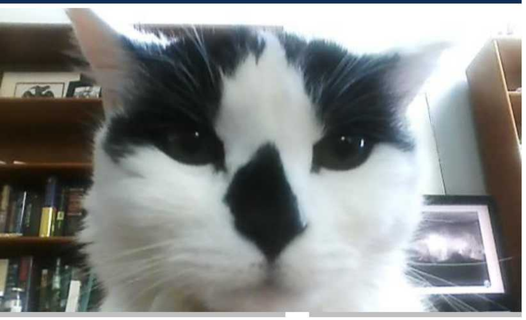
SAND2016-10804PE

Application of peridynamics to large deformations and soft materials



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Mechanical and Nuclear Engineering Seminar
Virginia Commonwealth University
October 21, 2016

Sandia National Laboratories

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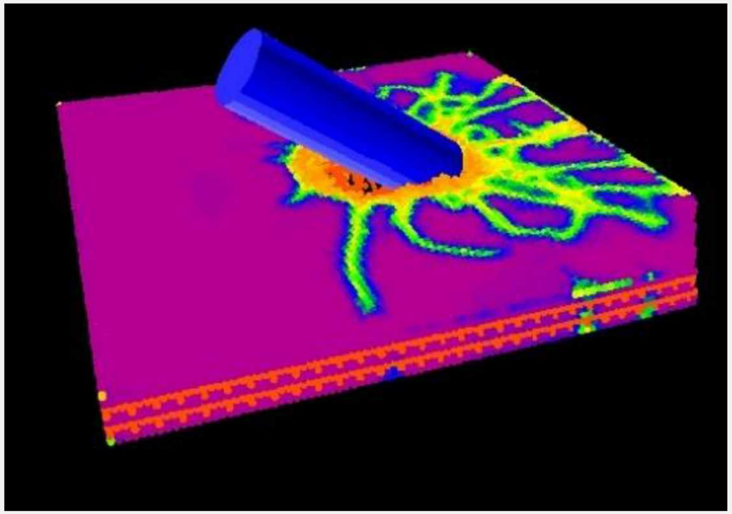
Outline

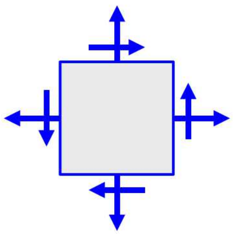
- Peridynamics background
  - Damage and fracture
- Geometric nonlinearity
  - Rubbery materials
- Thermodynamics and long-range forces
- Eulerian material models
  - Fluids and surface tension
  - Contact, friction, and wear
- Combining Lagrangian and Eulerian models
  - Gelatin
  - Bird strike simulant



Traditional application of peridynamics: Elastic-brittle material

Traditional solid mechanics

- The traditional mathematical model for solids and structures uses partial differential equations (PDEs):



$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + b_x = 0$$
$$\frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + b_y = 0$$

where $\sigma_{xx}\ldots$ are the stress components and b_x, b_y are the external loads.

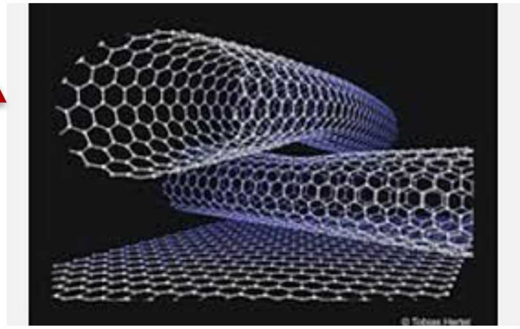
Augustin-Louis Cauchy, 1840

- Is this model up to the job of predicting material failure? Key assumptions:
- Contact forces
- Continuity

NO!

Fracture and fragmentation

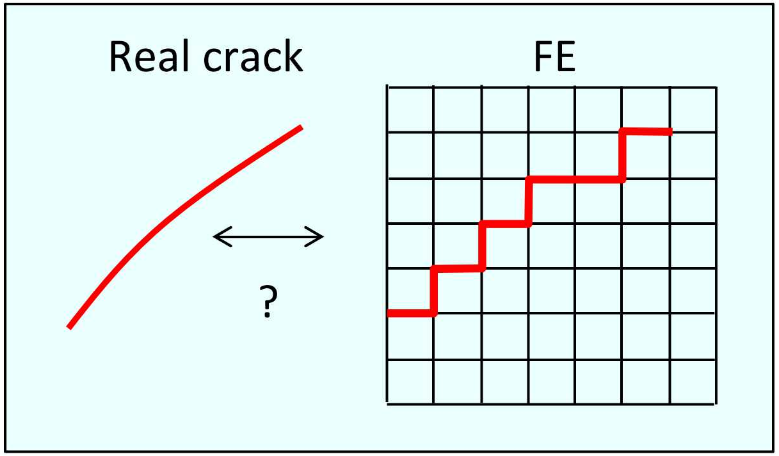
NO!



Nanoscale structures and metamaterials

These issues affect everything we "do"

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



Complex crack path in a composite

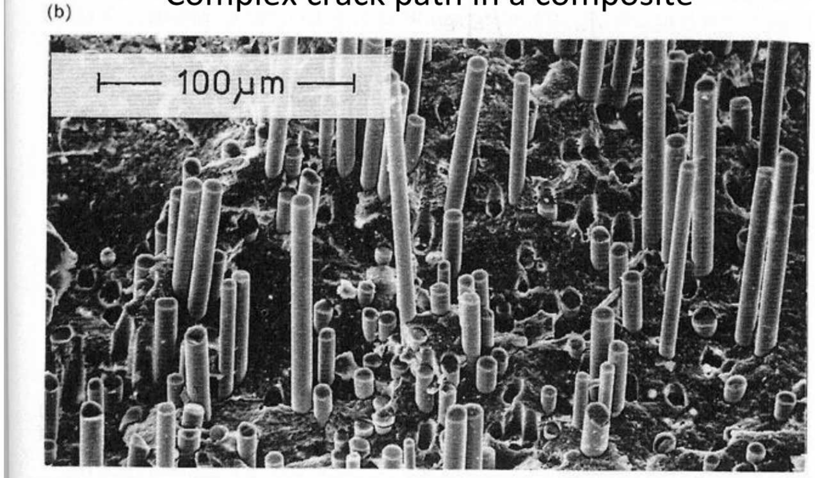


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of 'Silceram' glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

Purpose of peridynamics*

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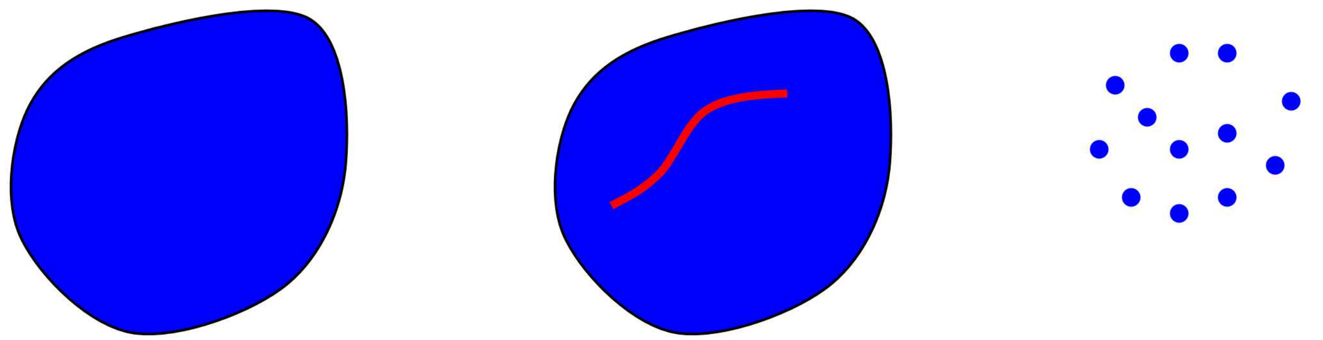
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



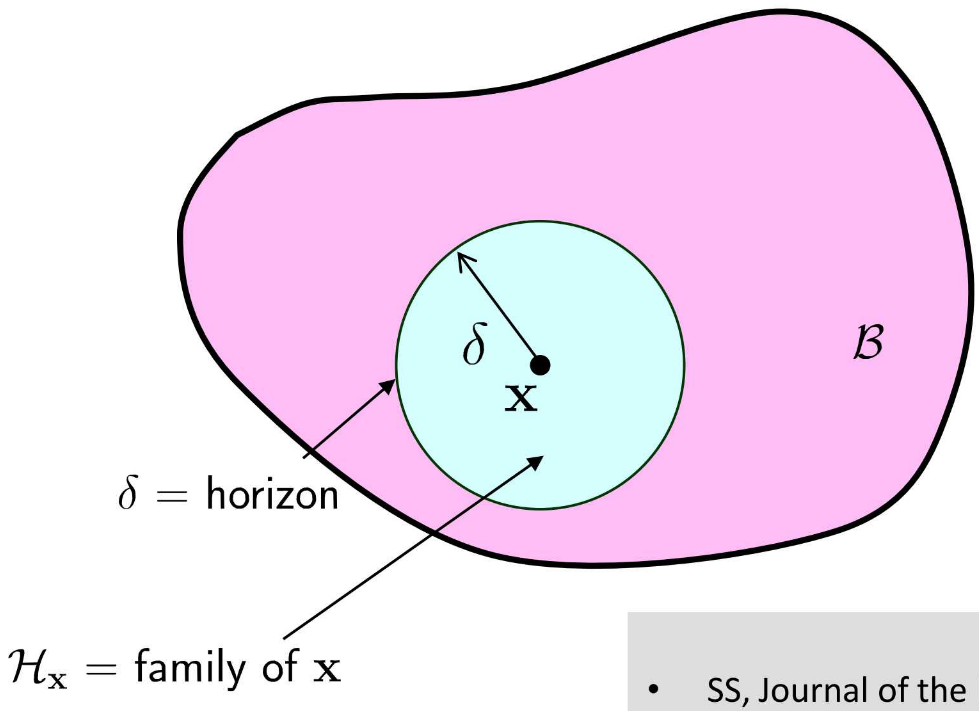
Continuous body | Continuous body with a defect | Discrete particles

- Why do this?
  - The standard theory (Cauchy, 1827) doesn’t always meet the needs of technology.
  - Model complex fracture patterns.
  - Communicate across length scales.

* Peri (near) + dyn (force)

Peridynamics basics: Horizon and family

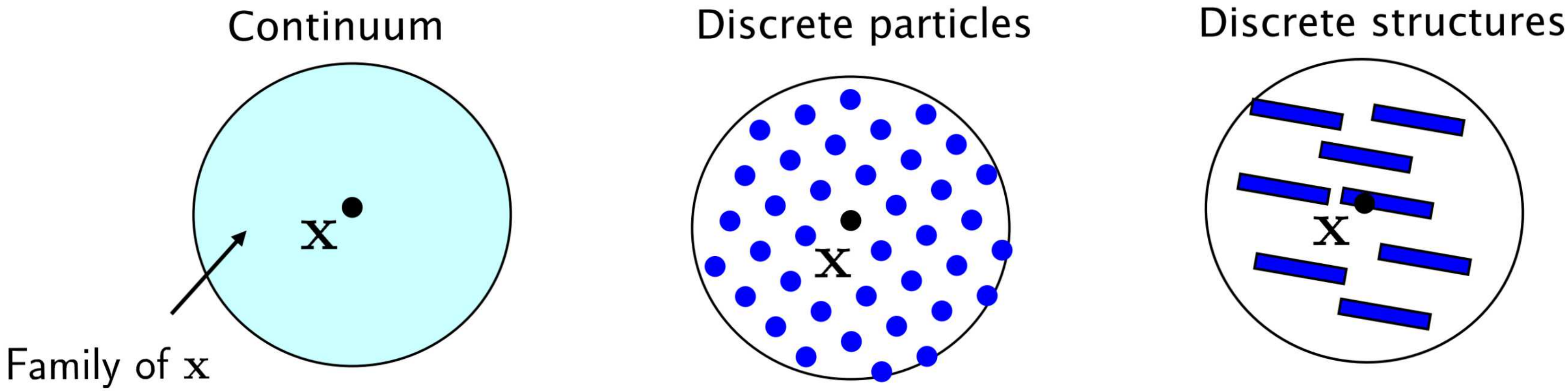
- Any point $\mathbf{x}$ interacts directly with other points within a distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}_{\mathbf{x}}$.

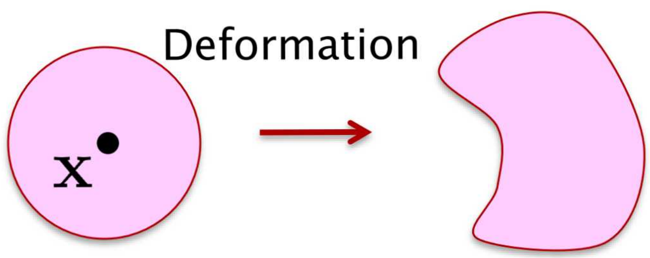


General references

- 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.

Equation of motion

- Write down the total potential energy in a body under the deformation y:

$$\Phi = \int_{\mathcal{B}} (W - \mathrm{b} \bullet \mathrm{y})\, dV.$$

- The Euler-Lagrange equation is

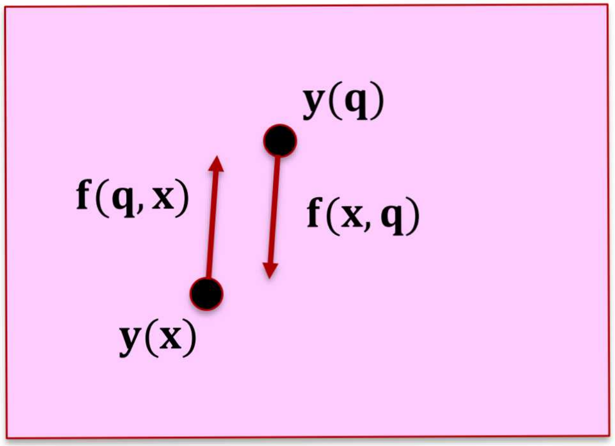
$$0 = \int_{\mathcal{H}_{\mathrm{x}}} \mathrm{f}(\mathrm{q}, \mathrm{x})\, dV_{\mathrm{q}} + \mathrm{b}(\mathrm{x}),$$

  which is the equilibrium equation of peridynamics.

- f is the pairwise bond force density, which comes from the material model.

- Dynamics:

$$\rho \ddot{\mathrm{y}}(\mathrm{x}, t) = \int_{\mathcal{H}_{\mathrm{x}}} \mathrm{f}(\mathrm{q}, \mathrm{x}, t)\, dV_{\mathrm{q}} + \mathrm{b}(\mathrm{x}, t).$$



Keeping track of the collective deformation of families: States

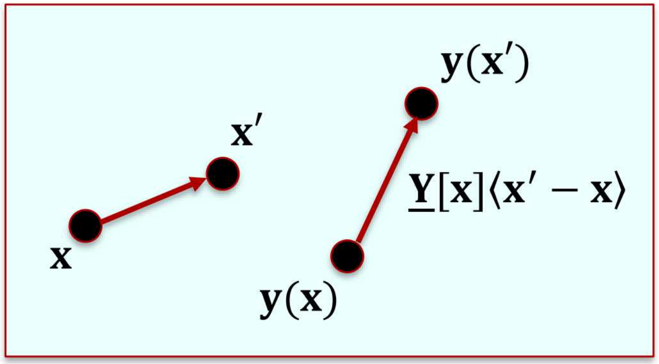
- A state is a mapping from bonds in a family to some other quantity. We write

$$\underline{A}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle = \text{something}.$$

- The *deformation state* maps each bond to its deformed image:

$$\underline{\mathbf{Y}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$$

where $\mathbf{y}$ is the deformation.



- Dot product of two states:

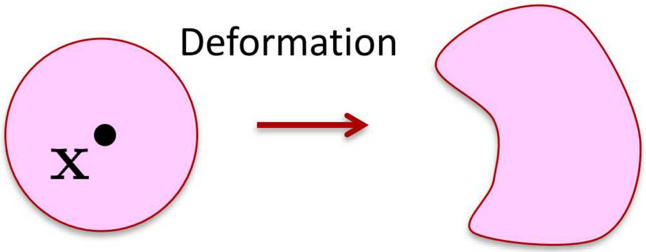
$$\underline{A} \bullet \underline{B} = \int_{\mathcal{H}} \underline{A}\langle \boldsymbol{\xi} \rangle \underline{B}\langle \boldsymbol{\xi} \rangle \, dV_{\boldsymbol{\xi}}.$$

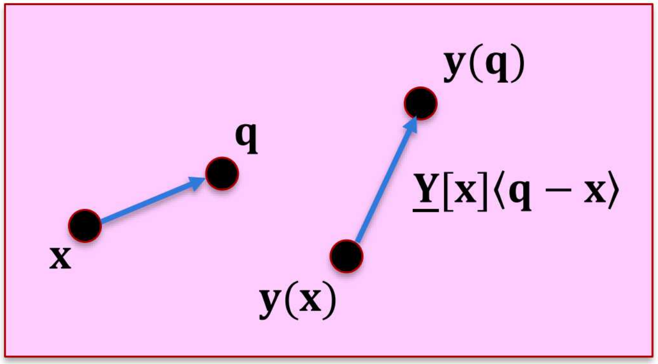
Energy density depends on the deformation state

- Strain energy at $\mathbf{x}$:

$$W(\underline{\mathbf{Y}}[\mathbf{x}]).$$

- Next figure out the bond forces.





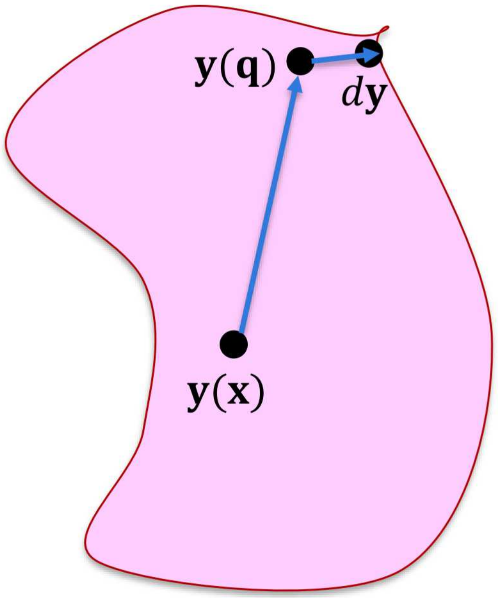
Bond forces from strain energy: Frechet derivatives

- Perturb the deformed point $\mathbf{y}(\mathbf{q})$ by a small additional displacement displacement $d\mathbf{y}$.
- The resulting change in strain energy is dW.
- The Fréchet derivative $W_{\underline{\mathbf{Y}}}$ is the state such that

$$dW = W_{\underline{\mathbf{Y}}} \bullet d\underline{\mathbf{Y}}.$$

- The bond forces are found from

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



Material models

- The *force state* $\underline{\mathbf{T}}$ associates a force density vector with each bond.
- For an elastic material, this is the Fréchet derivative of strain energy density:

$$\underline{\mathbf{T}}[\mathbf{x}]\langle\mathbf{x}' - \mathbf{x}\rangle = W_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}[\mathbf{x}])\langle\mathbf{x}' - \mathbf{x}\rangle.$$

- More generally, a *material model* is a state-valued function of a state:

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

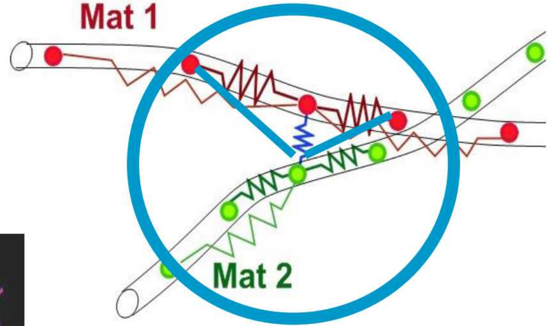
- Special case: in a *bond-based* material, each bond responds independently of all the other bonds.

$$\hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}[\mathbf{x}])\langle\mathbf{x}' - \mathbf{x}\rangle = \boldsymbol{\tau}(\underline{\mathbf{Y}}\langle\mathbf{x}' - \mathbf{x}\rangle)$$

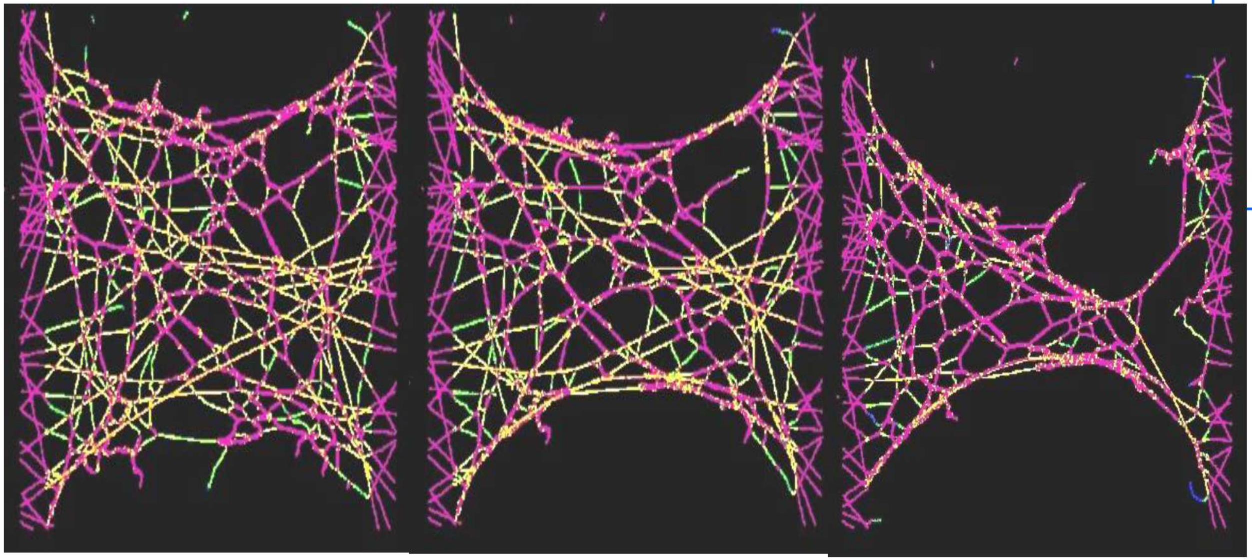
where $\boldsymbol{\tau}$ is a vector-valued function of a vector.

Nanofiber network: Long-range forces dominate response

- Multiple physical interactions with different length scales can all be included in a peridynamic material model.
- This makes it a natural way to treat van der Waals and surface forces.



Nanofiber interactions due to van der Waals forces



Nanofiber membrane (F. Bobaru, Univ. of Nebraska)

Connection with other theories

Connection to the local theory

- Start with the peridynamic equilibrium equation:

$$\int_{\mathcal{H}} (\underline{\mathbf{T}}\langle \mathbf{x}' - \mathbf{x}\rangle - \underline{\mathbf{T}}'\langle \mathbf{x} - \mathbf{x}'\rangle)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}. \qquad (*)$$

- Assume the deformation is smooth. Take $\delta \to 0$.

$$(*) \to \qquad \nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}.$$

Connection to Kunin's nonlocal theory

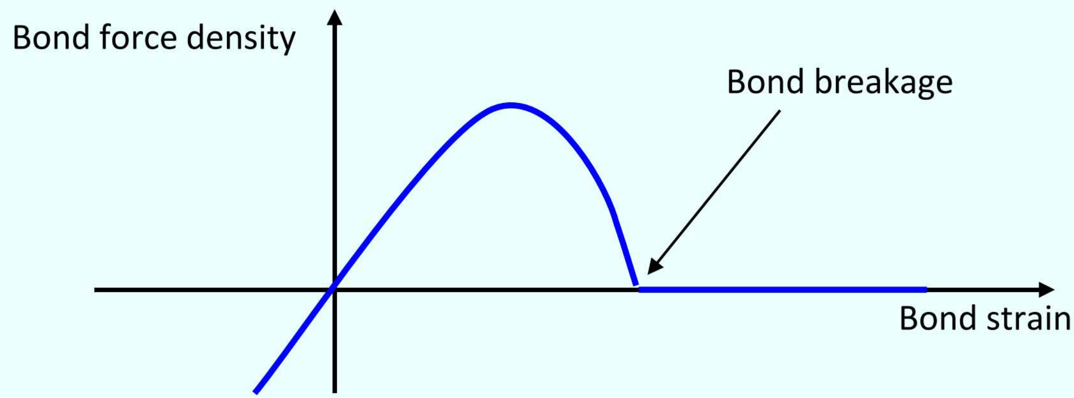
- Set $\delta = \infty$. Assume small displacements. Don't allow damage or other nonlinearity. Linearize.

$$(*) \to \qquad \int_{\mathcal{B}} \mathbf{C}(\mathbf{x}', \mathbf{x})(\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x}))\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}$$

where $\mathbf{C}$ is a tensor. This equation appears in Kunin's theory (1983).

Damage due to bond breakage

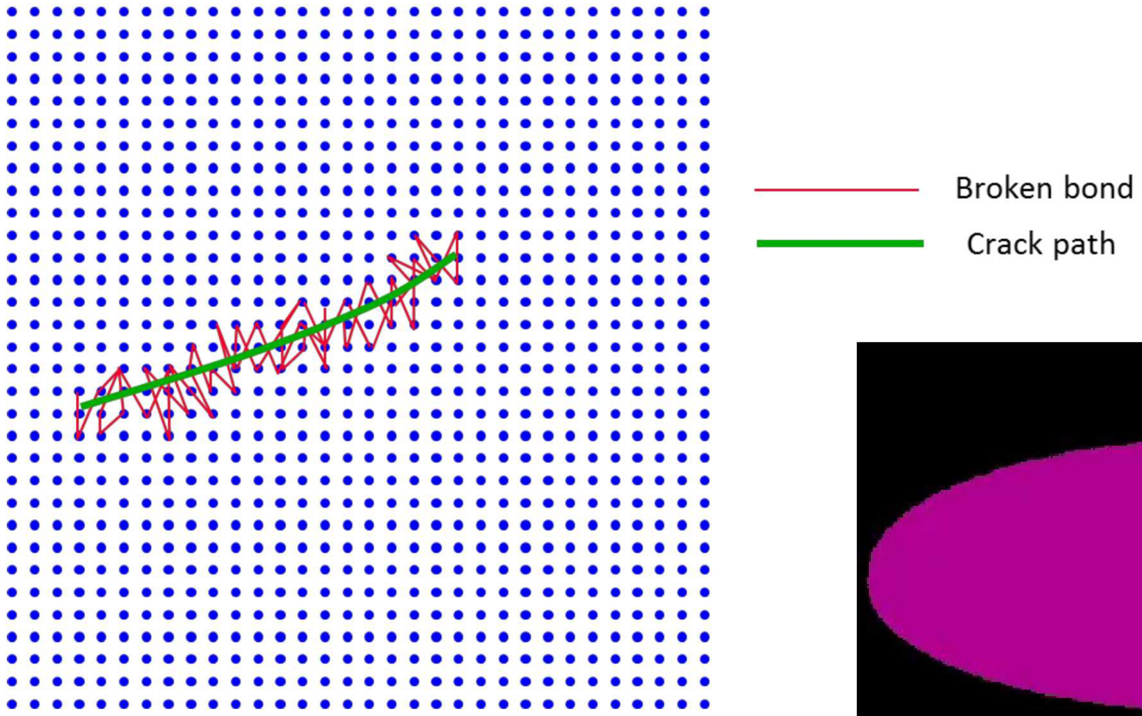
- Recall: each bond carries a force.
- Damage is implemented at the bond level.
  - Bonds break irreversibly according to some criterion.
  - Broken bonds carry no force.
- Examples of criteria:
  - Critical bond strain (brittle).
  - Hashin failure criterion (composites).
  - Gurson (ductile metals).

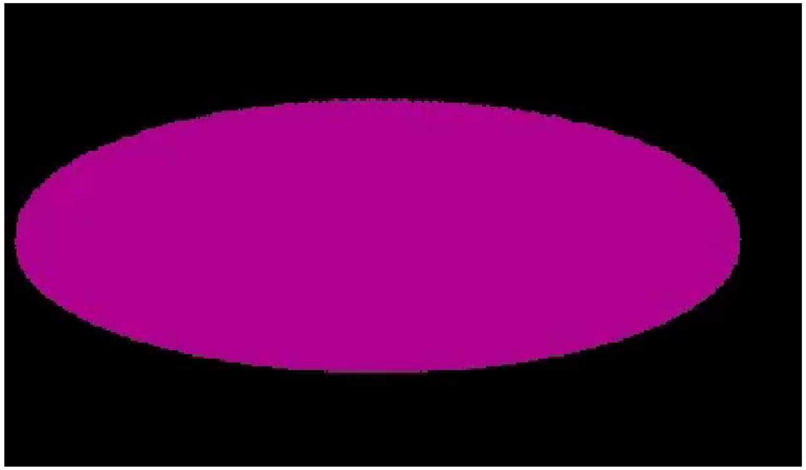


Critical bond strain damage model

Autonomous crack growth

- Bond breakage leads to fracture.
- Cracks do what they want (grow, arrest, branch, curve, oscillate, …)
- **Brittle** material model: Bond breaks when its strain reaches some critical value.

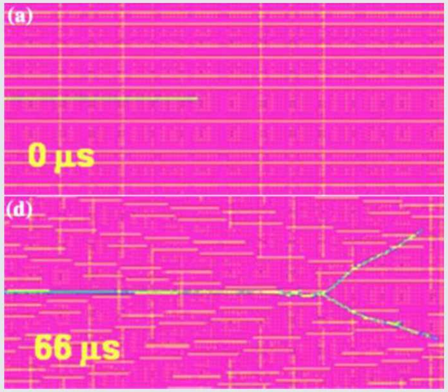




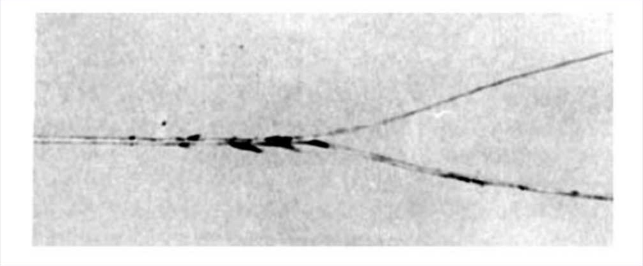
Brittle dynamic fracture

- The method reproduces many features of fracture in glass.

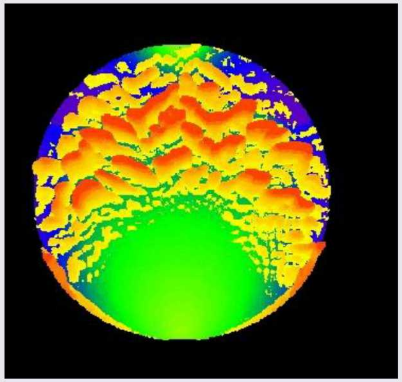
Crack branching



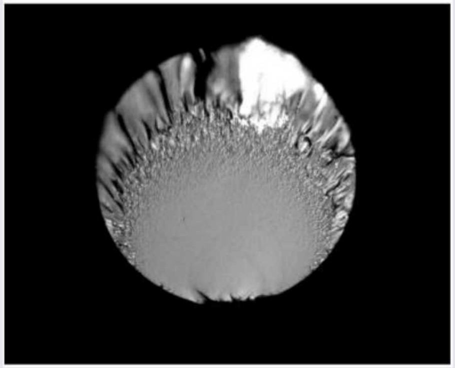
Agwai, Guven, & Madenci, Predicting crack propagation with peridynamics: a comparative study, Int. J. Fract. Int J Fract (2011) 171:65–78



Mirror-mist-hackle transition



3D peridynamic model



Optical fiber
(Castilone, Glaesemann & Hanson, Proc. SPIE (2002))

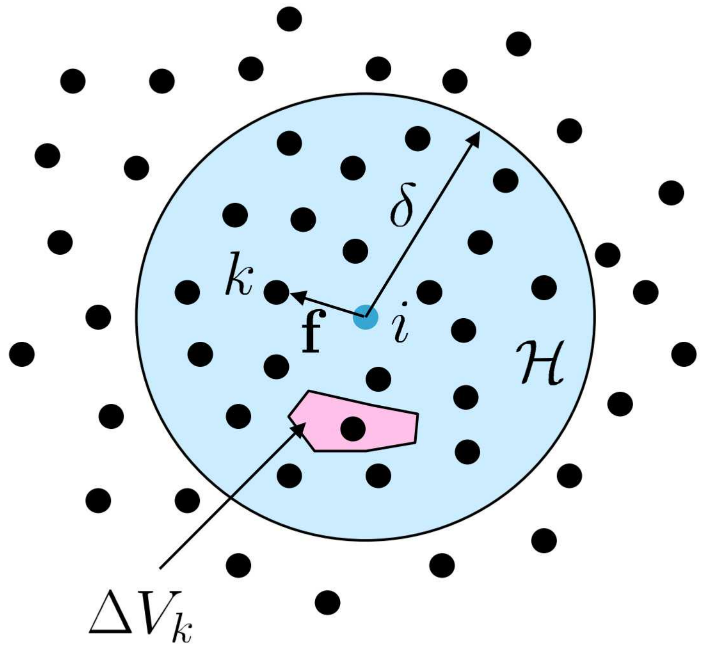
Particle discretization: Emu

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

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

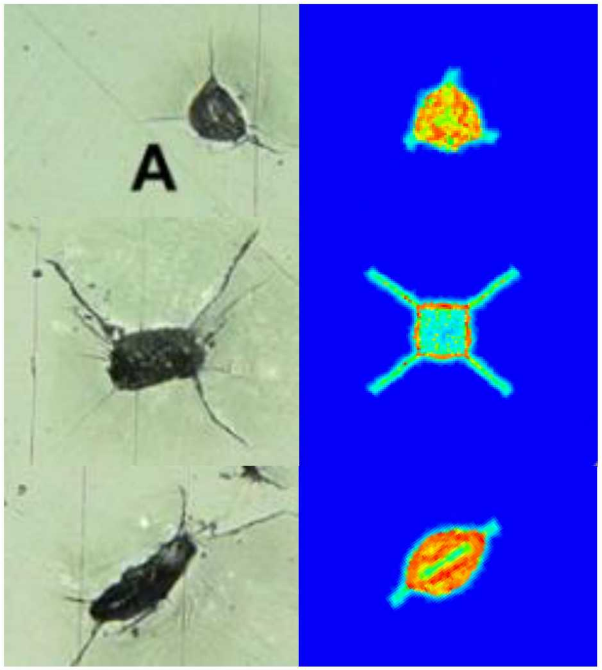
$$\approx$$

$$\rho\ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\,\Delta V_k + \mathbf{b}_i^n$$



- This discretization has a special affinity with the underlying mechanics.
- Convergence properties have been studied
  - Tian & Du, SIAM J. Numerical Analysis (2014).
- Discontinuous Galerkin is also viable (LS-DYNA).
  - Chen & Gunzburger, CMAME (2011).
  - Aksoy & and Şenocak, IJNME (2011).
  - Azdoud, Han, & Lubineau, Comp. Mech. (2014).
  - Ren, Wu, & Askari, Int. J. Impact Eng. (2016).

Simulation of impact damage



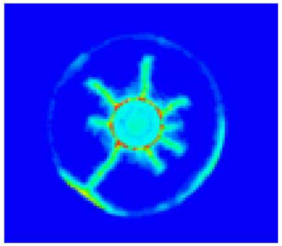
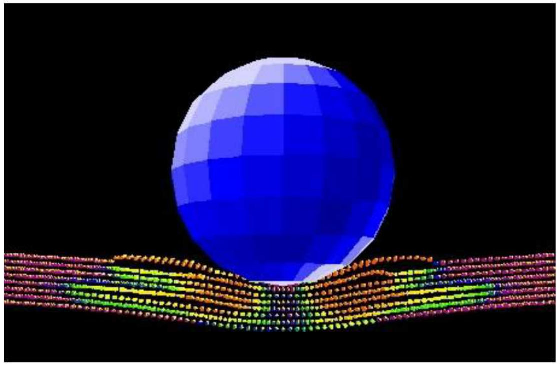
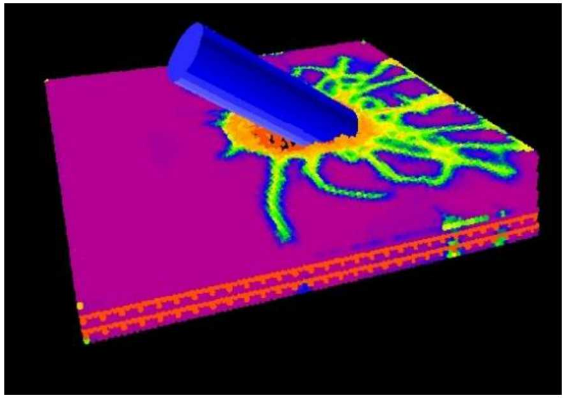


Image taken from Maekawa, 1991.

Particle impact on damage in glass (Guven)



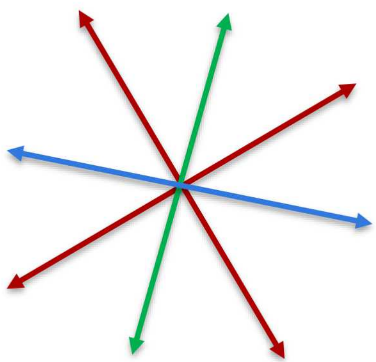
Hail against composite



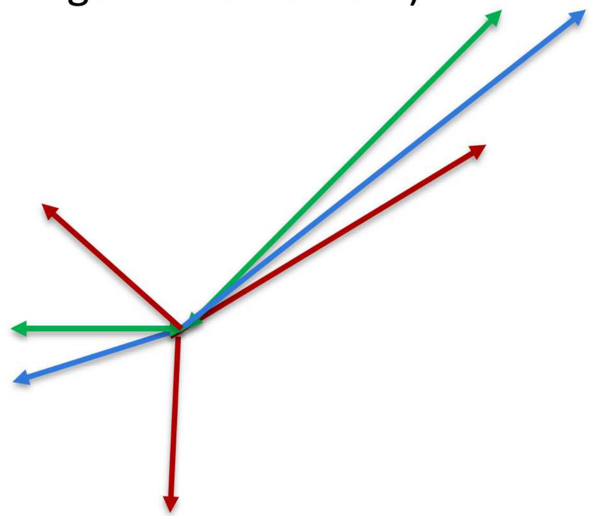
Impact on reinforced concrete

Soft materials: Geometrical nonlinearity comes "for free"

- Bond forces rotate with the bonds as the body deforms.
- Material models must be objective (invariant with respect to rotations).
- Material models must be nonpolar (balanced angular momentum).



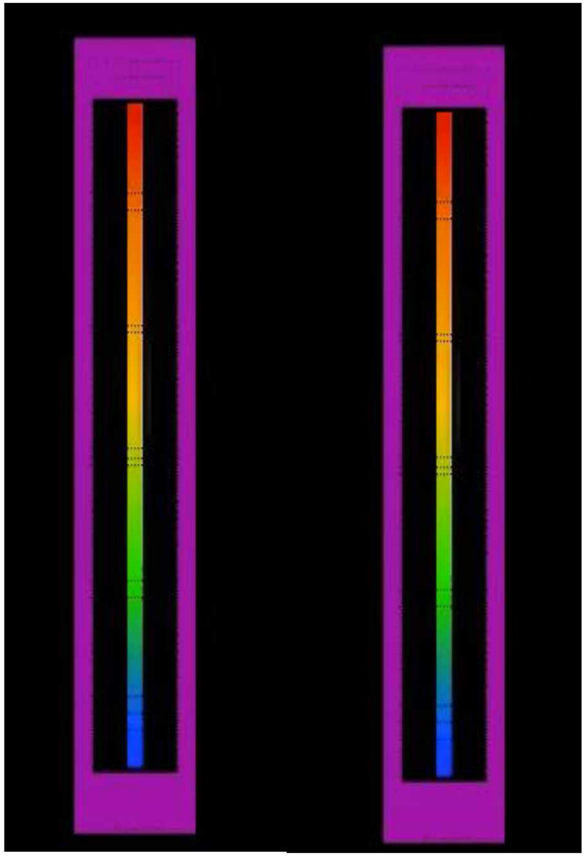
Undeformed bonds



Deformed bonds

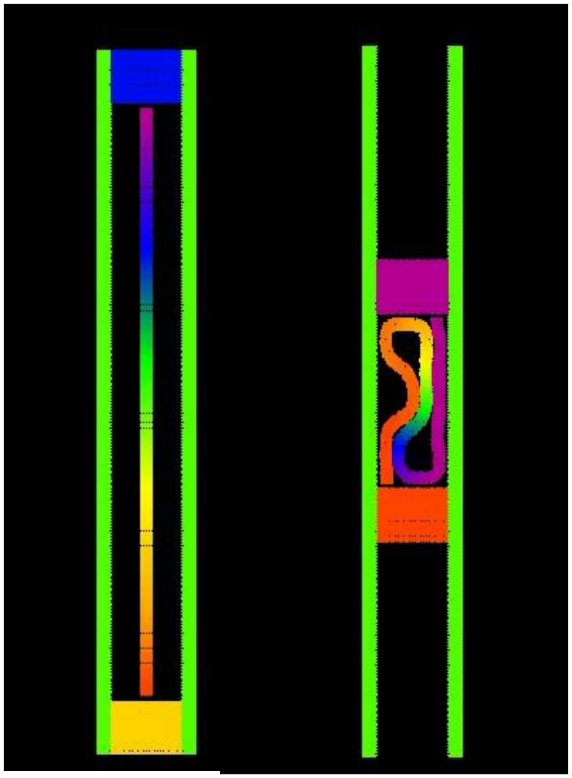
Example: Buckling and folding

VIDEOS
Axial compression of a beam



Linear peridynamic solid (LPS) | Microplastic

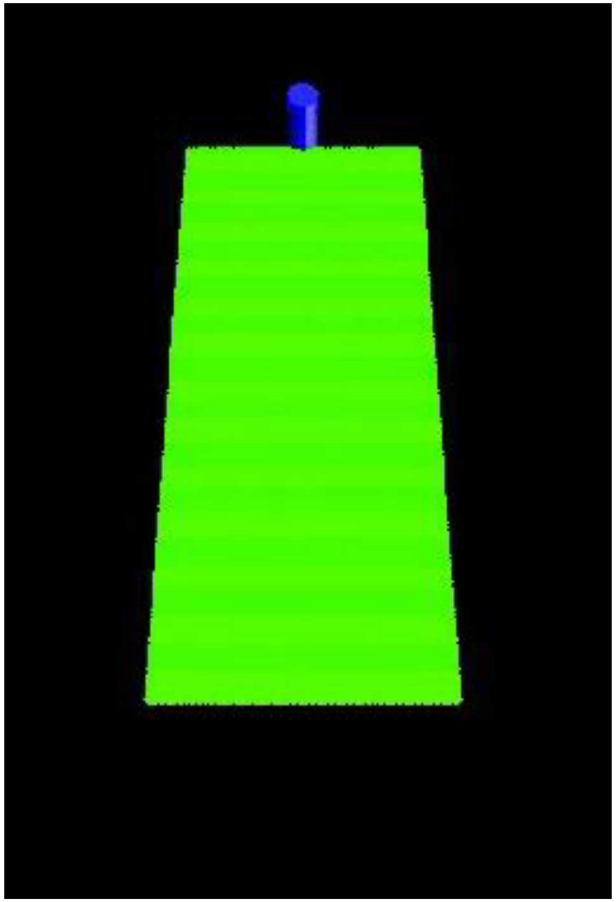
Example: Buckling and folding



Compression of an elastic strip
State-based material model:
Linear peridynamic solid (LPS)

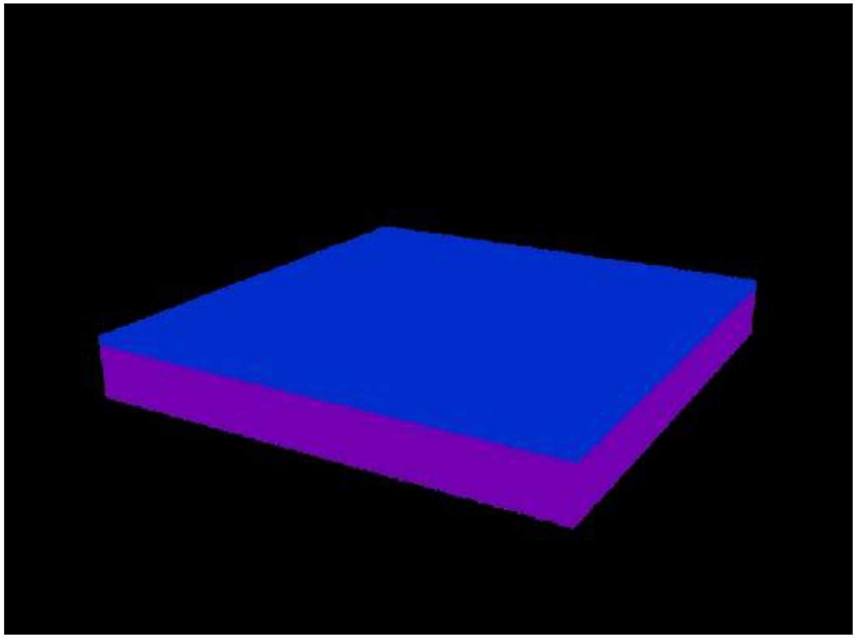
Method reproduces some subtleties in the fracture and debonding of membranes

Unstable crack path in a polyethylene membrane
(Silling & Bobaru, Int. J. Nonlin. Mech. 2005)



VIDEOS

Peeling of tape



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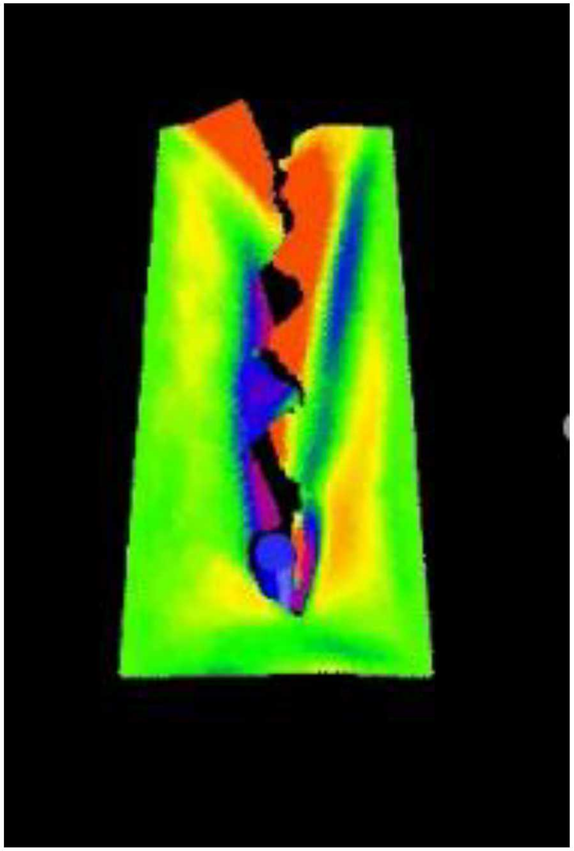

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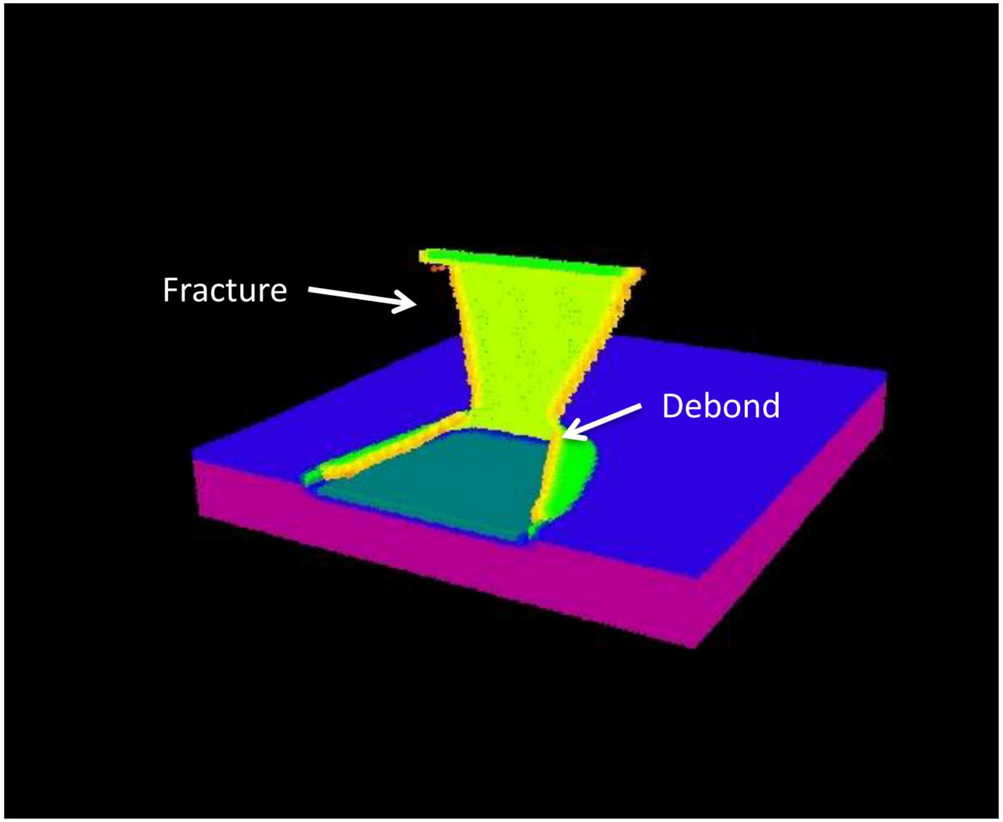
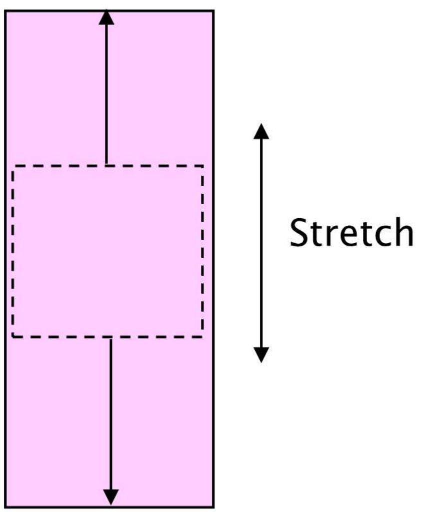
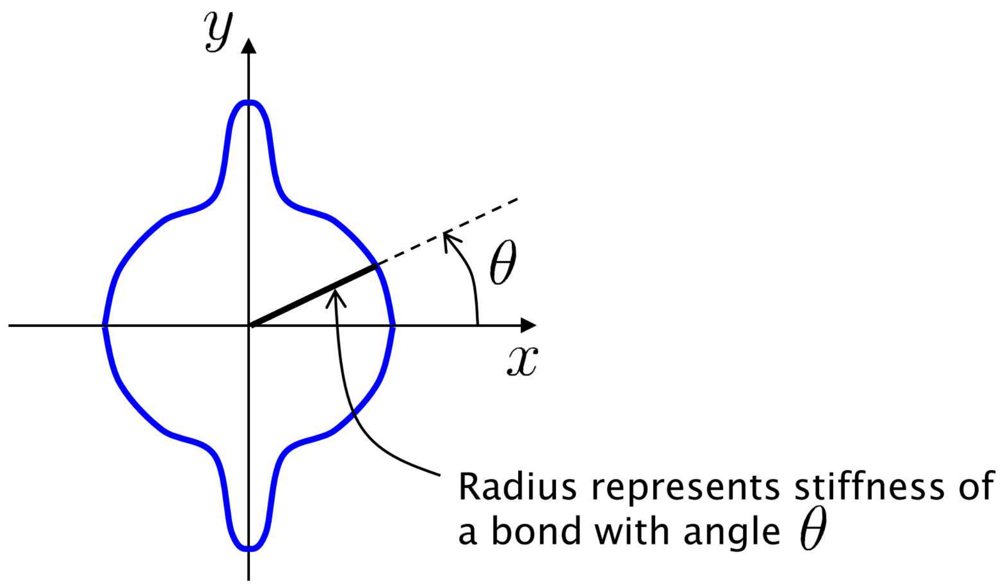


Nonlinearity in bond response can induce anisotropy: Rubber fracture

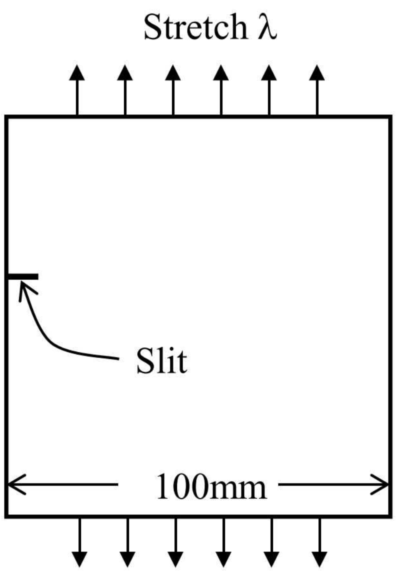
$$|\mathbf{f}| = c\Big[(1-a) + a|\sin\theta|^n\Big]s$$

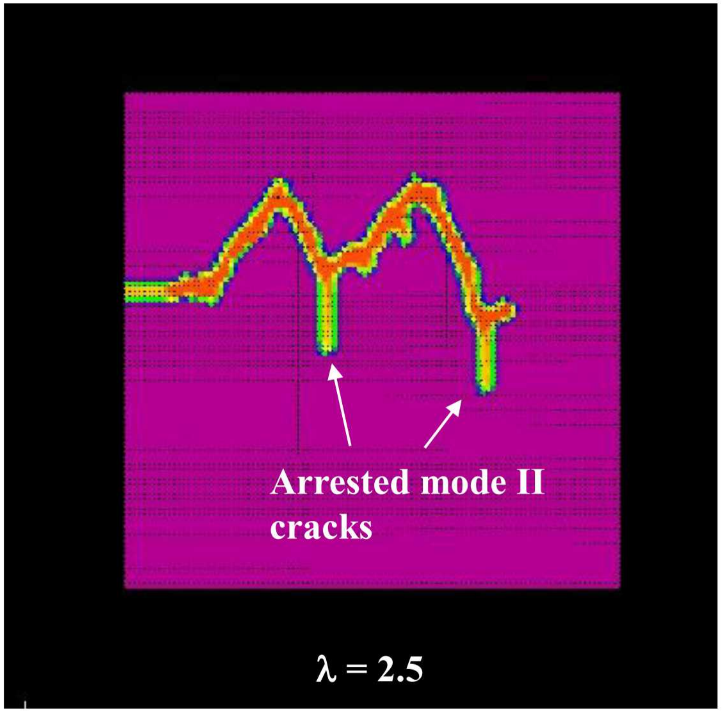


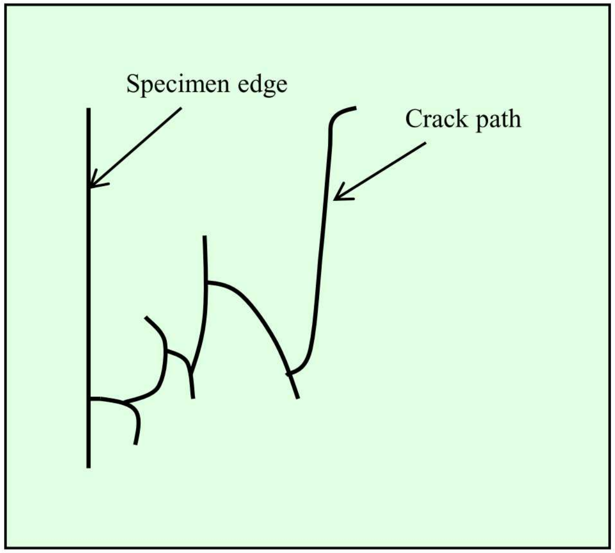


Crack turning in rubber

- Due to anisotropy, crack growth in mode II (parallel to loading) is competitive with mode I (straight ahead).
  - But the fields seen by a crack tip change as it grows.
  - Result: Cracks change direction and branches appear (then stop).







Experiment
(After Hamed et al. ,1996)

Nonlocal thermodynamics: Internal energy and stress power*

- First law statement:

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

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

- Compare this with the statement in the standard theory:

$$\dot{\varepsilon} = \sigma \cdot \dot{\mathrm{F}} + h + r.$$

- The stress power term sums up the work done on individual bonds:

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

- If the material is elastic, all of this work goes into the strain energy density:

$$W_{\underline{\mathbf{Y}}} \bullet \underline{\dot{\mathbf{Y}}} = \dot{W}.$$

* Joint work with Rich Lehoucq. See SS & Lehoucq, Adv. Appl. Mech. (2010)

Heat transport in bonds

- A bond-based nonlocal heat transport law:

$$h(\mathrm{x},t) = \int_{\mathcal{H}} K(\mathrm{q},\mathrm{x})(\theta(\mathrm{q},t) - \theta(\mathrm{x},t))\, dV_{\mathbf{q}}$$

  where θ is temperature, K is the bond conductivity.

-

$$K(\mathrm{x},\mathrm{q}) = K(\mathrm{q},\mathrm{x})$$

  ensures conservation of energy.

- Second law

$$\theta\dot{\eta} \geq h + r$$

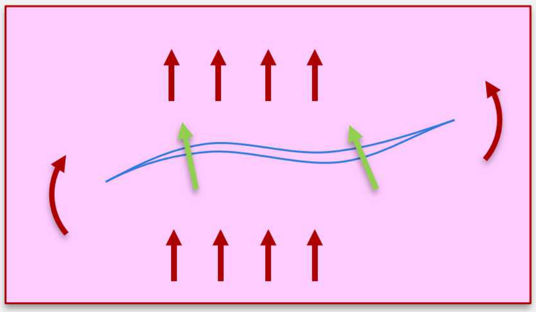
  where η is the entropy.

- Can show that the 2nd law implies $K \geq 0$ always.

Cracks and other singularities in heat transport

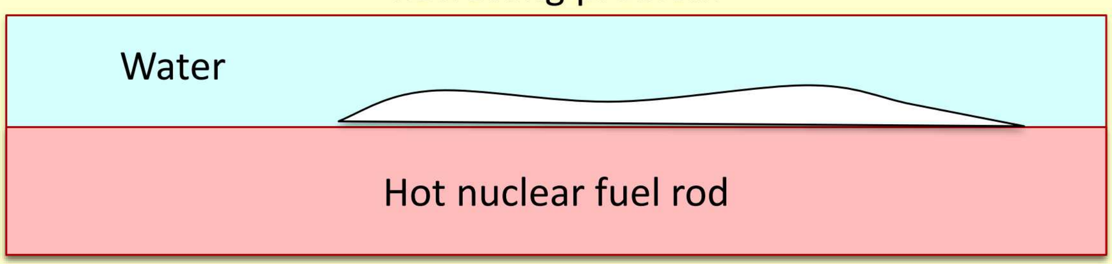
Heat conduction near a crack:

- Some heat goes around the corners where PDE heat equation blows up.
- Some heat jumps across the crack.



- F. Bobaru, & M. Duangpanya. "A peridynamic formulation for transient heat conduction in bodies with evolving discontinuities." *Journal of Computational Physics* (2012).
- S. Oterkus, E. Madenci, and A. Agwai. "Peridynamic thermal diffusion." *Journal of Computational Physics* (2014).

"Rewetting problem"



Fluids:
Effectively Eulerian material models

- A Lagrangian material model involves both the undeformed and deformed bond vectors. Example:

This term makes the model Lagrangian

$$\underline{\mathbf{T}}\langle\xi\rangle = (|\underline{\mathbf{Y}}\langle\xi\rangle| - |\xi|)\frac{\underline{\mathbf{Y}}\langle\xi\rangle}{|\underline{\mathbf{Y}}\langle\xi\rangle|}.$$

- An Eulerian material model has bond forces that depend only on the deformed bond vectors. Example:

$$\underline{\mathbf{T}}\langle\xi\rangle = |\underline{\mathbf{Y}}\langle\xi\rangle|^{-n}\frac{\underline{\mathbf{Y}}\langle\xi\rangle}{|\underline{\mathbf{Y}}\langle\xi\rangle|},$$

$n > 0$.

Using an equation of state to find the bond forces

- Define a nonlocal density by

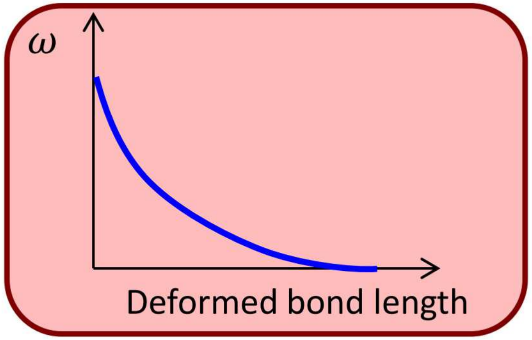
$$\rho = \rho_0 \int_{\mathcal{B}} \omega(|\underline{\mathbf{Y}}\langle\xi\rangle|)\, dV_{\xi}$$

where ρ_0 is the reference density and ω is a weighting function such that $\int \omega = 1$. Integration is in the reference configuration.

- Compute the pressure from

$$p = -\frac{1}{\rho^2}\frac{\partial\psi}{\partial\rho}.$$

where ψ is the free energy density.



- The force state is found from the Frechet derivative of ψ to be

$$\underline{\mathbf{T}}\langle\xi\rangle = \frac{\partial\psi}{\partial\underline{\mathbf{Y}}} = \frac{\partial\psi}{\partial\rho}\frac{\partial\rho}{\partial\underline{\mathbf{Y}}} = \frac{p\omega'(\xi)}{\rho^2}\frac{\underline{\mathbf{Y}}\langle\xi\rangle}{|\underline{\mathbf{Y}}\langle\xi\rangle|}.$$

Surface tension is implemented through nonlocal forces

- Surface tension arises from nonlocal forces between molecules.
- Peridynamic Eulerian model:

$$\underline{\mathbf{T}} = \underline{\mathbf{T}}^{\text{eos}} + \underline{\mathbf{T}}^{\text{surf}}$$

where

$$\underline{\mathbf{T}}^{\text{surf}} = \gamma \frac{\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|}$$

and γ is a constant.

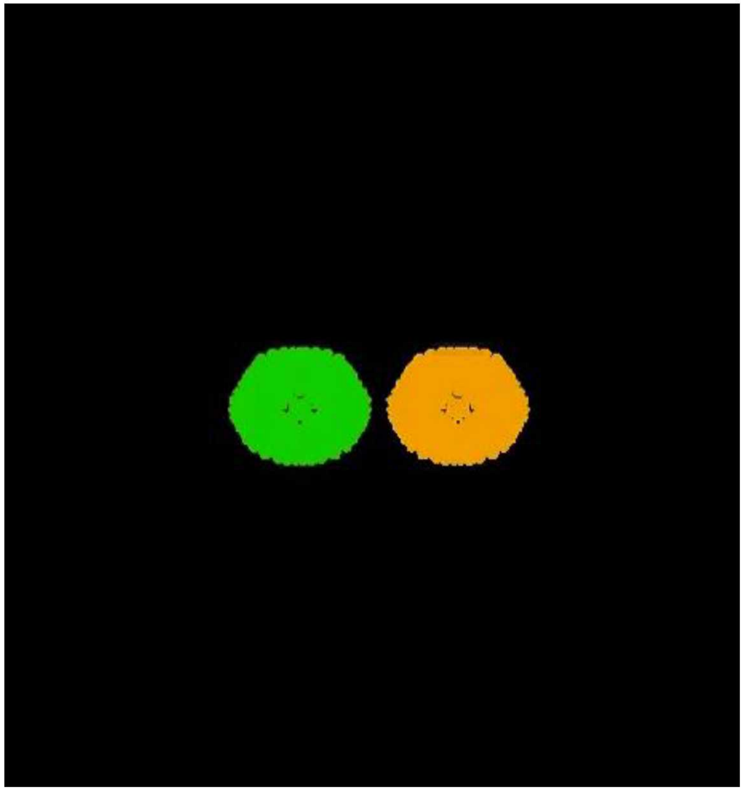
- Each pair of material particles within each other's family attracts.

Surface tension examples

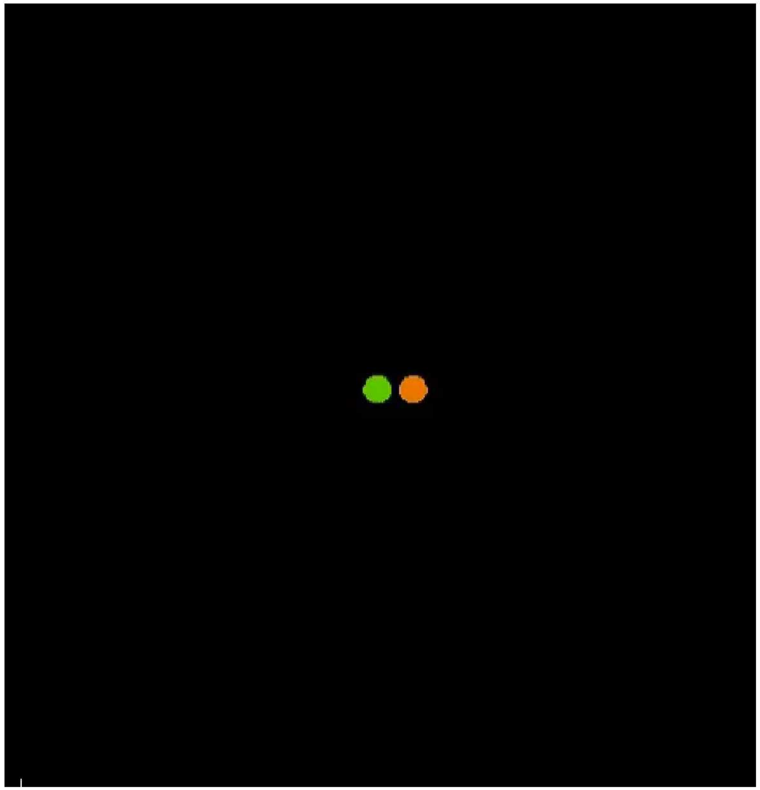
- Two droplets collide.
- Mie-Gruneisen EOS is used.

VIDEOS

THE BLOB (v=10)



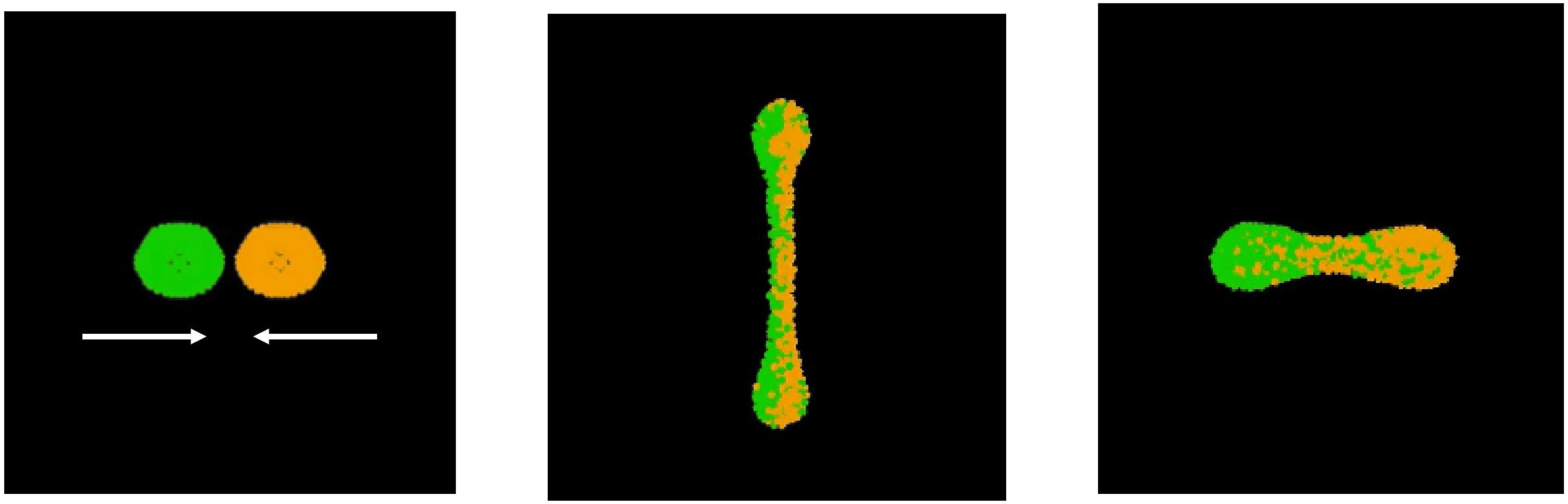
REVENGE OF THE BLOB (v=100)



Surface tension examples

- Two droplets collide.
- Mie-Gruneisen EOS is used.

THE BLOB (v=10)



Contact and friction forces as Eulerian material response

- Short-range contact and friction forces can be included within an Eulerian material model:

$$\underline{\mathbf{T}}^E = \underline{\mathbf{T}}^{\text{eos}} + \underline{\mathbf{T}}^{\text{contact}} + \underline{\mathbf{T}}^{\text{friction}}$$

where

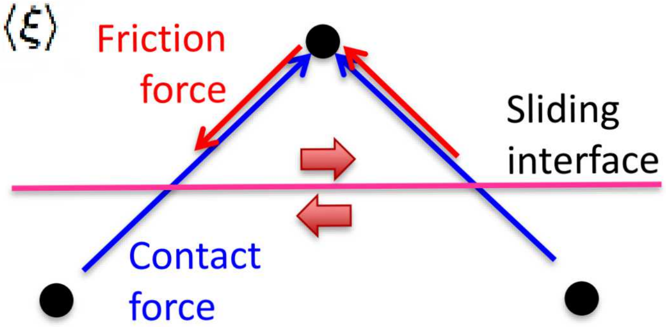
$$\underline{\mathbf{T}}^{\text{contact}}\langle\xi\rangle = \begin{cases} -c(r_c - |\underline{\mathbf{Y}}\langle\xi\rangle|)\mathbf{M} & \text{if } |\underline{\mathbf{Y}}\langle\xi\rangle| < r_c, \\ 0 & \text{otherwise.} \end{cases} , \qquad \mathbf{M} = \frac{\underline{\mathbf{Y}}\langle\xi\rangle}{|\underline{\mathbf{Y}}\langle\xi\rangle|}$$

where r_c is a cut-off distance for contact forces.

- The friction force state is

$$\underline{\mathbf{T}}^{\text{friction}}\langle\xi\rangle = -F \operatorname{sgn}\left(\frac{\partial}{\partial t}|\underline{\mathbf{Y}}\langle\xi\rangle|\right)\underline{\mathbf{T}}^{\text{contact}}\langle\xi\rangle$$

where F is the friction coefficient.



Combining Lagrangian and Eulerian response in a single material model

- We'd like to model both fluid-like and solid-like response in the same material model.
- Combine the two as a linear combination of force states:

$$\underline{\mathbf{T}} = \beta(p)\underline{\mathbf{T}}^E + (1 - \beta(p))\underline{\mathbf{T}}^L$$

where $\underline{\mathbf{T}}^E$ and $\underline{\mathbf{T}}^L$ are the Eulerian (fluid-like) and Lagrangian (solid-like) contributions respectively.

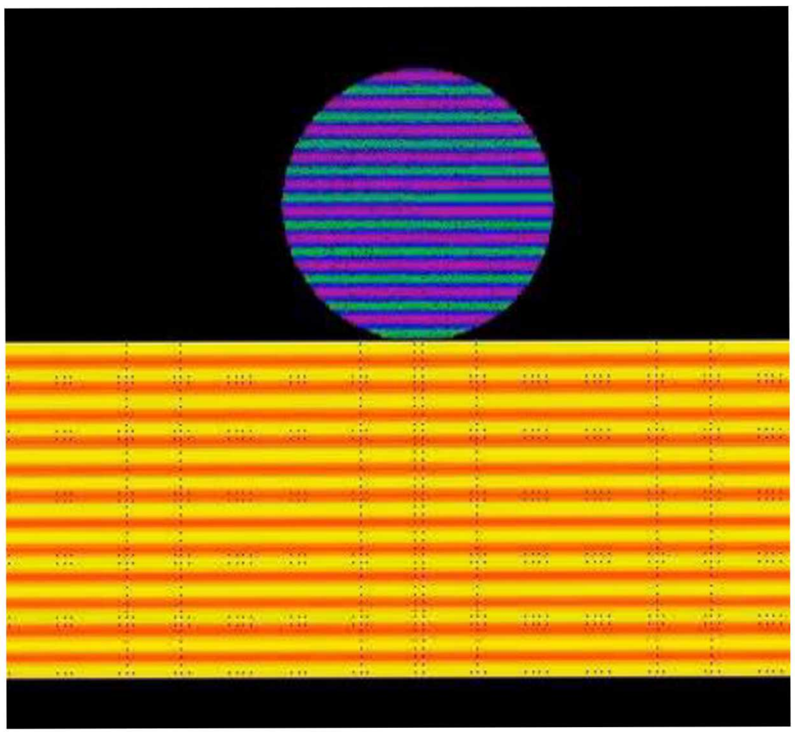
- $\beta(p)$ is a pressure-dependent interpolation parameter, $0 \leq \beta \leq 1$.
- Example: EOS & bond-based:

$$\underline{\mathbf{T}}\langle\xi\rangle = \left(\frac{\beta(p)p\omega'(\xi)}{\rho} + (1 - \beta(p))C(\xi)(|\underline{\mathbf{Y}}\langle\xi\rangle| - |\xi|)\right)\frac{\underline{\mathbf{Y}}\langle\xi\rangle}{|\underline{\mathbf{Y}}\langle\xi\rangle|}$$

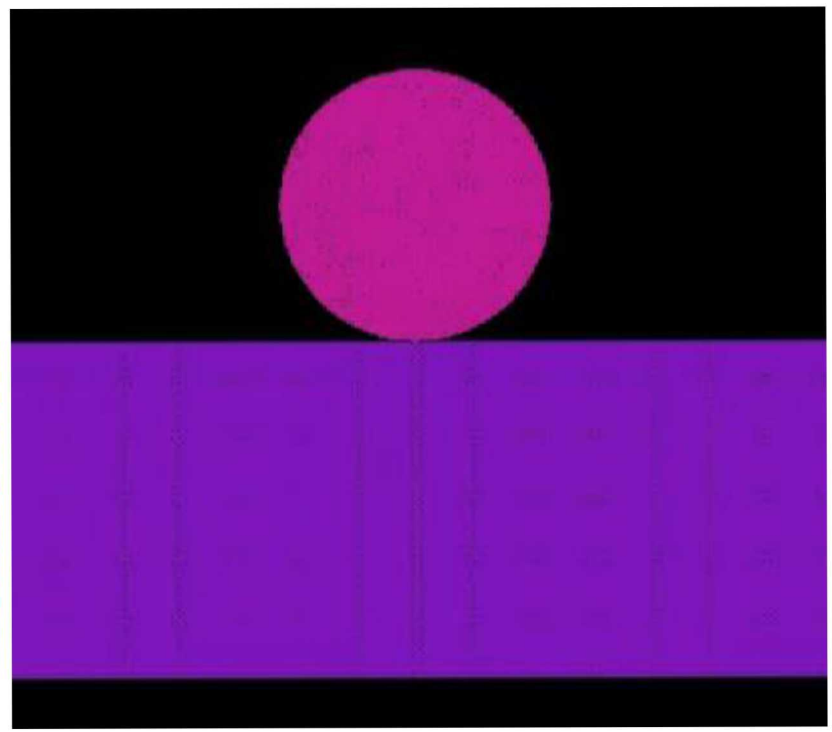
Example of Eulerian + Lagrangian material models: Wear

- Solid response and damage: Lagrangian
- Contact and friction: Eulerian

VIDEOS

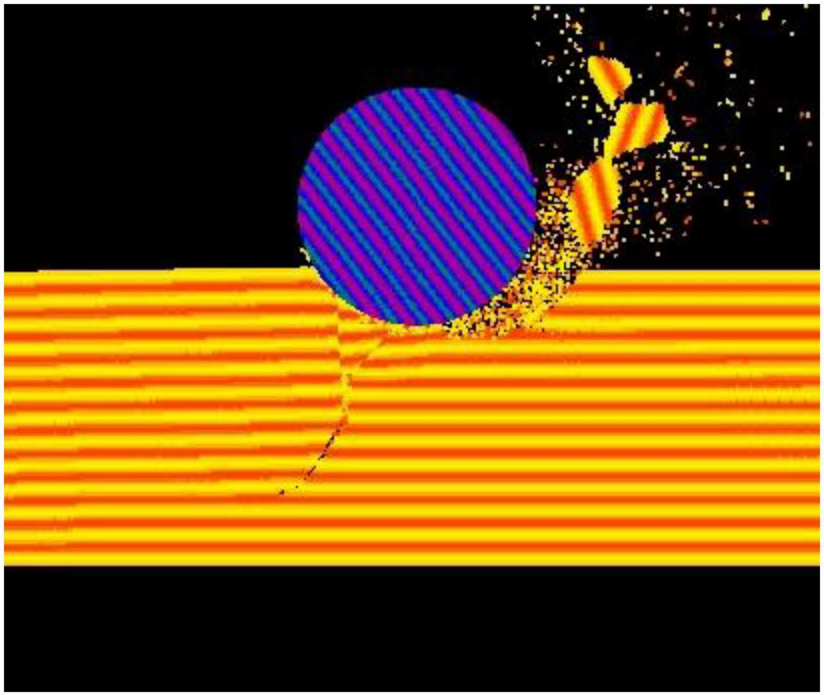


Material deformation

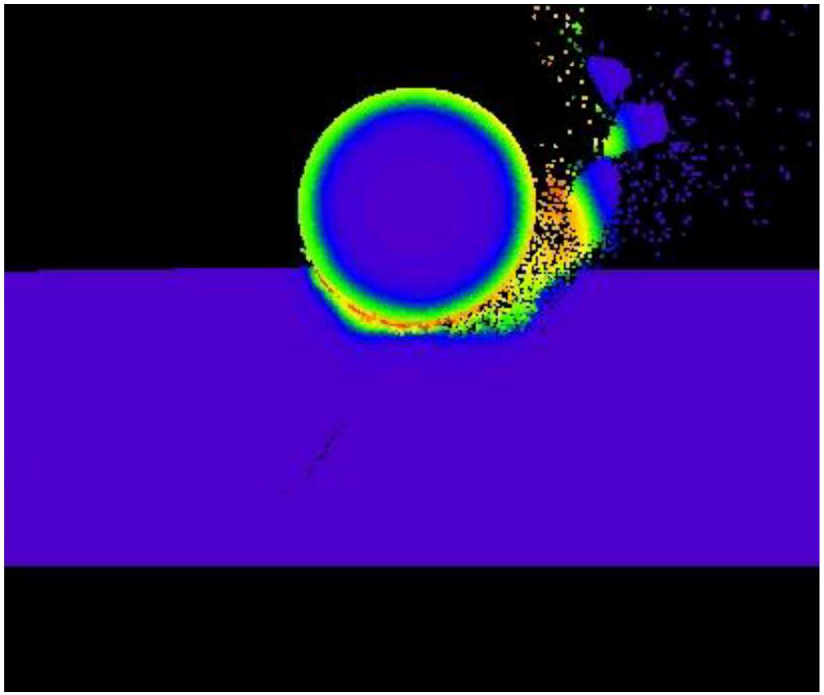


Damage

Friction forces appear in 1st law expression leading to heating



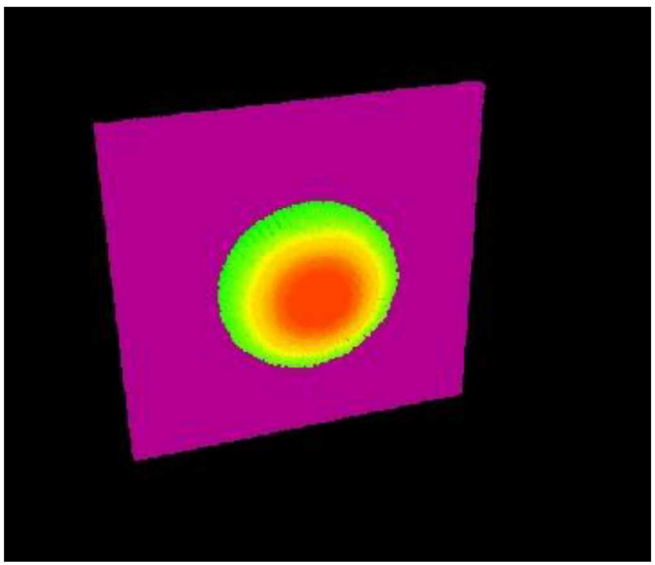
Material deformation



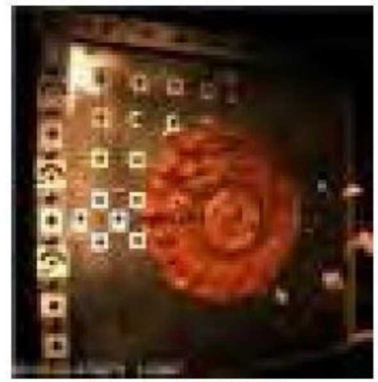
Temperature

Bird strike*
Peridynamics compared with SPH

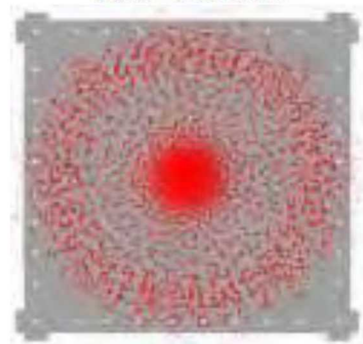
- Bird simulant (gelatin) vs. heavy plate
- The peridynamic model helps reduce the “spray” that is sometimes seen with SPH.



Peridynamics



Test - LG 997



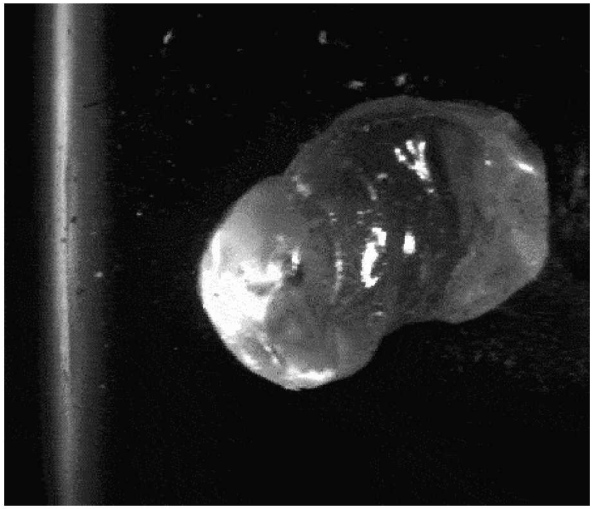
SPH

Olivares, NIS Document 09-039 (2010)

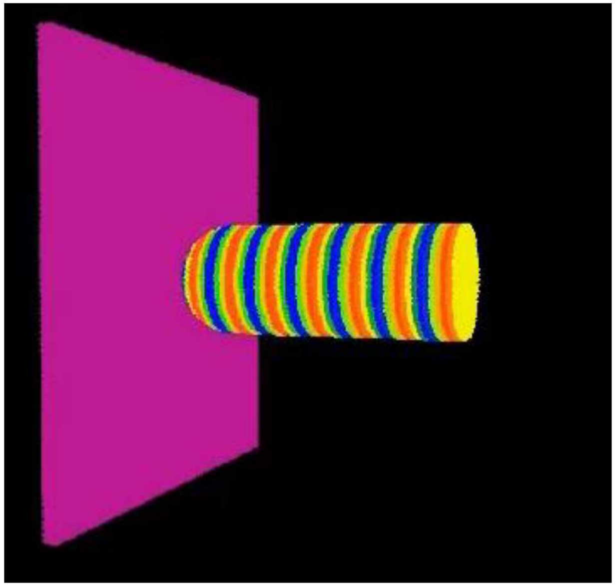
*Joint work with Boeing Research & Technology

Bird strike simulant (gelatin)

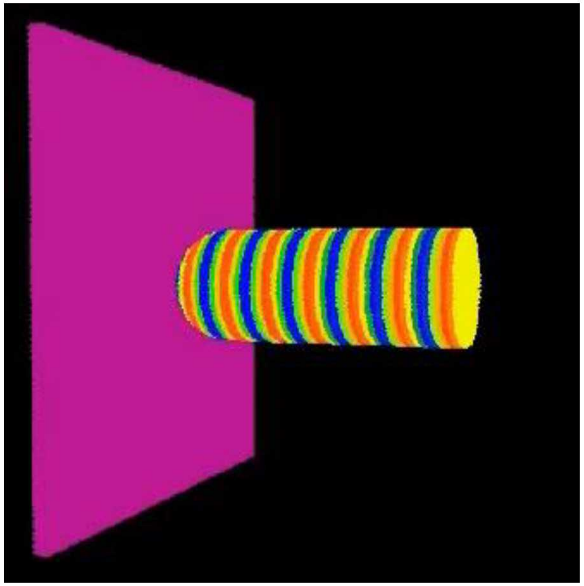
- Who cares?
  - The splash pattern helps determine loading on the structure, especially when the structure is itself highly deformable.



Typical test
(credit: Arthur Core)

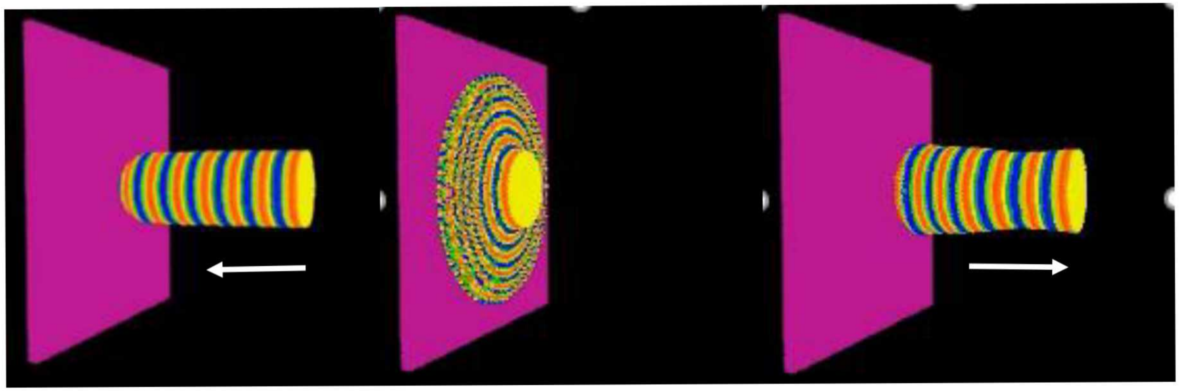


Meshless PD

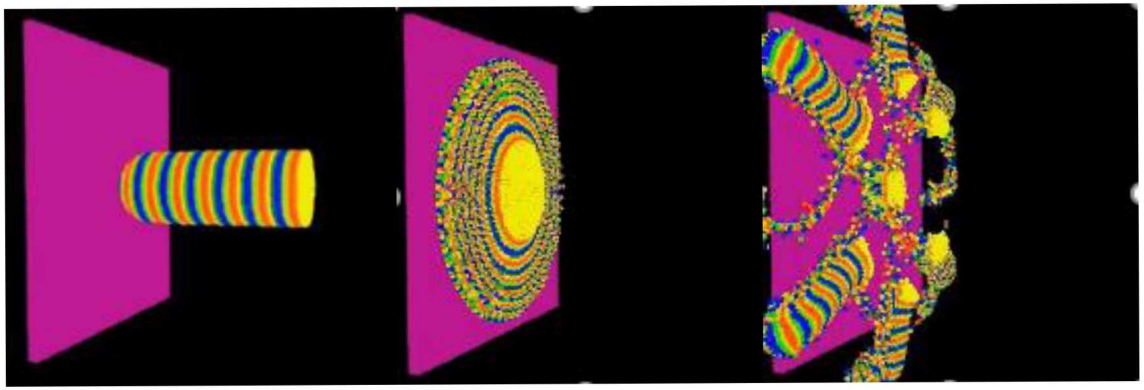


Meshless PD
with bond damage

Bird strike simulant (gelatin)



No fracture

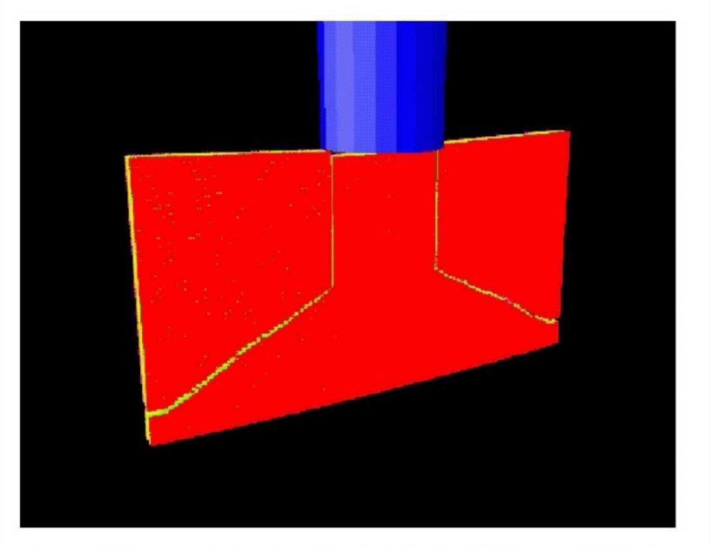


With fracture

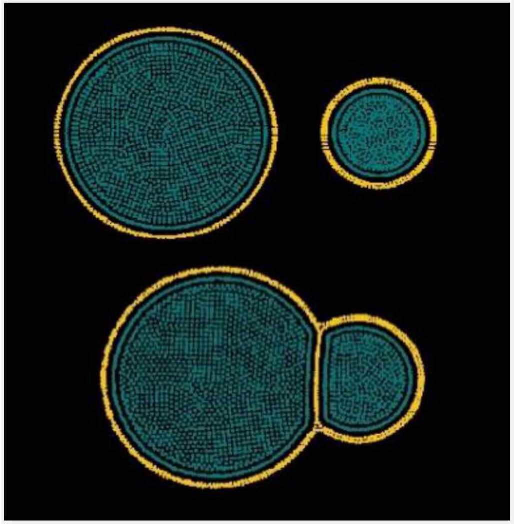
Summary

- Some techniques within peridynamics for studying large deformation and fracture in soft materials have been developed:
  - Eulerian material models.
  - Surface forces, contact, and friction as part of an Eulerian material model.
  - Combining Lagrangian & Eulerian material response.

The same theory encompasses a wide spectrum of phenomena, depending only on the choice of an appropriate material model.



Kalthoff-Winkler test



Soap bubbles