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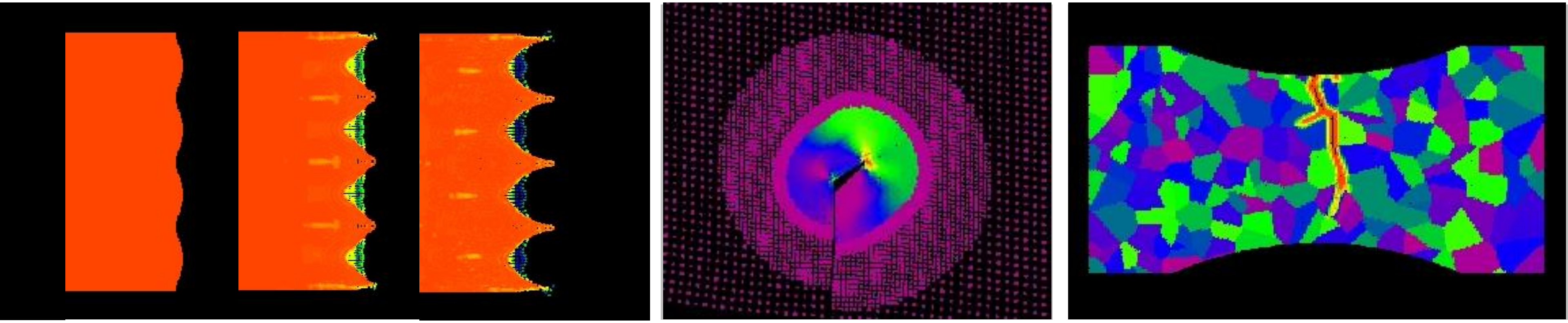

The thermodynamic form of peridynamics with application to phase transformations

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Outline

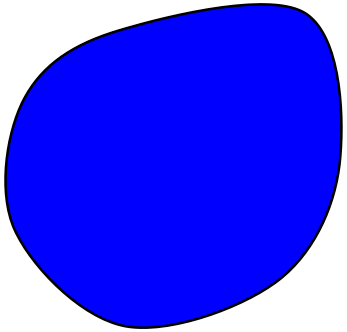
- Peridynamic mechanics summary
- Thermodynamic form of peridynamics
  - Frechet derivatives
  - First and second laws
  - Free energy and mechanics in a nonlocal model
  - Example: surface tension
- Peridynamic multiphase material models
  - Energy dissipation and kinetic relations
  - Computational example

Not covered in this talk: Peridynamic heat diffusion equations. But see

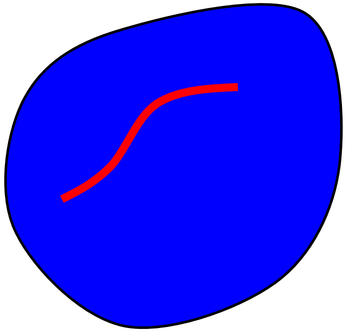
- Bobaru & Duangpanya. "The peridynamic formulation for transient heat conduction." International Journal of Heat and Mass Transfer 53 (2010) 4047-4059.
- Oterkus, Madenci, & Agwai. "Peridynamic thermal diffusion." Journal of Computational Physics 265 (2014) 71-96.
- Du, Gunzburger, Lehoucq, & Zhou, “Analysis and approximation of nonlocal diffusion problems with volume constraints” SIAM review, 54 (2012) 667-696.

Peridynamics:* What it is

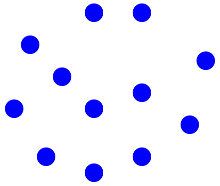
- It’s an extension of continuum mechanics to media with cracks and long-range forces.
- It unifies the mechanics of continuous and discontinuous media within a single, consistent set of equations.



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)

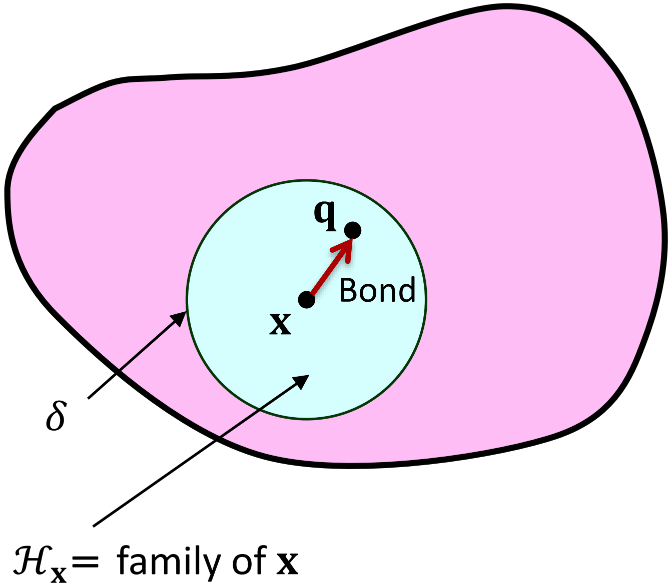
Peridynamics concepts: Horizon and family

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

Peridynamic equilibrium equation

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

$\mathbf{f}$ = bond force density

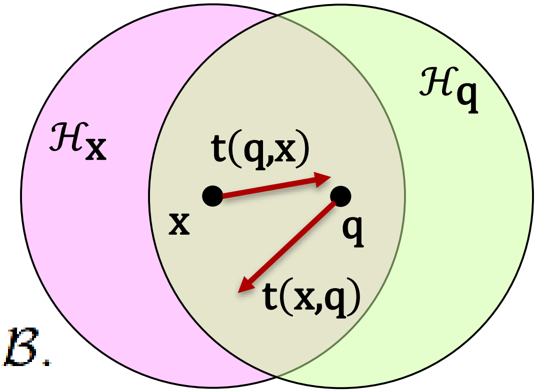


- The peridynamic field equations don't use spatial derivatives
  - so they are compatible with cracks.

General references

- SS, Journal of the Mechanics and Physics of Solids (2000)
- SS and R. Lehoucq, Advances in Applied Mechanics (2010)

Structure of the bond force



- Equilibrium equation:

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

- The pairwise bond force f has the following structure:

$$\mathrm{f}(\mathrm{q},\mathrm{x}) = \mathrm{t}(\mathrm{q},\mathrm{x}) - \mathrm{t}(\mathrm{x},\mathrm{q})$$

where the t terms are found from the material models at x and q separately:

$$\mathrm{t}(\mathrm{q},\mathrm{x}) = \underline{\mathrm{T}}[\mathrm{x}]\langle \mathrm{q}-\mathrm{x}\rangle, \qquad \mathrm{t}(\mathrm{x},\mathrm{q}) = \underline{\mathrm{T}}[\mathrm{q}]\langle \mathrm{x}-\mathrm{q}\rangle.$$

- This "state notation" is described next...

States

- A *state* is a mapping whose domain is a family.

$$\underline{A}\langle\xi\rangle = \text{something}$$

where ξ is a bond in a family $\mathcal{H}$.

- Famous states: Deformation state...

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

Force state...

$$\underline{\mathrm{T}}[\mathrm{x}]\langle\mathrm{q}-\mathrm{x}\rangle = \mathrm{t}(\mathrm{q},\mathrm{x}) = \text{force density within a bond}$$

- Dot product of states $\underline{A}$ and $\underline{B}$:

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

Functions of states

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

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

- Then $\Psi_{\underline{A}}(\underline{A})$ is the *Fréchet derivative* of Ψ at $\underline{A}$.
- Famous Fréchet derivative: Force state in an elastic material...

$$\underline{\mathbf{T}} = W_{\underline{\mathbf{Y}}}$$

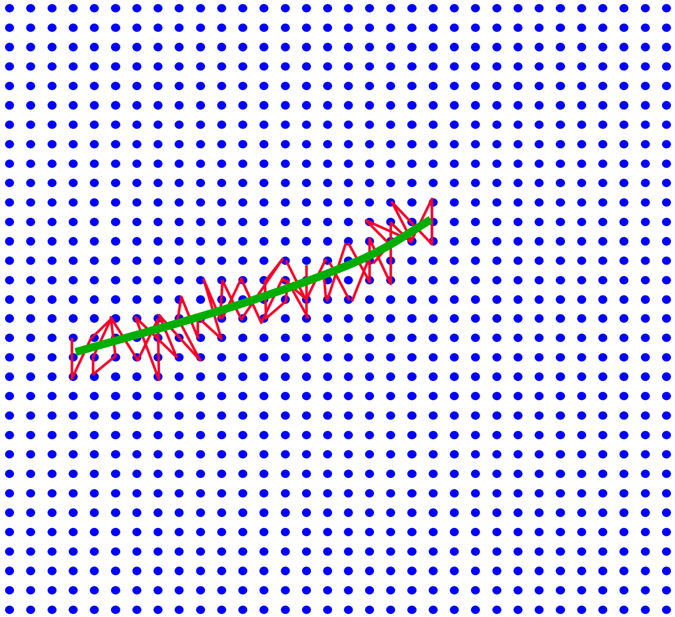
where W is the strain energy density.

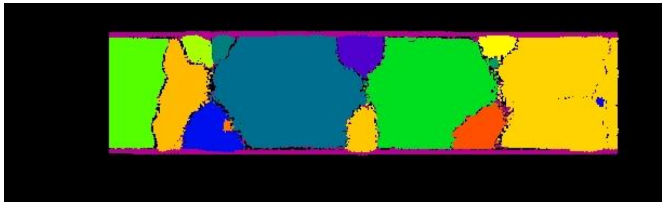
$$dW = \underline{\mathbf{T}} \bullet d\underline{\mathbf{Y}}$$

sums up the work done by bond forces through incremental bond deformation.

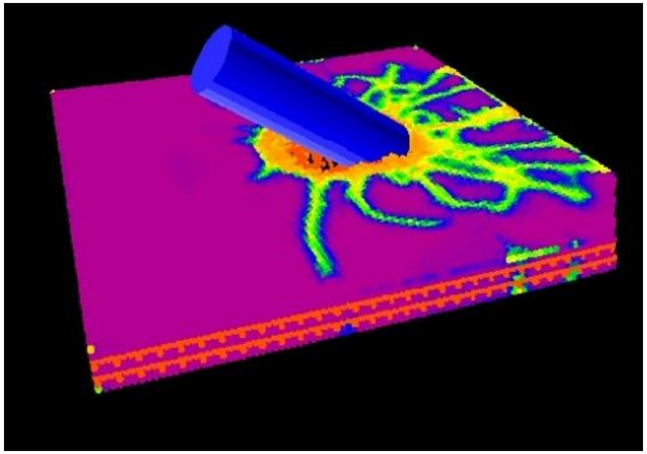
Discontinuities are treated within the basic field equations

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





Cracking in a composite lamina



Impact against reinforced concrete

Peridynamic form of the thermodynamic laws

- First law expression:

$$\begin{aligned}\dot{\varepsilon} &= \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + r + h \\ &= \int_{\mathcal{H}} \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \cdot \underline{\dot{\mathbf{Y}}}\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} + r + h,\end{aligned}$$

  where ε is the internal energy density, r is the source rate, h is the rate of heat transport.

- Second law expression:

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

  where θ is the temperature and η is the entropy.

Additivity of the internal energy density

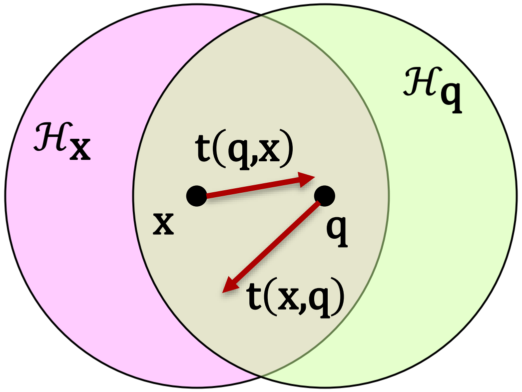
- How to distribute the rate of work done by nonlocal forces acting between subregions $\mathcal{B}_1$ and $\mathcal{B}_2$?

- A 50/50 allocation between the subregions leads to a non-additive concept of ε (Williams & Gurtin, 1971).

- Peridynamic approach: each point owns the work done through the forces in its own force state:

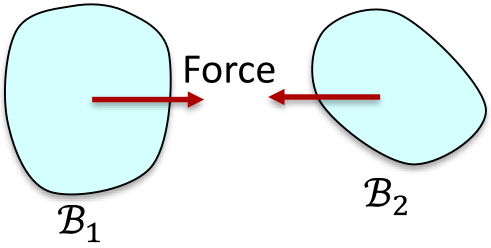
$$\dot{\varepsilon}(\mathrm{x}) = \underline{\mathbf{T}}[\mathrm{x}] \bullet \underline{\dot{\mathbf{Y}}}[\mathrm{x}] + r(\mathrm{x}) + h(\mathrm{x})$$

$$\dot{\varepsilon}(\mathrm{q}) = \underline{\mathbf{T}}[\mathrm{q}] \bullet \underline{\dot{\mathbf{Y}}}[\mathrm{q}] + r(\mathrm{q}) + h(\mathrm{q}).$$



- The resulting ε is additive:

$$\int_{\mathcal{B}_1} \dot{\varepsilon} + \int_{\mathcal{B}_1} \dot{\varepsilon} = \int_{\mathcal{B}_1 \cup \mathcal{B}_2} \dot{\varepsilon}.$$



Forces and entropy in terms of free energy

SS & Lehoucq, Adv Appl Mech (2010)
Oterkus, Madenci & Agwai, JMPS (2014)

- Free energy:

$$\psi = \varepsilon - \theta\eta.$$

- Simple material:

$$\psi(\underline{\mathbf{Y}}, \theta)$$

- First + second laws imply (through Coleman-Noll or similar method):

$$\underline{\mathbf{T}} = \psi_{\underline{\mathbf{Y}}}, \qquad \eta = -\psi_\theta.$$

- If a rate-dependent term is included,

$$\underline{\mathbf{T}} = \psi_{\underline{\mathbf{Y}}} + \underline{\mathbf{T}}^{\mathrm{d}}(\dot{\underline{\mathbf{Y}}})$$

then it can be shown that the following dissipation inequality must hold:

$$\dot{\underline{\mathbf{Y}}} \bullet \underline{\mathbf{T}}^{\mathrm{d}}(\dot{\underline{\mathbf{Y}}}) \geq 0.$$

- It is sufficient but *not necessary* that

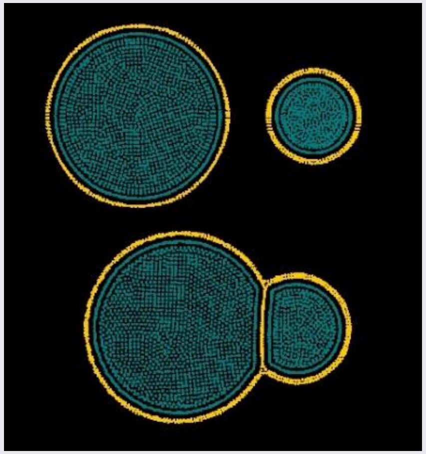
$$\dot{\underline{\mathbf{Y}}}\langle\xi\rangle \bullet \underline{\mathbf{T}}^{\mathrm{d}}(\dot{\underline{\mathbf{Y}}})\langle\xi\rangle \geq 0 \qquad \forall \xi \in \mathcal{H}_{\mathbf{x}}.$$

Examples of how nonlocality in thermodynamics could be useful

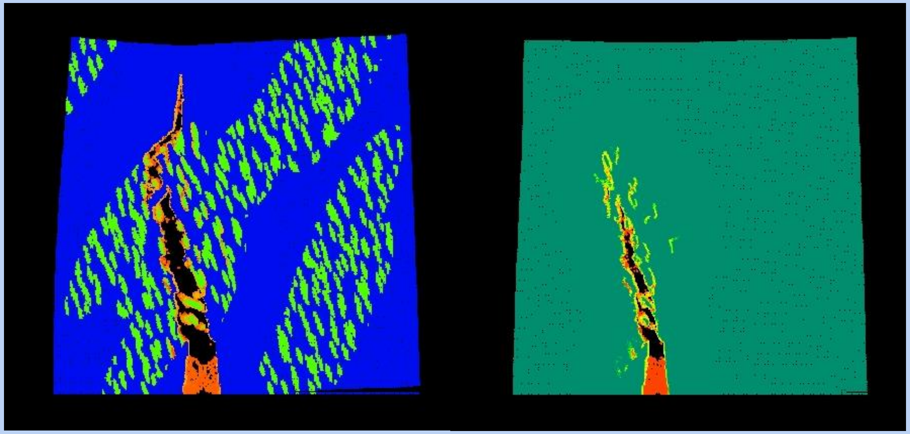
A peridynamic material model of the form

$$\underline{\mathbf{T}} = -(p(\vartheta) + \sigma)\frac{\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|}$$

where p is pressure, ϑ is dilatation, and σ is a constant qualitatively models surface tension.

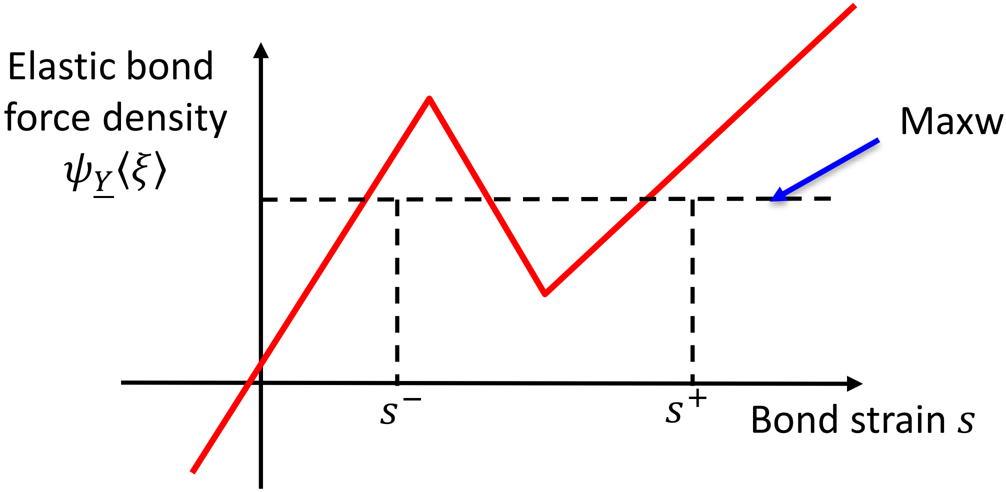


Soap bubbles



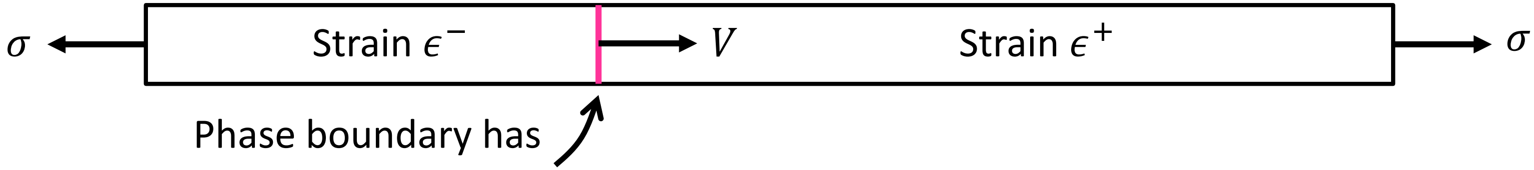
Multiscale model of crack growth

Equilibrium between phases (elastic, isothermal)



Examples of phase transformations in different settings:

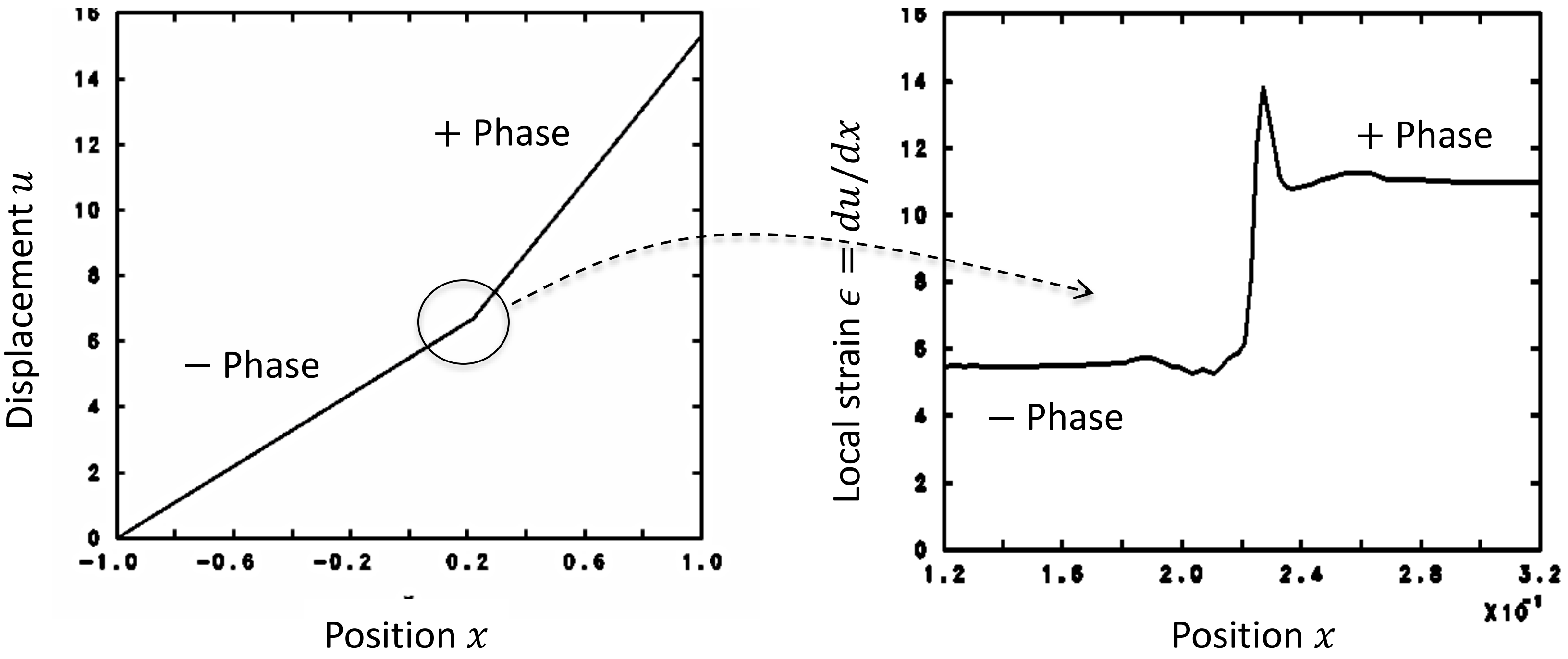
- Elastic bars: Ericksen
- Crystals: James
- Strings: Purohit & Bhattacharya
- Lattices: Truskinovsky & Vainchtein
- Inelastic continuum: Levitas



Phase boundary has
internal structure in a
nonlocal model

Structure of the phase boundary in a peridynamic model (Emu)

- Hard load problem in a bar.
- Similar results to Dayal & Bhattacharya (2006).
- The phase boundary contains internal structure, finite width and energy.



Energy dissipation model for a bond

- A moving phase boundary must dissipate energy (e.g. Abeyaratne and Knowles, 1991).
- Introduce a dissipative term into the material model:

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

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.

Scaling of the damping coefficient with horizon

- Set $u(x,t) = U(z)$, $z = x - Vt$.

- Can show that the total rate of energy dissipation is

$$\dot{\Phi}^{\text{diss}} = \frac{\gamma V^2 \delta^3}{6} \int_{-\infty}^{\infty} (U''')^2 \, dz.$$

- Suppose we want to change horizon δ but keep $\dot{\Phi}^{\text{diss}}$ the same.

- Since $U''' \propto \delta^{-2}$, and the phase boundary width is of order δ, it follows that γ is independent of δ.

The peridynamic dissipation model generates a kinetic relation

- Conjecture: V depends only on the total rate of energy dissipation through the *kinetic relation* (Abeyaratne & Knowles, 1991):

  $$\dot{\Phi}^{\text{diss}} := \mathcal{F} V(\mathcal{F})$$

  where $\mathcal{F}$ is the *driving force*,

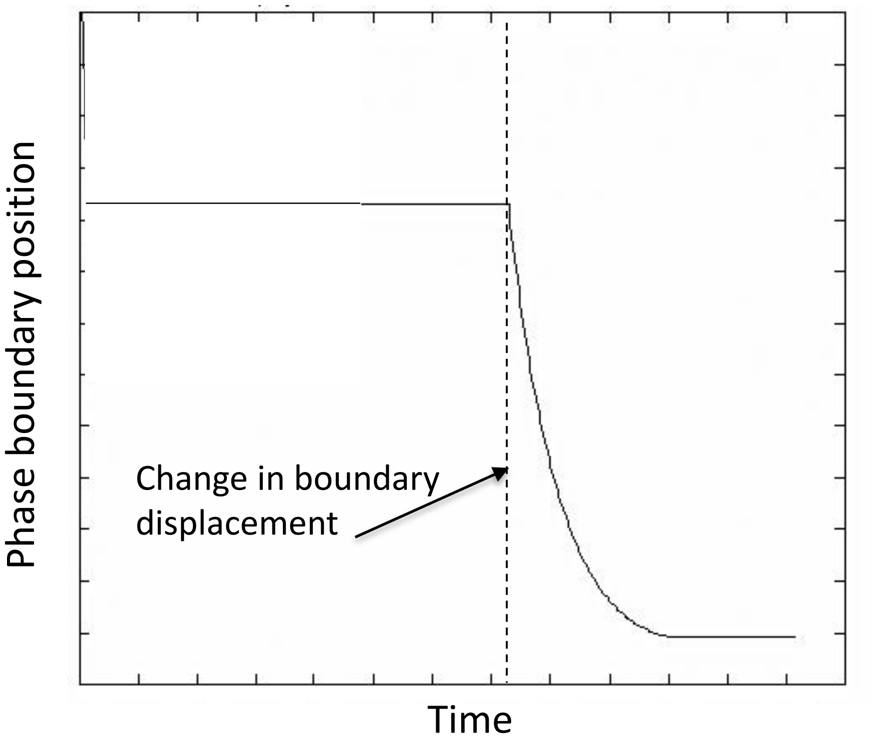
  $$\mathcal{F} = (\varepsilon^{+} - \varepsilon^{-})(\sigma - \sigma_{\text{equil}}).$$

- We found $\dot{\Phi}^{\text{diss}} = KV^2$ if γ is scaled appropriately, hence

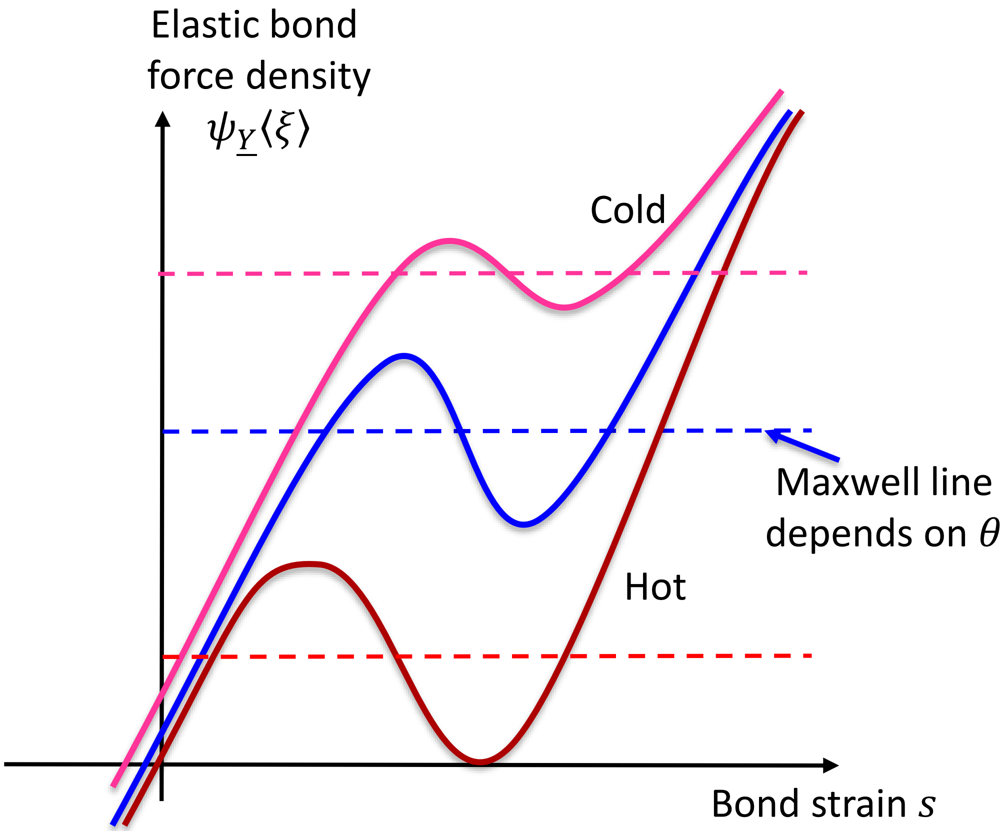
  $$V(\mathcal{F}) = \frac{\mathcal{F}}{K}.$$

Phase boundary subjected to a small change in remote loading (Emu)

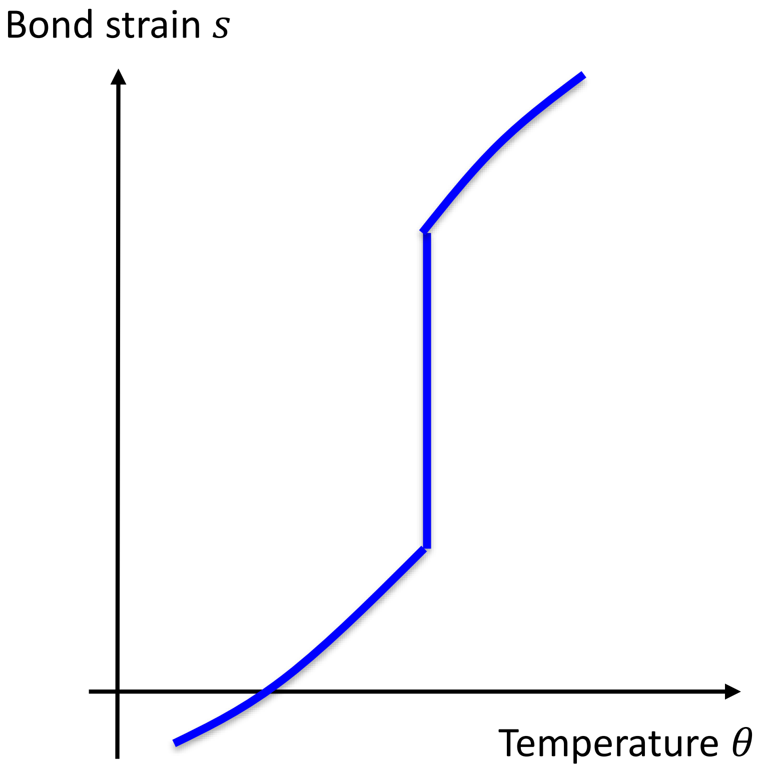
- Peridynamic simulation of a bar using the dissipation model discussed above.
- Perturb the boundary conditions and watch the phase boundary motion.
- Decaying exponential motion tends to confirm the kinetic relation derived above.



Including temperature dependence



Thermoelastic material model



Strain at constant bond force

Conclusions

- Consistent strongly nonlocal thermodynamics is apparently possible in peridynamics.
    - Applications include nanoscale forces and fracture processes.
- New way of modeling dissipation takes advantage of state-based material modeling.
    - With a suitable elastic material model, it leads to a kinetic relation and stable phase boundary motion.
    - Open question: how to treat static metastable states.