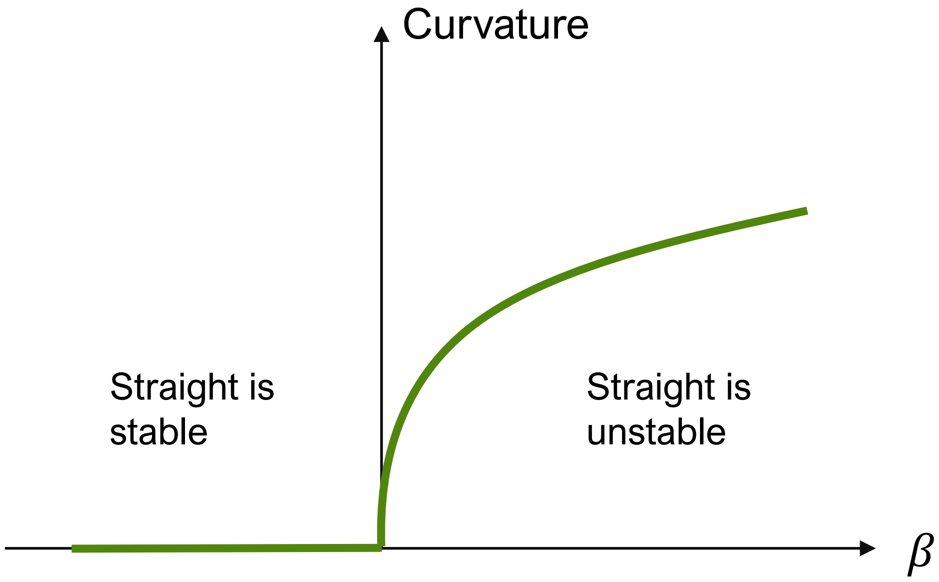
$$A_4 = \frac{a\lambda_0^2}{8}\int_0^\delta \left[c(\xi)\left(\frac{\lambda_0}{3} + \varepsilon_0\right) + f_i(\xi)\right] \xi^3 \, \mathrm{d}\xi.$$

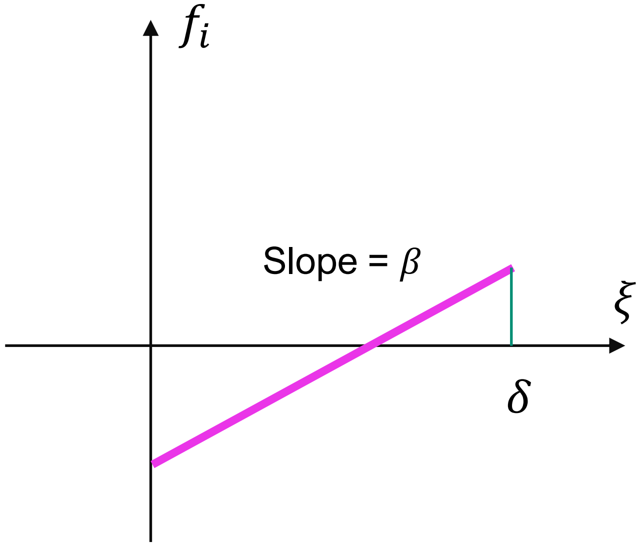
If a straight fiber is unstable, what does equilibrium look like?

- For a given material, find the ϵ and κ that minimize W:

$$\kappa_{eq} = \max\left\{0, \frac{EA_1}{2EA_3 - A_4^2}\right\}, \qquad \varepsilon_{eq} = \frac{A_4 \kappa_{eq}}{E}$$

where E is the Young's modulus.

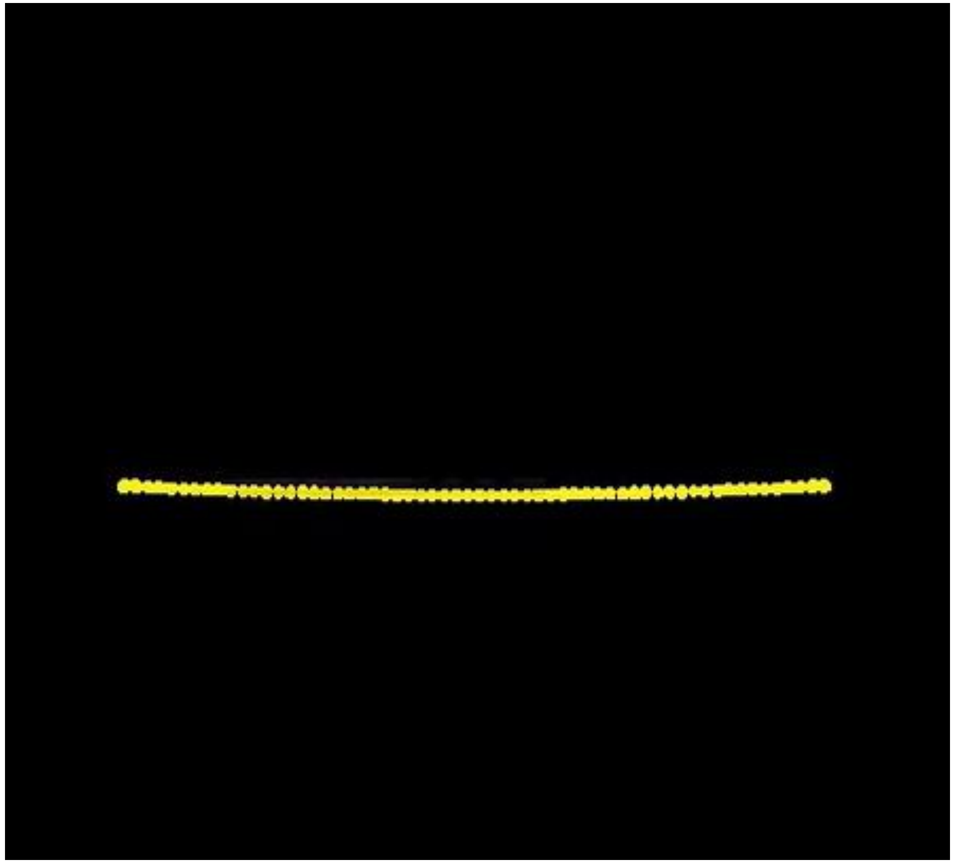




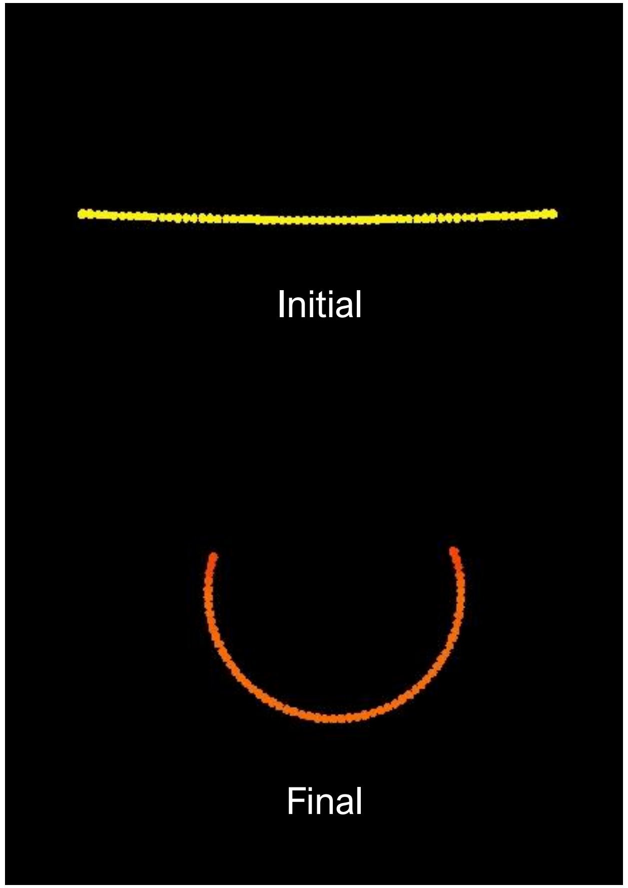
Emu simulation of an internally loaded fiber

- Internal loading is turned on suddenly.

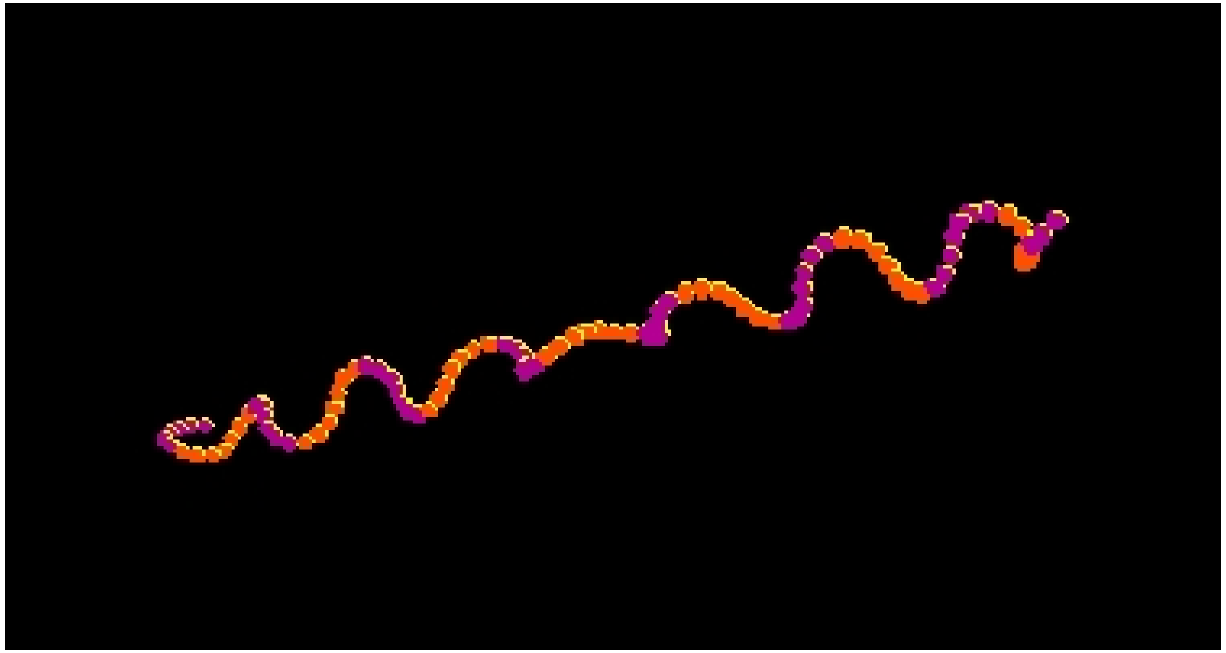
VIDEO



Colors show strain
(red = 0.01)



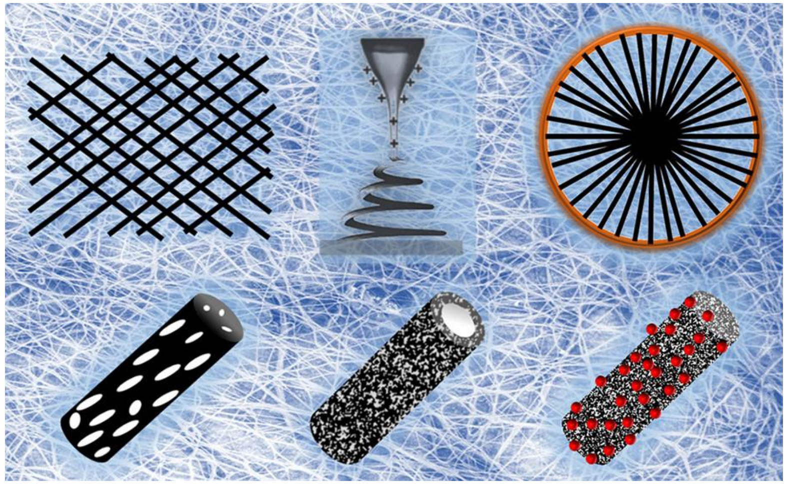
More complex internal loading leads to more complex shapes



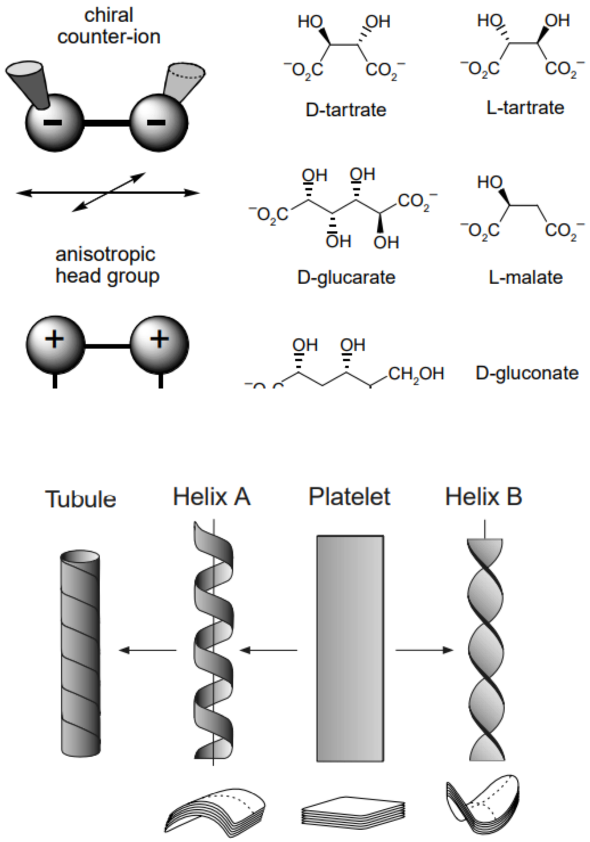
- Purple and red attract.
- Purple repels purple.
- Red repels red.

Possible uses

- There is a lot of interest in self-assembly of nanomaterials.
- Extending the model to an Eulerian description would be the next step.***



Concepts for structures built up by manipulating charge and composition in electrospun nanofibers*



Chemical composition of a ribbon induces internal forces**

*J. Xue et al., *Acc. Chem. Res.* (2017)
** R. Oda et al., *Nature* (1999)
*** SS et al., *Int. J. Impact. Engin.* (2017)

Conclusions

- Peridynamics allows long-range forces that can change the shape of a structure.
- The internal forces compete with the elastic bond response in determining the stability of the system.
- In simple cases, the equilibrium curvature can be computed explicitly.

This work:
SS, Self-Induced Curvature in an Internally Loaded Peridynamic Fiber, SAND2022-5539 (2022).