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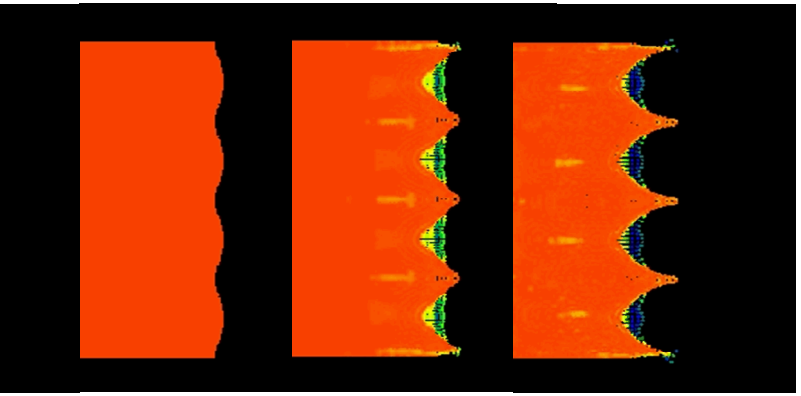
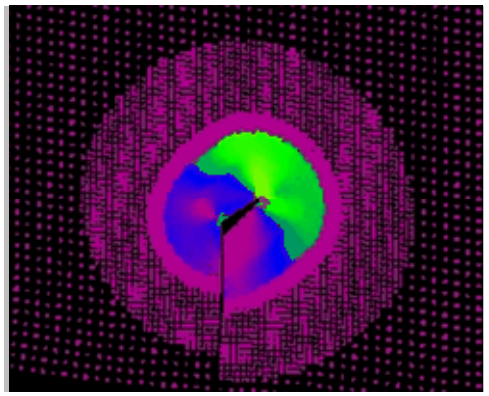
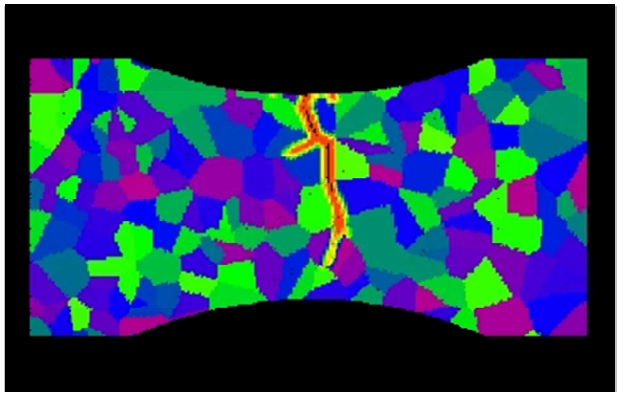

# Energy Balance and Transport in Peridynamics


Stewart Silling

Multiscale Science Departiment

Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

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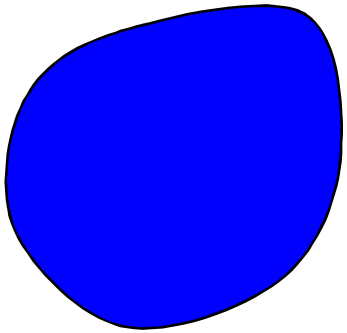
# Outline

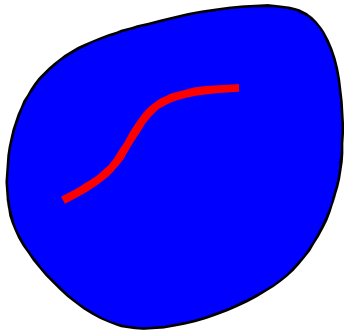
- Peridynamics: review of the mechanical theory.
- First law.
- Heat transport.
- Second law, dissipation, and damage.
- Energy balance near a crack tip (J-integral).

# Purpose of peridynamics

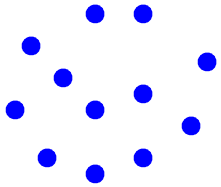
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body with a defect

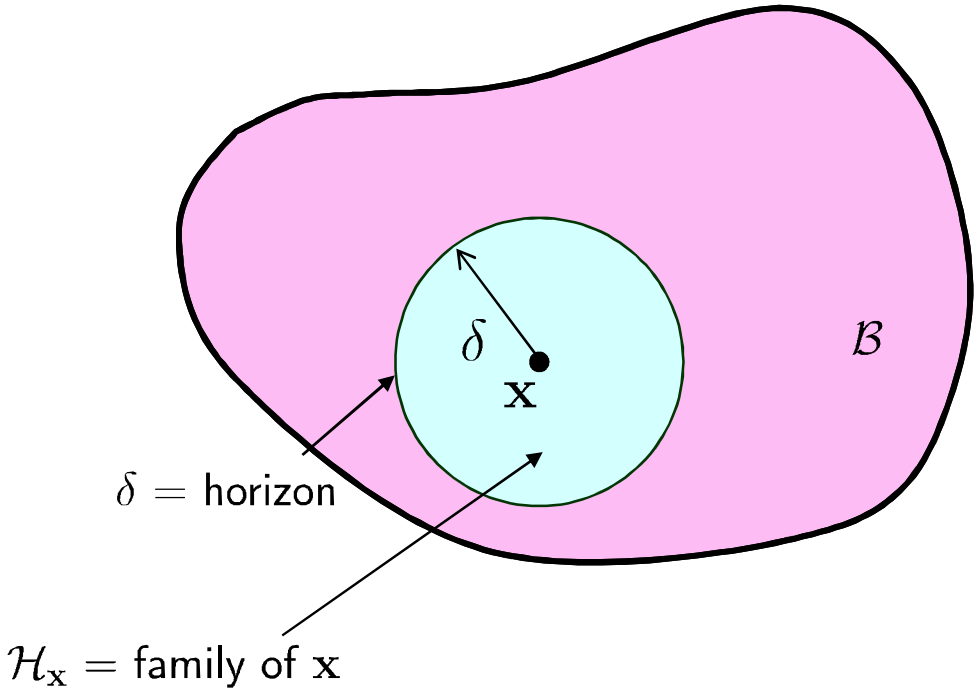


Discrete particles

- Why do this?
  - Avoid coupling dissimilar mathematical systems (A to C).
  - Model complex fracture patterns.
  - Communicate across length scales.

# Peridynamics basics: Horizon and family

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



# 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:

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

# Frechet derivatives

- Let $\psi(\underline{A})$ be a function of a state.
- The Fréchet derivative $\psi_{\underline{A}}$ describes how small changes in each bond affect $\psi$:

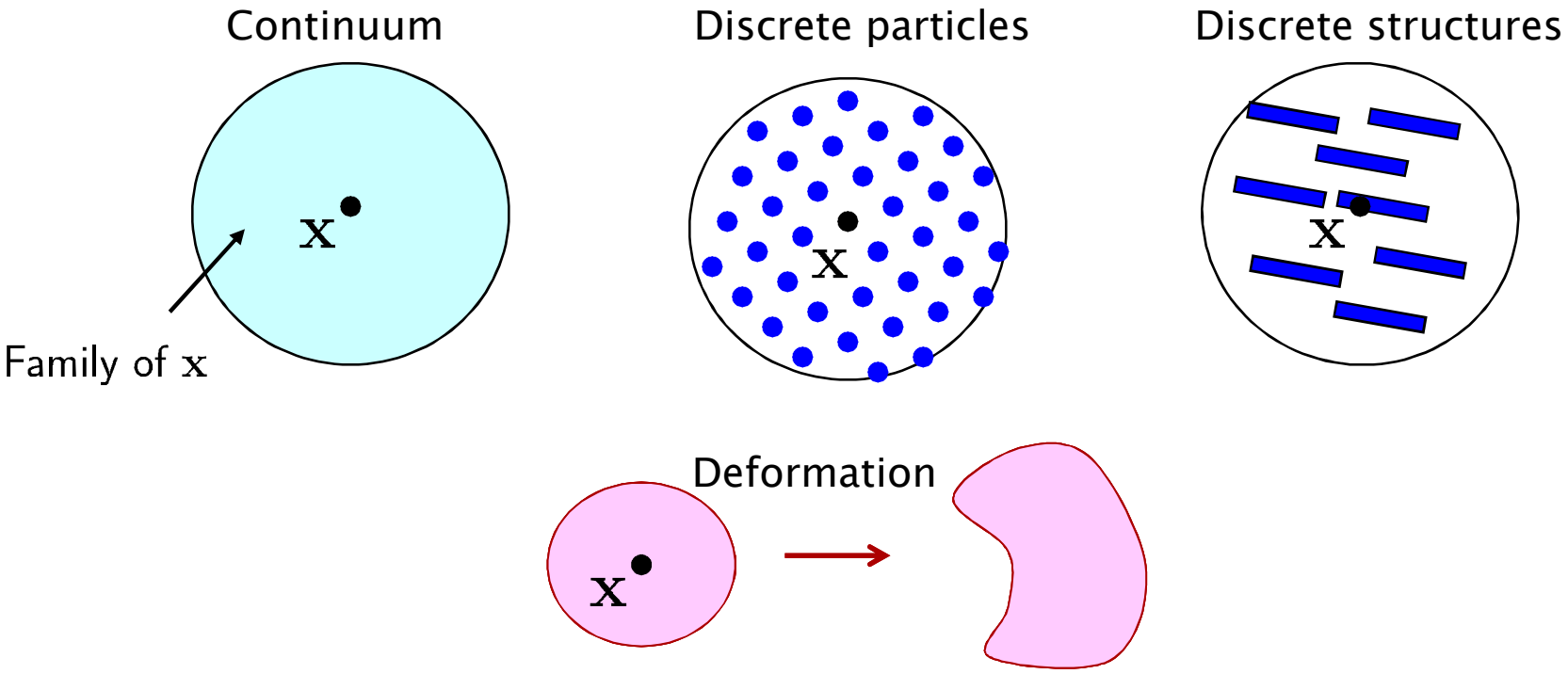
$$\psi(\underline{A} + \Delta\underline{A}) - \psi(\underline{A}) = \psi_{\underline{A}}(\underline{A}) \bullet \Delta\underline{A} + o(\|\Delta\underline{A}\|)$$

  where $\Delta\underline{A}$ is a small increment and $\|\Delta\|$ is the norm

$$\|\underline{A}\| = \sqrt{\underline{A} \bullet \underline{A}}.$$

- Note that $\psi_{\underline{A}}$ is itself a state.

# Strain energy at a point




- Key assumption: the strain energy density at $\mathbf{x}$ is determined by the deformation of its family.

# Potential energy minimization yields the peridynamic equilibrium equation

- Potential energy in a body:

$$\Phi = \int_{\mathcal{B}} (W - \mathbf{b} \cdot \mathbf{y}) \, dV_{\mathbf{x}}$$

where $W$=strain energy density, $\mathbf{b}$=body force density, and $\mathbf{y}$=deformation.

- Take the first variation of $\Phi$ with respect to $\mathbf{y}$.
- The equilibrium equation is the Euler-Lagrange equation:

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

where $\mathbf{f}$ is the *pairwise force density*,

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

# 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:

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

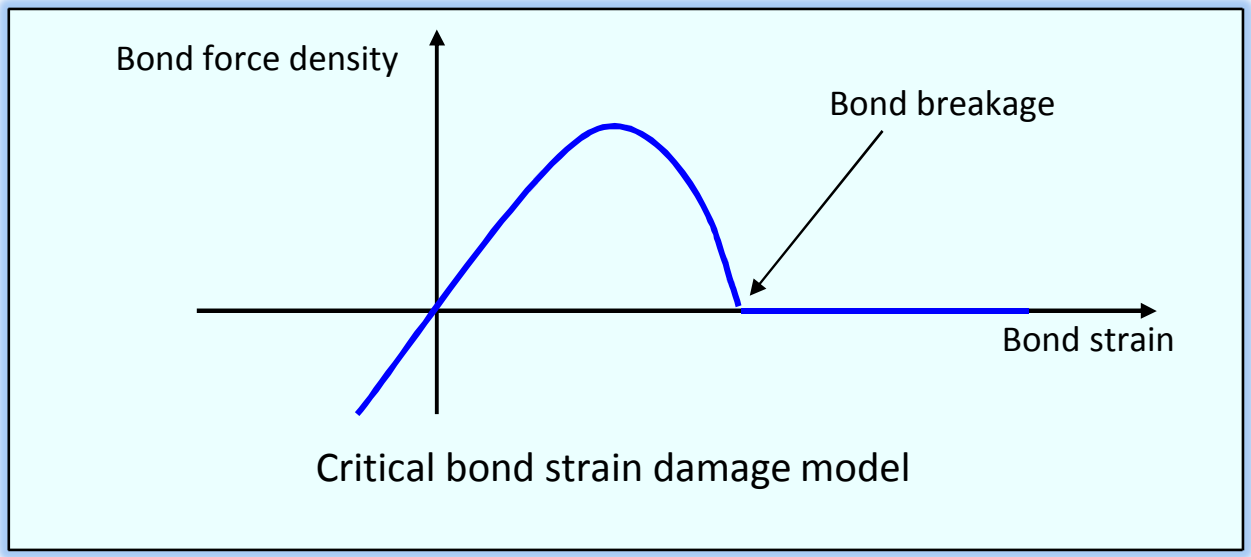
- Special case: in a *bond-based* material, each bond responds independently of all the other bonds.

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

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

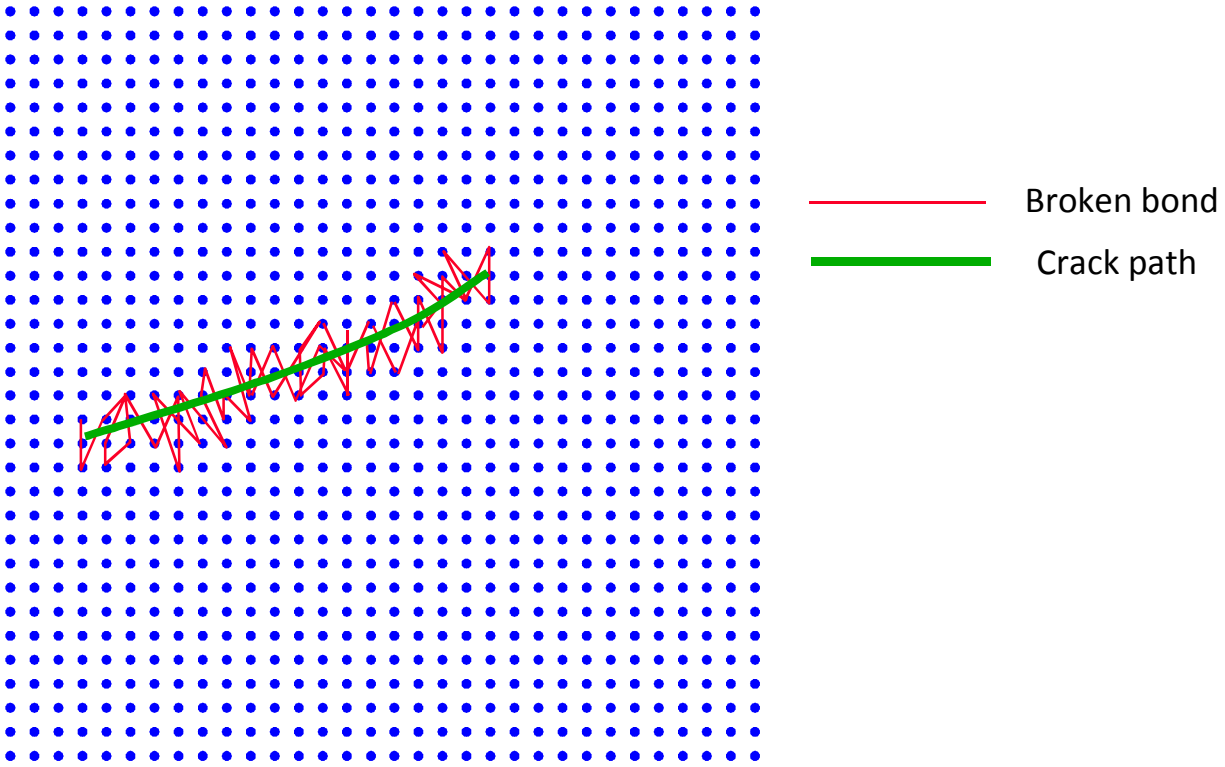
# Damage due to bond breakage

- 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

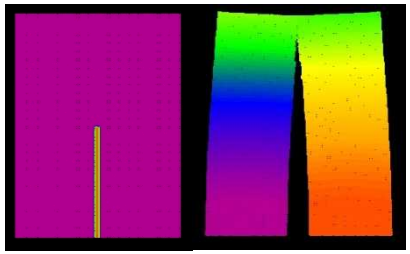
# Autonomous crack growth

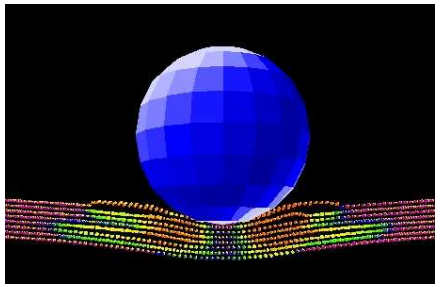


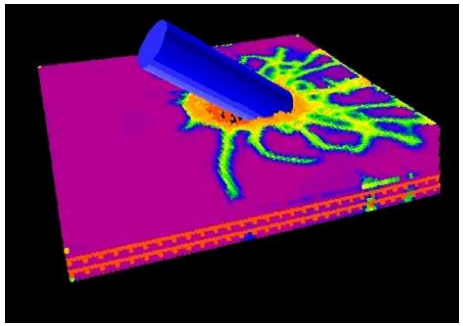

- When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.

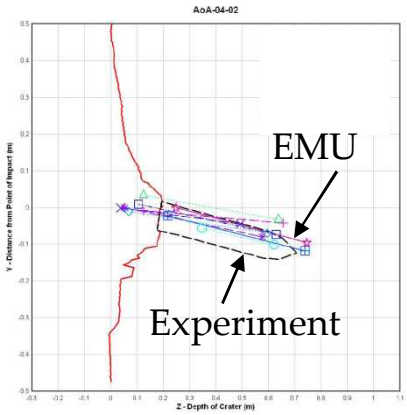
# Examples of validation for peridynamics

- Single crack brittle energy balance
- 3-point bend test
- Dynamic fracture
  - Crack growth velocity
  - Trajectory
  - Branching
- Impact into concrete and aluminum
  - Residual velocity
  - Penetration depth
  - Crater size
- Fatigue
  - S-N curves for aluminum and epoxy
  - Paris law curves for aluminum
- Composite impact, damage, and fracture
  - Delaminations (compare NDE)
  - Residual strength in OHC, OHT
  - Stress concentration profile in OHT
  - Bird strike loading
  - Lamina tensile fracture










# Internal energy density

- First law statement:

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

  where $\varepsilon$=internal energy density, $r$=energy source rate, $q$=energy transport rate.

- Compare this with the statement in the standard theory:

$$\dot{\varepsilon} = \boldsymbol{\sigma} \cdot \dot{\mathbf{F}} + r + q.$$

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

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

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

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

  by the properties of the Fréchet derivative.

# Heat transport: variation form

- Define a functional $I$ by:

$$I = \int_{\mathcal{B}} Z(\nabla\theta)\, dV_{\mathbf{x}} + \int_{\mathcal{B}} r\theta\, dV_{\mathbf{x}}$$

where

$$Z(\nabla\theta) = \frac{1}{2}\nabla\theta \cdot (\mathbf{K}\nabla\theta)$$

and where $\theta$=temperature, $\mathbf{K}$=conductivity tensor, $r$=source rate.

- The Euler-Lagrange equation for this $I$ is the steady-state anisotropic heat equation:

$$\nabla \cdot \mathbf{h} + r = 0, \qquad \mathbf{h} = \mathbf{K}\nabla\theta$$

where $\mathbf{h}$ is the heat flux vector.

- We will postulate a peridynamic version of this variational form...

# Peridynamic heat transport

- Define the *temperature state* by:

$$\underline{\Theta}[\mathbf{x}]\langle\boldsymbol{\xi}\rangle = \theta(\mathbf{x}+\boldsymbol{\xi}) - \theta(\mathbf{x})$$

- Let $Z$ be a scalar valued function of a state.
- Recall that a state is the peridynamic analogue of the gradient.
- Define a functional $I$ by

$$I = \int_{\mathcal{B}} Z(\underline{\Theta}[\mathbf{x}])\, dV_{\mathbf{x}} + \int_{\mathcal{B}} r\theta\, dV_{\mathbf{x}}.$$

# Peridynamic heat equation

- The Euler-Lagrange equation for $I$ is

$$\int_{\mathcal{B}} \left( \underline{Q}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{Q}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + r(\mathbf{x}) = 0$$

  where $\underline{Q}$ is the Fréchet derivative of $Z$:

$$\underline{Q}(\underline{\Theta}) = Z_{\underline{\Theta}}(\underline{\Theta}).$$

- Time-dependent form: If the heat capacity $c$ is constant,

$$\rho c \dot{\theta}(\mathbf{x}, t) = \int_{\mathcal{B}} \left( \underline{Q}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{Q}[\mathbf{x}', t]\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + r(\mathbf{x}, t).$$

# Bond heat transport

- Rewrite the above as

$$\rho c\dot{\theta}(\mathbf{x},t) = \int_{\mathcal{B}} q(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + r(\mathbf{x},t).$$

where

$$q(\mathbf{x}',\mathbf{x},t) = \underline{Q}[\mathbf{x},t]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{Q}[\mathbf{x}',t]\langle \mathbf{x}-\mathbf{x}'\rangle.$$

- $q$ is the rate of heat transport along the bond $\mathbf{x}'-\mathbf{x}$.
- Dimensions are energy/volume$^2$.
- Observe that $q$ is antisymmetric:

$$q(\mathbf{x}',\mathbf{x},t) = -q(\mathbf{x},\mathbf{x}',t)$$

from which it follows that total energy is conserved:

$$\int_{\mathcal{B}} \rho c\dot{\theta}\, dV_{\mathbf{x}} = \int_{\mathcal{B}} r\, dV_{\mathbf{x}}.$$

# Bond-based heat transport model

- Recall that the bond heat transport is derived from $Z$:

$$\underline{Q}\langle\boldsymbol{\xi}\rangle = Z_{\underline{\Theta}}\langle\boldsymbol{\xi}\rangle.$$

- Special case:

$$Z(\underline{\Theta}) = \frac{1}{2}\underline{\Theta} \bullet \underline{\omega\Theta} = \frac{1}{2}\int_{\mathcal{B}} \underline{\omega}\langle\boldsymbol{\xi}\rangle\underline{\Theta}^2\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}}.$$

- Leads to

$$\underline{Q}\langle\boldsymbol{\xi}\rangle = \underline{\omega}\langle\boldsymbol{\xi}\rangle\underline{\Theta}\langle\boldsymbol{\xi}\rangle = \underline{\omega}\langle\boldsymbol{\xi}\rangle(\theta(\mathbf{x}+\boldsymbol{\xi}) - \theta(\mathbf{x})).$$

- The heat flow in each bond is independent of the temperature drop in the other bonds.

For further results and computational examples:
F. Bobaru, and M. Duangpanya, International Journal of Heat and Mass Transfer (2010)
F. Bobaru, and M. Duangpanya, Journal of Computational Physics (2012)

# State-based heat transport model allows interaction between bonds: example

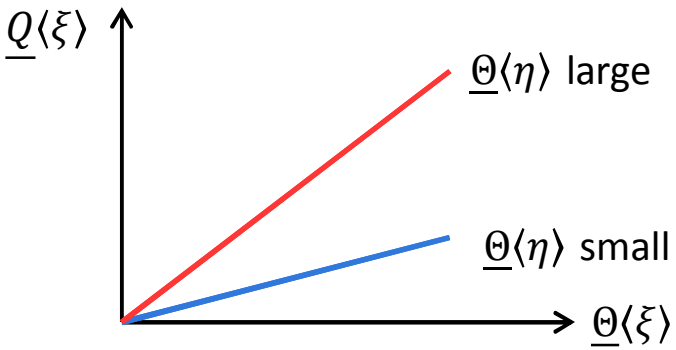
- Suppose there is one special bond $\eta$ that affects the heat flow in the other bonds:

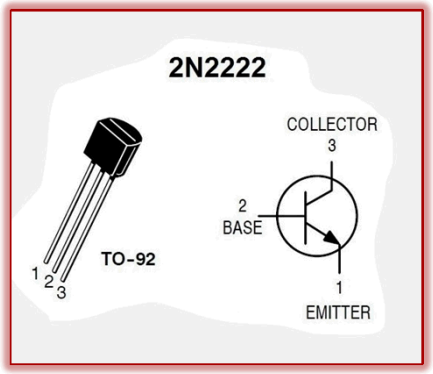
$$Z(\underline{\Theta}) = (\underline{\Theta} \bullet \underline{\omega\Theta})e^{\underline{\Theta}\langle\boldsymbol{\eta}\rangle}.$$

- From Fréchet derivative, find

$$\underline{Q}\langle\boldsymbol{\xi}\rangle = \begin{cases} \underline{\omega}\langle\boldsymbol{\xi}\rangle\underline{\Theta}\langle\boldsymbol{\xi}\rangle e^{\underline{\Theta}\langle\eta\rangle} & \text{if } \boldsymbol{\xi} \neq \boldsymbol{\eta}, \\ \underline{\omega}\langle\boldsymbol{\eta}\rangle\underline{\Theta}\langle\boldsymbol{\eta}\rangle(1 + \underline{\Theta}^2\langle\boldsymbol{\eta}\rangle)e^{\underline{\Theta}\langle\eta\rangle} & \text{if } \boldsymbol{\xi} = \boldsymbol{\eta}. \end{cases}$$

- The special bond $\eta$ acts like a valve that controls the conductivity in the other bonds: "peridynamic transistor."



# Heat flux vector

- Define the *heat flux vector* by

$$\mathbf{H}(\mathbf{x}) = \frac{1}{2}\int_{\mathcal{S}}\int_0^\infty\int_0^\infty (v+w)^2 \underline{Q}(\mathbf{x}+v\mathbf{m}, \mathbf{x}-w\mathbf{m})\mathbf{m}\, dw\, dv\, d\Omega_{\mathbf{m}}$$

  where $\mathcal{S}$ is the unit sphere and $d\Omega_{\mathbf{m}}$ is differential solid angle in the direction of unit vector $\mathbf{m}$.

- By direct differentiation, can show that

$$\nabla\cdot\mathbf{H}(\mathbf{x}) = \int_{\mathcal{B}} q(\mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}'}$$

  so we can write the heat equation as

$$\rho c\dot{\theta} = \nabla\cdot\mathbf{H} + r.$$

- If the horizon gets small and the fields are smooth enough,

$$\mathbf{H} \to \int_{\mathcal{H}} \underline{Q}\langle\boldsymbol{\xi}\rangle\boldsymbol{\xi}\, dV_{\boldsymbol{\xi}}.$$

# Thermodynamic form of a peridynamic material model

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- First law expression:

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

where $\varepsilon$ is the internal energy density, $r$ is the source rate, $h$ is the rate of heat transport.

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

- Second law expression:

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

where $\theta$ is the temperature and $\eta$ is the entropy.

- Free energy:

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

- Assume a material model of the form

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

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

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

# Bond damage

- Each bond is endowed with a damage variable collectively represented as the *damage state*

$$\underline{\phi}\langle\boldsymbol{\xi}\rangle.$$

- Damage cannot decrease:

$$\dot{\underline{\phi}} \geq 0.$$

# Thermodynamic form of damage

- Free energy:

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

where $\varepsilon$=internal energy density, $\theta$=temperature, $\eta$=entropy.

- Assume a material model of the form

$$\psi(\underline{\mathbf{Y}}, \theta, \underline{\phi}), \qquad \eta(\underline{\mathbf{Y}}, \theta, \underline{\phi}).$$

- In addition to

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

the second law leads to the restriction

$$\psi_{\underline{\phi}} \leq 0$$

- The dissipation due to damage growth is

$$\dot{\psi}^{\mathrm{d}} = -\psi_{\underline{\phi}} \bullet \dot{\underline{\phi}}.$$

# Mechanical (only) material model

- Assume a given thermodynamic path (e.g. isothermal).
- By convention, $\psi$ is now called $W$, the strain energy density.
- Assume the dependence on $\underline{\mathbf{Y}}$ is only through bond extension state

$$\psi = W(\underline{e}, \underline{\phi})$$

where $\underline{e}$ is the *extension state* defined by

$$\underline{e}\langle\boldsymbol{\xi}\rangle = |\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|$$

in other words the change in length of a bond.

# Ordinary state model with damage: Thermodynamic force state

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- Assume a strain energy density of the form

$$W(\underline{e}, \underline{\phi})$$

- The force state is given by

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \underline{t}\langle\boldsymbol{\xi}\rangle\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle, \qquad \underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle = \frac{\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|}$$

  where $\underline{t}$ is the scalar force state,

$$\underline{t} = W_{\underline{e}}.$$

- The *thermodynamic force state* is defined by

$$\underline{z} = -W_{\underline{\phi}}.$$

# Condition for damage growth: Failure surface

- Assume a failure criterion of the form

$$S(\underline{z}, \underline{\phi}) = 0$$

  where $S < 0$ for undamaged, unstressed material.

- Assume that damage evolves according to normality:

$$d\underline{\phi} = S_{\underline{z}} d\lambda$$

  where $d\lambda$ is a differential scalar.

- Consistency condition: failure surface and damage evolve such that $S \leq 0$ always.

# Incremental form of bond damage growth

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- Consistency condition implies

$$\begin{aligned} dS = 0 &= \underline{S_z} \bullet d\underline{z} + \underline{S_\phi} \bullet d\underline{\phi} \\ &= \underline{S_z} \bullet (-\underline{\underline{W_{\phi e}}} \bullet d\underline{e} - \underline{\underline{W_{\phi\phi}}} \bullet d\underline{\phi}) + \underline{S_\phi} \bullet d\underline{\phi} \\ &= -\underline{S_z} \bullet \underline{\underline{W_{\phi e}}} \bullet d\underline{e} + (-\underline{S_z} \bullet \underline{\underline{W_{\phi\phi}}} + \underline{S_\phi}) \bullet \underline{S_z} d\lambda \end{aligned}$$

- Solve this for $d\lambda$, find

$$d\underline{\phi} = \underline{S_z} \frac{\underline{S_z} \bullet \underline{\underline{W_{\phi e}}} \bullet d\underline{e}}{\underline{S_z} \bullet \underline{S_\phi} - \underline{S_z} \bullet \underline{\underline{W_{\phi\phi}}} \bullet \underline{S_z}}.$$

- We now know how the bond damage evolves in response to a small change in deformation of the family.

# Example: Linear microelastic material with continuous bond damage

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- Suppose

$$\begin{aligned} W(\underline{e}, \underline{\phi}) &= \int_{\mathcal{H}} w(\underline{e}\langle\boldsymbol{\xi}\rangle)(1 - \underline{\phi}\langle\boldsymbol{\xi}\rangle)d\boldsymbol{\xi} \\ &= \underline{w} \bullet (1 - \underline{\phi}) \end{aligned}$$

  where $w$ is the undamaged micropotential (example: $\underline{w} = C\underline{e}^2/2$).

- This is a bond-based material written in the form of an ordinary state-based model.

- Stuff we need:

$$\underline{t} = w_{\underline{e}}(1 - \underline{\phi}), \qquad \underline{z} = \underline{w}, \qquad W_{\underline{\phi e}} = w_{\underline{e}}\underline{\Delta}, \qquad W_{\underline{\phi\phi}} = 0.$$

# Example ctd: Failure surface

- Further suppose the failure surface is given by

$$S(\underline{z}, \underline{\phi}) = \underline{\mu} \bullet \underline{z} - k(1 + \eta D), \qquad D = \underline{\tau} \bullet \underline{\phi}$$

  where $k$ and $\eta$ are constants; $\underline{\mu}$, $\underline{\tau}$ are scalar influence functions, $\int \underline{\tau} = 1$.

- More stuff:

$$S_{\underline{z}} = \underline{\mu}, \qquad S_{\underline{\phi}} = -k\eta\underline{\tau}.$$

# Example ctd: Explicit form of damage state evolution

- Damage can grow when

$$\underline{\tau} \bullet \underline{w} = \int_{\mathcal{H}} \underline{\tau}\langle\boldsymbol{\xi}\rangle w(\underline{e}\langle\boldsymbol{\xi}\rangle)\, d\boldsymbol{\xi} = k(1+\eta D)$$

  meaning when the weighted average of the bond stored energies is high enough.

- In response to a small change in extension $d\underline{e}$,

$$d\underline{\phi} = \frac{(\underline{\tau} w_{\underline{e}}) \bullet d\underline{e}}{k\eta \underline{\tau} \bullet \underline{\mu}}\, \underline{\mu}.$$

- The relative rate of damage growth among bonds is dictated by the form of $S$, in this case by $\underline{\mu}$.

# Peridynamic CDM derived from standard CDM

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- Suppose we have a classical model:

$$W'(\mathbf{F}, D), \qquad S'(Z, D)$$

where $D$ is a scalar damage variable and $\mathbf{F} = \partial \mathbf{y} / \partial \mathbf{x}$.

- To get a peridynamic version of this, set (as with correspondence models):

$$W(\underline{\mathbf{Y}}, \underline{\phi}) = W'(\bar{\mathbf{F}}(\underline{\mathbf{Y}}), D), \qquad \bar{\mathbf{F}}(\underline{\mathbf{Y}}) = ((\underline{\omega \mathbf{Y}}) * \underline{\mathbf{X}})((\underline{\omega \mathbf{X}}) * \underline{\mathbf{X}})^{-1}.$$

where $\bar{\mathbf{F}}$ is the approximate deformation gradient tensor. Then set

$$S(\underline{z}, \underline{\phi}) = S'(Z(\underline{z}), D(\underline{\phi}))$$

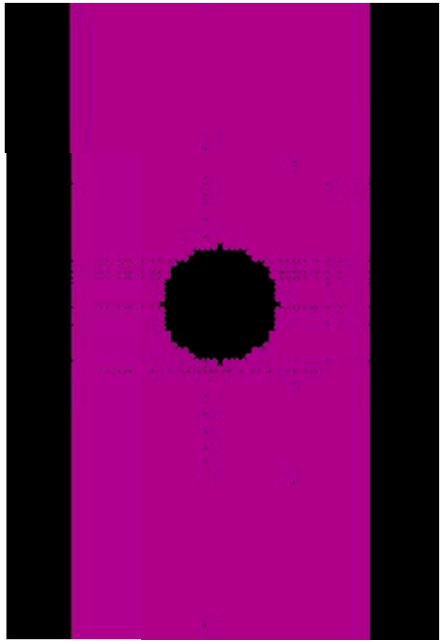
where the classical parameters $D$, $Z$ are found from

$$D(\underline{\phi}) = \underline{\tau} \bullet \underline{\phi}, \qquad Z = -W'_D.$$

- Now we can apply the previous relations to the peridynamic failure surface $S$.

# Computational example

VIDEO



Scalar damage $D$

- Bond-based microelastic, bulk modulus is $\kappa = 100\text{GPa}$.
- Failure surface:

$$S(\underline{z}, \underline{\phi}) = \underline{\mu} \bullet \underline{z} - k(1 + \eta D), \qquad D = \underline{\tau} \bullet \underline{\phi}$$

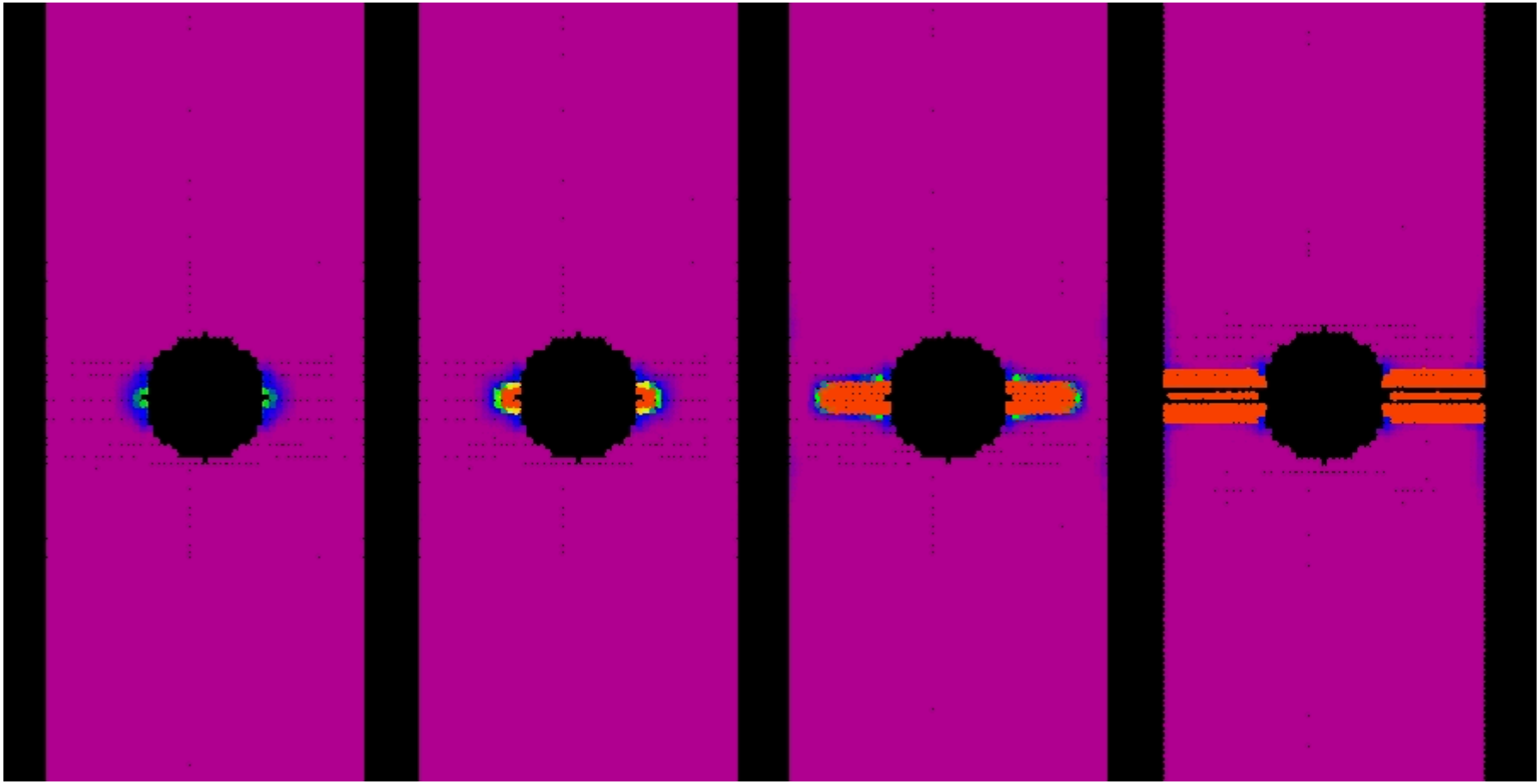
$$\eta = 10, \qquad k = \frac{\kappa \varepsilon_0^2}{2V}, \qquad \varepsilon_0 = 0.01$$

$$\underline{\mu} = \underline{\tau} = \frac{1}{V}$$

where $V$ is the family volume.

- Damage evolution is stable for awhile, then suddenly becomes unstable.

# Computational example, ctd



# Entropy production and energy dissipation

- Again using Coleman-Noll, the rate of entropy production is

$$\dot{\eta} = \frac{\dot{\psi}^{\mathrm{d}}}{\theta}$$

where the *rate of energy dissipation* is given by

$$\begin{aligned}\dot{\psi}^{\mathrm{d}} &= -\psi_{\underline{\phi}} \bullet \underline{\dot{\phi}} \\ &:= -\int_{\mathcal{H}} \psi_{\underline{\phi}}\langle \mathbf{x}' - \mathbf{x}\rangle \; \underline{\dot{\phi}}\langle \mathbf{x}' - \mathbf{x}\rangle \; dV'\end{aligned}$$

where $\underline{\phi}$ is the Fréchet derivative of $\psi$ with respect to $\underline{\phi}$.

- For an isothermal process, therefore

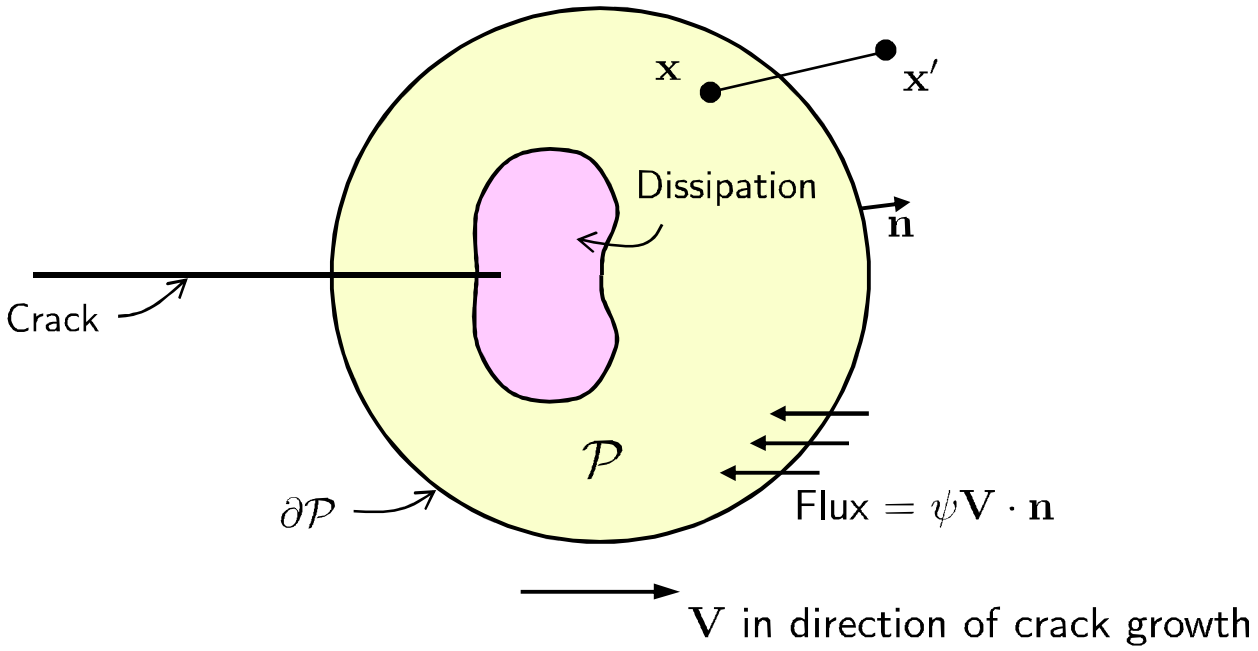
$$\dot{\psi} = \dot{\varepsilon} - \theta\dot{\eta}$$

so that

$$\dot{\psi} = \dot{\varepsilon} - \dot{\psi}^{\mathrm{d}}.$$

# Energy dissipation near a defect

- Assume a homogeneous body.
- Assume a constant defect velocity .
- $\mathcal{P}$ moves with the defect through the reference configuration $\mathcal{B}$.

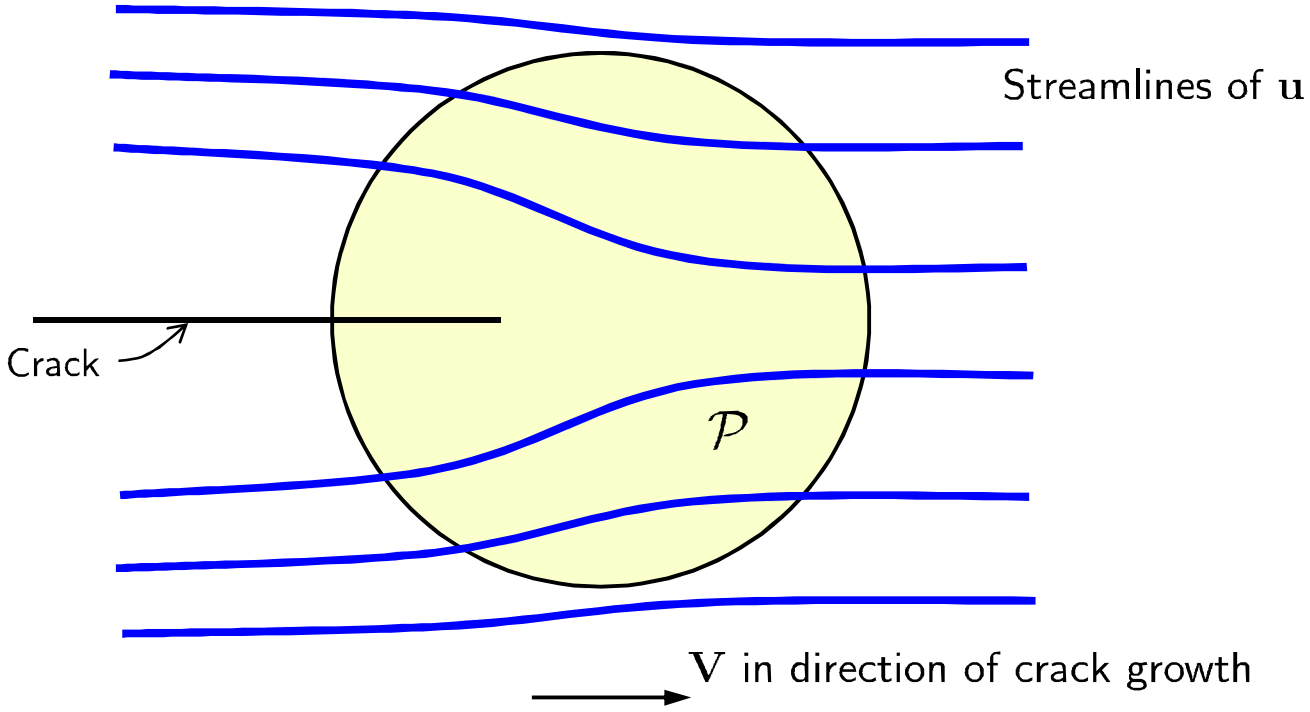


# Steady-state defect growth

- Assumed motion is

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

where $\mathbf{u}$ is a given function and $|\mathbf{V}|$ is small.



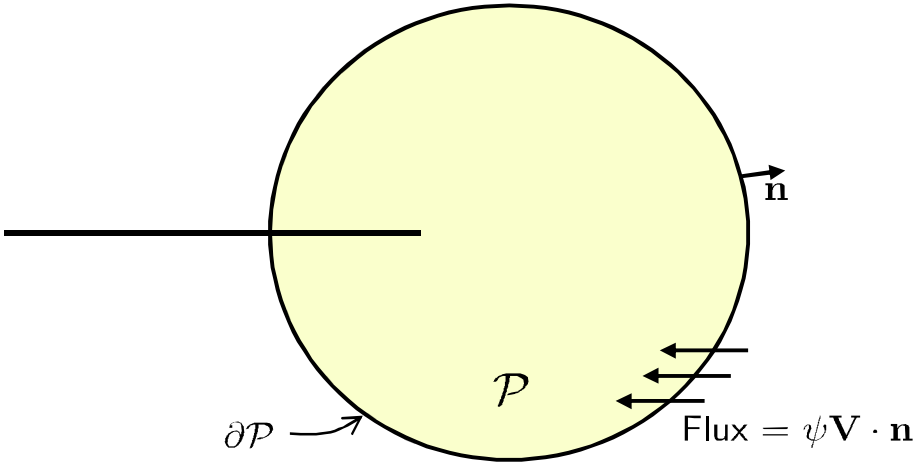
# Free energy balance

- Reynolds transport theorem implies

$$\frac{d}{dt}\int_{\mathcal{P}} \psi \, dV = \int_{\mathcal{P}} \dot{\psi} \, dV + \int_{\partial\mathcal{P}} \psi \mathbf{V} \cdot \mathbf{n} \, dA$$

but steady-state implies

$$\frac{d}{dt}\int_{\mathcal{P}} \psi \, dV = 0.$$



# Work done through the contour

- Recall

$$\dot{\psi} = \dot{\varepsilon} - \dot{\psi}^{\mathrm{d}}.$$

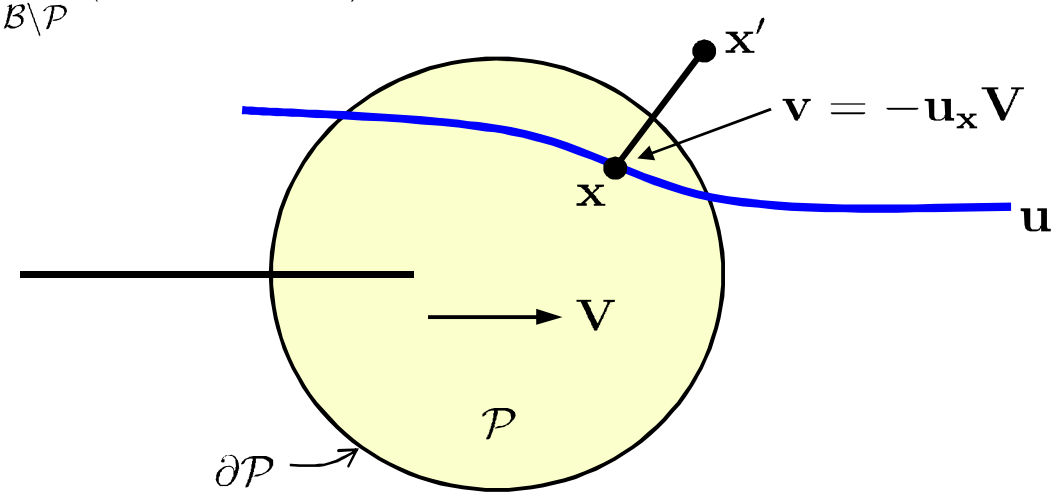
hence

$$\int_{\mathcal{P}} \left(\dot{\varepsilon} - \dot{\psi}^{\mathrm{d}}\right) \, dV + \int_{\partial\mathcal{P}} \psi \mathbf{V} \cdot \mathbf{n} \, dA = 0$$

- Global first law under present assumptions reduces to

$$\int_{\mathcal{P}} \dot{\varepsilon} \, dV = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \left(\mathbf{t} \cdot \mathbf{v}' - \mathbf{t}' \cdot \mathbf{v}\right) \, dV' \, dV$$

$$\mathbf{u}_{\mathbf{x}} = \operatorname{grad} \mathbf{u}(\mathbf{x})$$
$$\mathbf{u}'_{\mathbf{x}} = \operatorname{grad} \mathbf{u}(\mathbf{x}')$$



# Total rate of energy dissipation

- Eliminate $\dot{\varepsilon}$ term to find

$$\int_{\mathcal{P}} \dot{\psi}^{\mathrm{d}}\, dV = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \left(\mathbf{t}\cdot(-\mathbf{u}'_{\mathbf{x}}\mathbf{V}) - \mathbf{t}'\cdot(-\mathbf{u}_{\mathbf{x}}\mathbf{V})\right)\, dV'\, dV + \int_{\partial\mathcal{P}} \psi\mathbf{V}\cdot\mathbf{n}\, dA$$

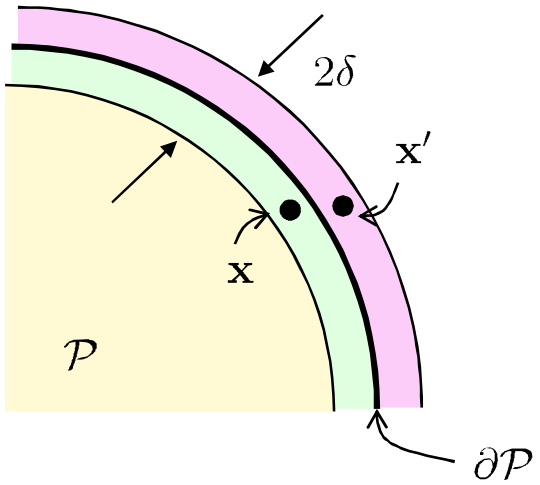
or

$$\int_{\mathcal{P}} \dot{\psi}^{\mathrm{d}}\, dV = \mathbf{J}\cdot\mathbf{V}$$

where

$$\mathbf{J} = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \left(\mathbf{u}_{\mathbf{x}}^{T}\mathbf{t}' - (\mathbf{u}'_{\mathbf{x}})^{T}\mathbf{t}\right)\, dV'\, dV + \int_{\partial\mathcal{P}} \psi\mathbf{n}\, dA$$

**Peridynamic J-integral (3D)**

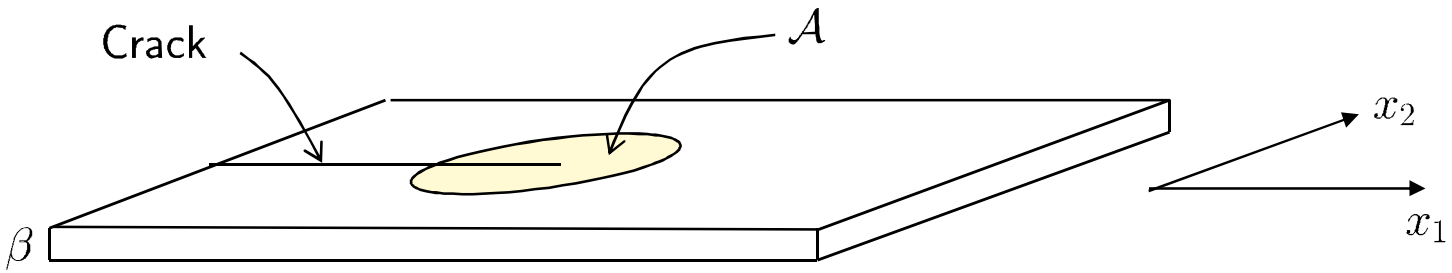



Integrand is nonzero only if $\mathbf{x}$ and $\mathbf{x}'$ are sufficiently close to $\partial\mathcal{P}$.

# Crack in a plate

- Apply to a plate of thickness $\beta$. $\mathcal{A}$ is the interior of a curve in the plane.
- Assume crack grows in the $x_1$ direction.

$$J_1 = \beta^2 \int_{\mathcal{A}} \int_{\mathcal{B}\setminus\mathcal{A}} \left( \frac{\partial \mathbf{u}}{\partial x_1} \cdot \mathbf{t}' - \frac{\partial \mathbf{u}'}{\partial x_1} \cdot \mathbf{t} \right) \, dA' \, dA + \beta \int_{\partial \mathcal{A}} \psi n_2 \, ds$$




For further results and computational examples:
Hu, W., Ha, Y. D., Bobaru, F., & Silling, S. A., International Journal of Fracture (2012).

# Limit of small horizon

- Small horizon:

$$\frac{\partial \mathbf{u}}{\partial x_1} \approx \frac{\partial \mathbf{u}'}{\partial x_1}$$

hence

$$J_1 \approx \beta^2 \int_{\mathcal{A}} \frac{\partial \mathbf{u}}{\partial x_1} \cdot \left[ \int_{\mathcal{B}\setminus\mathcal{A}} (\mathbf{t}' - \mathbf{t}) \, dA' \right] \, dA + \beta \int_{\partial\mathcal{A}} \psi n_2 \, ds$$
$$= \beta \int_{\partial\mathcal{A}} \left[ -\frac{\partial \mathbf{u}}{\partial x_1} \cdot \boldsymbol{\tau} \, ds + \psi n_2 \right] \, ds$$

where $\boldsymbol{\tau}$ is the traction vector on $\partial\mathcal{A}$.

- This is the same as Rice's $J$-integral in the standard theory (except for factor of $\beta$).

# Significance of the peridynamic J-integral

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$$\mathbf{J} = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \left(\mathbf{u}_{\mathbf{x}}^{T}\mathbf{t}' - (\mathbf{u}_{\mathbf{x}}')^{T}\mathbf{t}\right) dV'\, dV + \int_{\partial\mathcal{P}} \psi\mathbf{n}\, dA$$

- Directly computed the free energy dissipated by a defect based on the first law and on steady-state assumptions.
- Did not need to assume anything about the physical dissipative mechanism.
- Did not assume that dissipation is confined to a small process zone.
- Defect may or may not involve a discontinuity in $\mathbf{u}$ (consistent with the "spirit of peridynamics").
- For more info: SS & RL, "Peridynamic Theory of Solid Mechanics," to appear in *Advances in Applied Mechanics*, vol. 44 (2010).

# Extra slides

# Rate of work on a subregion

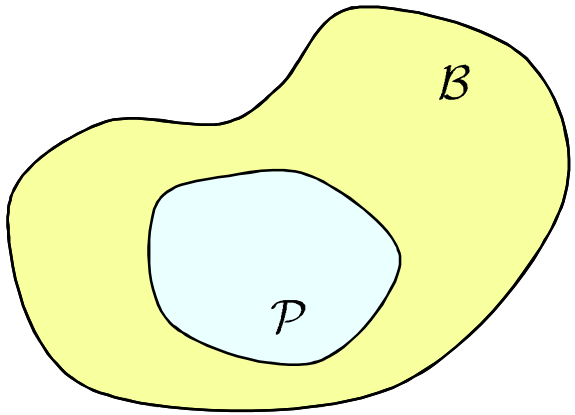
- Recall the balance of linear momentum, multiply through by $\mathbf{v}(\mathbf{x})$, integrate over subregion $\mathcal{P}$:

$$\rho(\mathbf{x})\dot{\mathbf{v}}(\mathbf{x}) - \mathbf{b}(\mathbf{x}) = \int_{\mathcal{B}} \Big(\mathbf{t}(\mathbf{x}', \mathbf{x}) - \mathbf{t}(\mathbf{x}, \mathbf{x}')\Big)\, dV_{\mathbf{x}'}$$

$$\int_{\mathcal{P}} \Big(\rho(\mathbf{x})\dot{\mathbf{v}}(\mathbf{x}) - \mathbf{b}(\mathbf{x})\Big) \cdot \mathbf{v}(\mathbf{x})\, dV = \int_{\mathcal{P}} \int_{\mathcal{B}} \Big(\mathbf{t}(\mathbf{x}', \mathbf{x}) - \mathbf{t}(\mathbf{x}, \mathbf{x}')\Big) \cdot \mathbf{v}(\mathbf{x})\, dV_{\mathbf{x}'}\, dV_{\mathbf{x}}$$

Shorthand:

$$\int_{\mathcal{P}} (\rho\dot{\mathbf{v}} - \mathbf{b}) \cdot \mathbf{v}\, dV = \int_{\mathcal{P}} \int_{\mathcal{B}} (\mathbf{t} - \mathbf{t}') \cdot \mathbf{v}\, dV'\, dV$$



# Rate of work on a subregion, ctd.

- Add $\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}\cdot\mathbf{v}'$ to the double integral, rearrange:

$$\int_{\mathcal{P}} (\rho\dot{\mathbf{v}} - \mathbf{b})\cdot\dot{\mathbf{v}}\, dV = \int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}} (\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v})\, dV'\, dV - \int_{\mathcal{P}}\int_{\mathcal{B}} \mathbf{t}\cdot(\mathbf{v}'-\mathbf{v})\, dV'\, dV$$

- Rewrite this as

$$\dot{\mathcal{K}}(\mathcal{P}) + \mathcal{W}_{\text{abs}}(\mathcal{P}) = \mathcal{W}_{\text{sup}}(\mathcal{P})$$

  where the kinetic energy in $\mathcal{P}$ is $\mathcal{K}(\mathcal{P}) = \int_{\mathcal{P}} \rho\mathbf{v}\cdot\mathbf{v}/2\, dV$,

- the power *supplied to* $\mathcal{P}$ is

$$\mathcal{W}_{\text{sup}}(\mathcal{P}) = \int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}} (\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v})\, dV'\, dV + \int_{\mathcal{P}} \mathbf{b}\cdot\mathbf{v}\, dV,$$

  and the power *absorbed by* $\mathcal{P}$ is

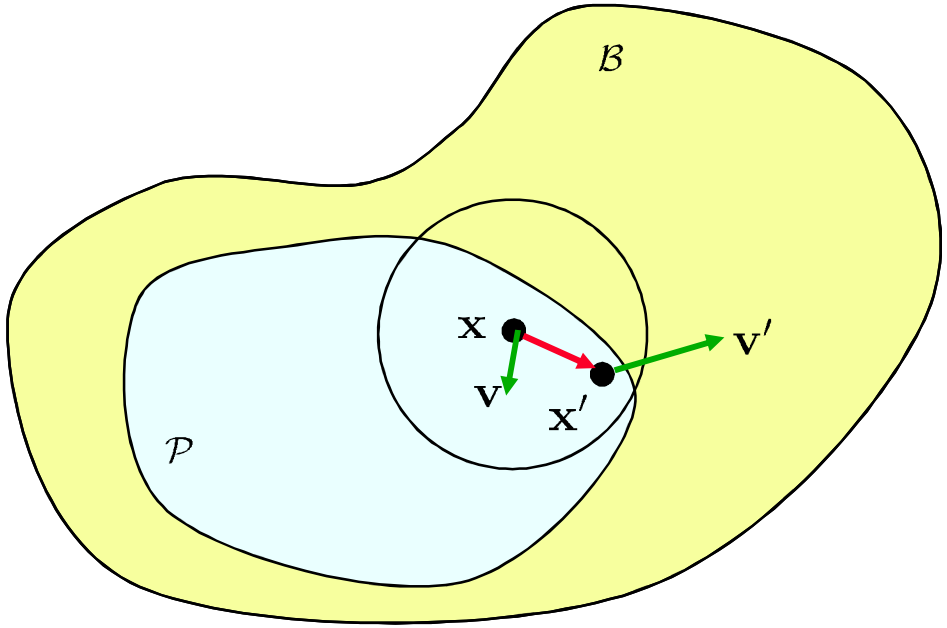
$$\mathcal{W}_{\text{abs}}(\mathcal{P}) = \int_{\mathcal{P}}\int_{\mathcal{B}} \mathbf{t}\cdot(\mathbf{v}'-\mathbf{v})\, dV'\, dV.$$

# Power absorbed: the cartoon

- The power absorbed by $\mathcal{P}$ is

$$\mathcal{W}_{\text{abs}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v}) \, dV' \, dV.$$

- This is the rate of work done *by the entire body* in stretching *all* bonds of $\mathcal{P}$.
- Work done on the bond $\mathbf{x}' - \mathbf{x}$ "belongs to" $\mathcal{P}$ even if $\mathbf{x}'$ is not in $\mathcal{P}$.

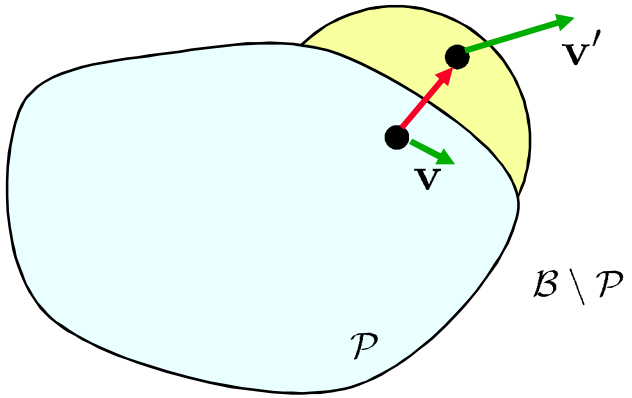


# Power supplied: the cartoon

- The power supplied to $\mathcal{P}$ is

$$\begin{aligned}\mathcal{W}_{\text{sup}}(\mathcal{P}) &= \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} (\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v})\, dV'\, dV + \int_{\mathcal{P}} \mathbf{b}\cdot\mathbf{v}\, dV \\ &= \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \mathbf{t}\cdot(\mathbf{v}' - \mathbf{v})\, dV'\, dV + \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} (\mathbf{t} - \mathbf{t}')\cdot\mathbf{v}\, dV'\, dV + \int_{\mathcal{P}} \mathbf{b}\cdot\mathbf{v}\, dV\end{aligned}$$

- This is the rate of work done *by the exterior of* $\mathcal{P}$ in stretching bonds of $\mathcal{P}$...
- plus the rate of work done *by the exterior of* $\mathcal{P}$ in accelerating $\mathcal{P}$...
- plus the rate of work done by $\mathbf{b}$ on $\mathcal{P}$.



# Global first law expression

- Recall the mechanical energy balance:

$$\dot{\mathcal{K}}(\mathcal{P}) + \mathcal{W}_{\text{abs}}(\mathcal{P}) = \mathcal{W}_{\text{sup}}(\mathcal{P}).$$

- Let $\mathcal{Q}(\mathcal{P})$ be the rate of heat transport into $\mathcal{P}$:

$$\dot{\mathcal{K}}(\mathcal{P}) + \big(\mathcal{W}_{\text{abs}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P})\big) = \mathcal{W}_{\text{sup}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}).$$

- Postulate there exists an *internal energy density* $\mathcal{E}$ such that

$$\dot{\mathcal{E}}(\mathcal{P}) = \mathcal{W}_{\text{abs}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}).$$

- The first law then takes the form

$$\dot{\mathcal{K}}(\mathcal{P}) + \dot{\mathcal{E}}(\mathcal{P}) = \mathcal{W}_{\text{sup}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P})$$

# Additivity of the internal energy

- Let $\mathcal{P}_1$ and $\mathcal{P}_2$ be disjoint subregions of $\mathcal{B}$. Recall

$$\dot{\mathcal{E}}(\mathcal{P}) = \mathcal{W}_{\text{abs}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}), \qquad \mathcal{W}_{\text{abs}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v}) \, dV' \, dV.$$

- Require $\mathcal{Q}(\mathcal{P}_1) + \mathcal{Q}(\mathcal{P}_2) = \mathcal{Q}(\mathcal{P}_1 \cup \mathcal{P}_2)$.
- Compute directly

$$\begin{aligned} \mathcal{W}_{\text{abs}}(\mathcal{P}_1) + \mathcal{W}_{\text{abs}}(\mathcal{P}_2) &= \int_{\mathcal{P}_1} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v}) \, dV' \, dV + \int_{\mathcal{P}_2} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v}) \, dV' \, dV \\ &= \mathcal{W}_{\text{abs}}(\mathcal{P}_1 \cup \mathcal{P}_2) \end{aligned}$$

  hence $\mathcal{E}$ is *additive*:

$$\mathcal{E}(\mathcal{P}_1) + \mathcal{E}(\mathcal{P}_2) = \mathcal{E}(\mathcal{P}_1 \cup \mathcal{P}_2).$$

- It follows there exists an *internal energy density* $\varepsilon$ such that

$$\mathcal{E}(\mathcal{P}) = \int_{\mathcal{P}} \varepsilon \, dV.$$

# Structure of the energy balance

- Let $q(\mathbf{x}', \mathbf{x})$=heat transport rate, $r$=source rate. Write the first law in the form

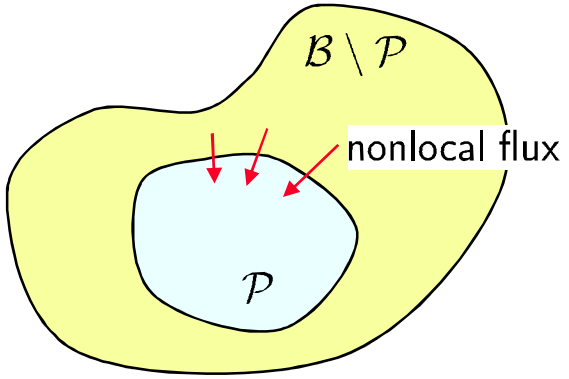
$$\frac{d}{dt}\int_{\mathcal{P}}\left(\frac{\rho\mathbf{v}\cdot\mathbf{v}}{2}+\varepsilon\right)\,dV=\int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}}\left(\mathbf{t}\cdot\mathbf{v}'-\mathbf{t}'\cdot\mathbf{v}+q\right)\,dV'\,dV+\int_{\mathcal{P}}\left(\mathbf{b}\cdot\mathbf{v}+r\right)\,dV.$$

- Assume $q$ is antisymmetric, *i.e.*, $q(\mathbf{x}, \mathbf{x}') = -q(\mathbf{x}', \mathbf{x})$.
- So the first law has the general form

$$\frac{d}{dt}\int_{\mathcal{P}}\text{intensive quantity}\,dV=\int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}}\text{nonlocal flux}\,dV'\,dV+\int_{\mathcal{P}}\text{source rate}\,dV$$

  where the nonlocal flux is antisymmetric.

- This general form was anticipated by Noll (1955).
- Additivity of the left hand side depends on the double integral being $\int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}}$ (or equivalently $\int_{\mathcal{P}}\int_{\mathcal{B}}$).



# Local form of the first law

- Recall that for all choices of $\mathcal{P} \subset \mathcal{B}$,

$$\dot{\mathcal{E}}(\mathcal{P}) = \mathcal{W}_{\text{abs}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P})$$

or

$$\int_{\mathcal{P}} \dot{\varepsilon}\, dV = \int_{\mathcal{P}} \left( r + \int_{\mathcal{B}} \left( \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v}) + q \right) dV' \right) dV$$

- Localize to get the local form of the first law:

$$\dot{\varepsilon} = r + h + \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v})\, dV'$$

where $h = \int_{\mathcal{P}} q\, dV'$.

# Peridynamic "stress power"

- Recall the definitions

$$\mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x}) = \underline{\mathbf{Y}}\langle \mathbf{x}' - \mathbf{x}\rangle, \qquad \mathbf{t}(\mathbf{x}', \mathbf{x}) = \underline{\mathbf{T}}\langle \mathbf{x}' - \mathbf{x}\rangle.$$

- Define at any point $\mathbf{x}$

$$\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} = \int_{\mathcal{B}} \underline{\mathbf{T}}\langle \mathbf{x}' - \mathbf{x}\rangle \cdot \underline{\dot{\mathbf{Y}}}\langle \mathbf{x}' - \mathbf{x}\rangle \, dV'.$$

- So the local first law can be written as

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

- Compare this with standard theory:

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

- Conclude that $\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}}$ is the (nonlocal) peridynamic version of the stress power.
- It represents the rate of work done in stretching the bonds of $\mathbf{x}$.

# Second law and its implications (Coleman-Noll)

- Postulate the second law has the form

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

  where $\theta$=temperature and $\eta$=entropy density.

- Define the free energy by

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

- Combine this with first and second laws to find

$$\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} - \dot{\theta}\eta - \dot{\psi} \geq 0. \tag{1}$$

- Suppose

$$\psi = \psi(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta), \qquad \eta = \eta(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta).$$

- Take time derivative:

$$\dot{\psi} = \psi_{\underline{\mathbf{Y}}} \bullet \underline{\dot{\mathbf{Y}}} + \psi_{\underline{\dot{\mathbf{Y}}}} \bullet \underline{\ddot{\mathbf{Y}}} + \psi_\theta \dot{\theta} \tag{2}$$

  where $\psi_{\mathbf{Y}}$ indicates the Fréchet derivative.

# Second law and its implications (Coleman-Noll), ctd.

- Combine (1), (2) to obtain

$$\left(\underline{\mathbf{T}} - \psi_{\underline{\mathbf{Y}}}\right) \bullet \underline{\dot{\mathbf{Y}}} + \psi_{\underline{\dot{\mathbf{Y}}}} \bullet \underline{\ddot{\mathbf{Y}}} - (\psi_\theta + \eta)\dot{\theta} \geq 0.$$

- Coleman-Noll: Assume $\underline{\dot{\mathbf{Y}}}$, $\underline{\ddot{\mathbf{Y}}}$, and $\dot{\theta}$ can be varied independently. Inequality above must hold in all such cases.

- Conclude:

$$\underline{\mathbf{T}} = \psi_{\underline{\mathbf{Y}}}, \qquad \psi_{\underline{\dot{\mathbf{Y}}}} = 0, \qquad \eta = -\psi_\theta.$$

- This doesn't say that $\underline{\mathbf{T}}$ is independent of $\underline{\dot{\mathbf{Y}}}$.

- By following Fried (2010), we can similarly derive a dissipation inequality:

$$\underline{\mathbf{T}} = \underline{\mathbf{T}}^e(\underline{\mathbf{Y}}, \theta) + \underline{\mathbf{T}}^d(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta) \quad \Longrightarrow \quad \underline{\mathbf{T}}^d \bullet \underline{\dot{\mathbf{Y}}} \geq 0.$$

- Can treat damage evolution similarly.