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The Peridynamic Model and Nonlocality

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Purposes of the peridynamic model

- To treat material with cracks using the same equations as without cracks.
- To treat discrete particles using the same equations as continua.

- Why do this?
  - The standard theory is not a good tool for modeling cracks.
  - PDEs do not apply on discontinuities or to discrete particles.
  - This leads to the need for special techniques when cracks are present.
  - No natural way to couple atoms to continua.

Strategy

Replace the standard PDEs with integral equations.

- The integral equations involve interaction between points separated by finite distances (nonlocality).
- The integral equations are not derivable from the PDEs.
    - But they converge to the PDEs in the limit of small length scales.

Bond–based peridynamic model

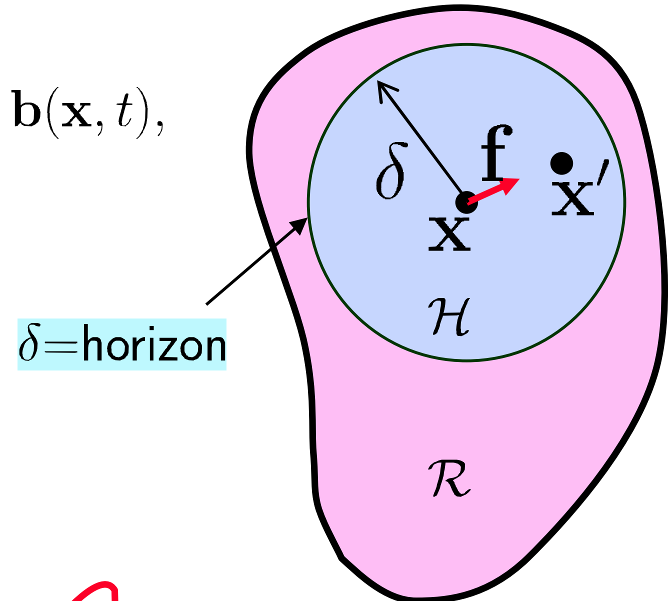
The original (2000) peridynamic model...

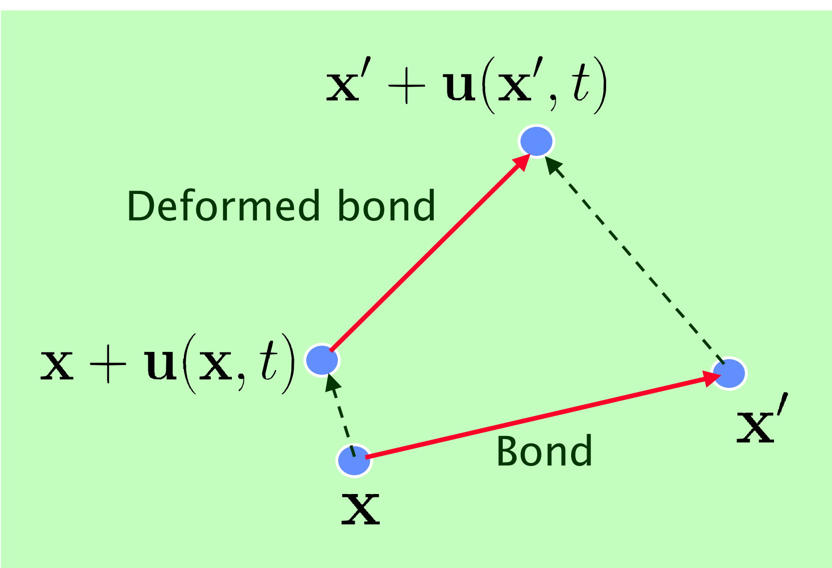
$$\rho \ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{u}(\mathbf{x}',t) - \mathbf{u}(\mathbf{x},t), \mathbf{x}' - \mathbf{x}) \, dV_{\mathbf{x}} + \mathbf{b}(\mathbf{x},t),$$

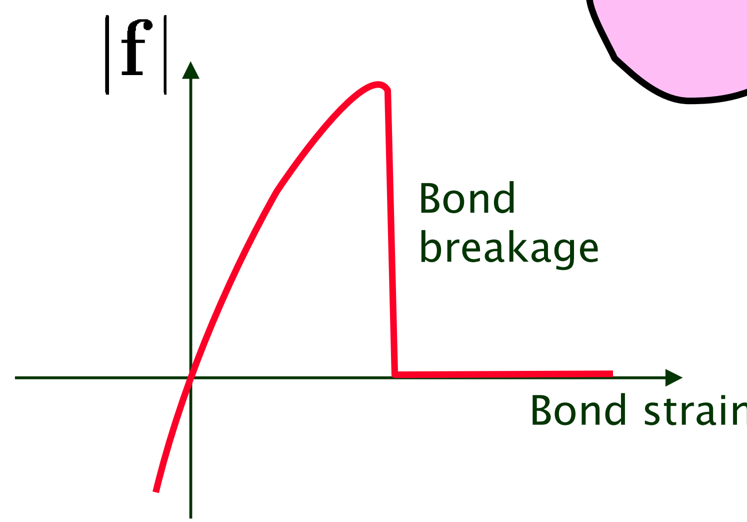
$\mathbf{u}$=displacement, $\mathbf{b}$=body force density

$\mathbf{f}$=pairwise force function (force/volume^2)

Sums up the forces that all the $\mathbf{x}'$ exert on $\mathbf{x}$.







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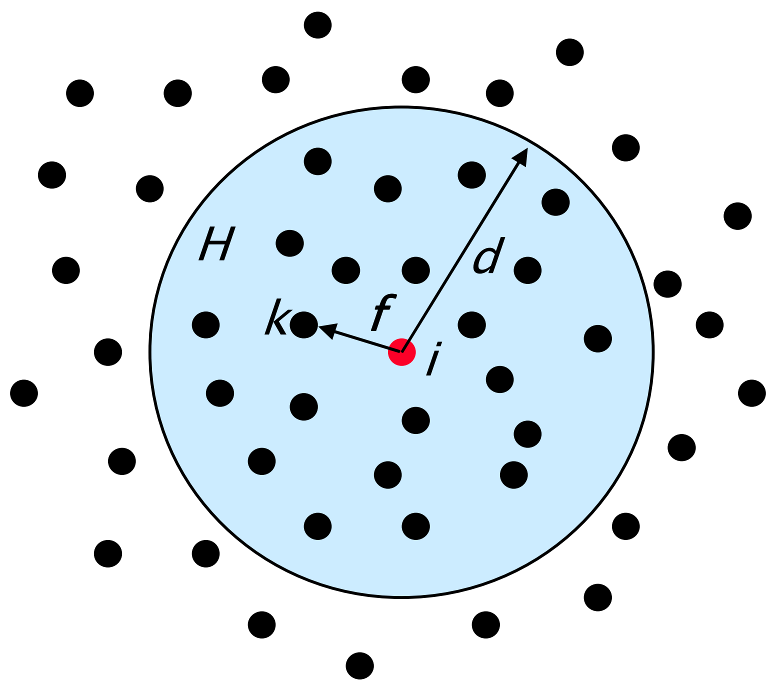
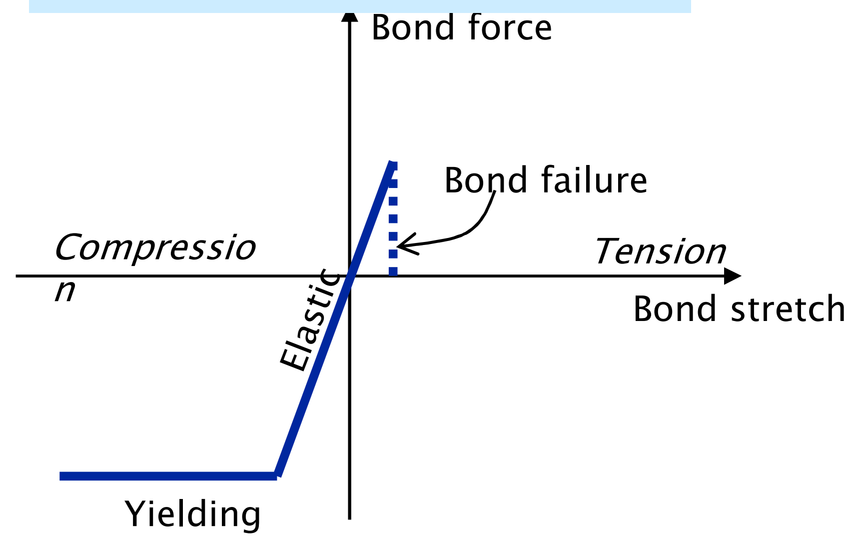
EMU numerical method and material model incorporate damage at the bond level

- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.
- Parameters come from measurable elastic-plastic and fracture data for materials.

$$\rho \ddot{\boldsymbol{u}}_i^n = \sum_{k \in H} \boldsymbol{f}(\boldsymbol{u}_k^n - \boldsymbol{u}_i^n, \boldsymbol{x}_k - \boldsymbol{x}_i) \Delta V_i + \boldsymbol{b}(\boldsymbol{x}_i, t)$$



All material-specific behavior is contained in the function *f*.



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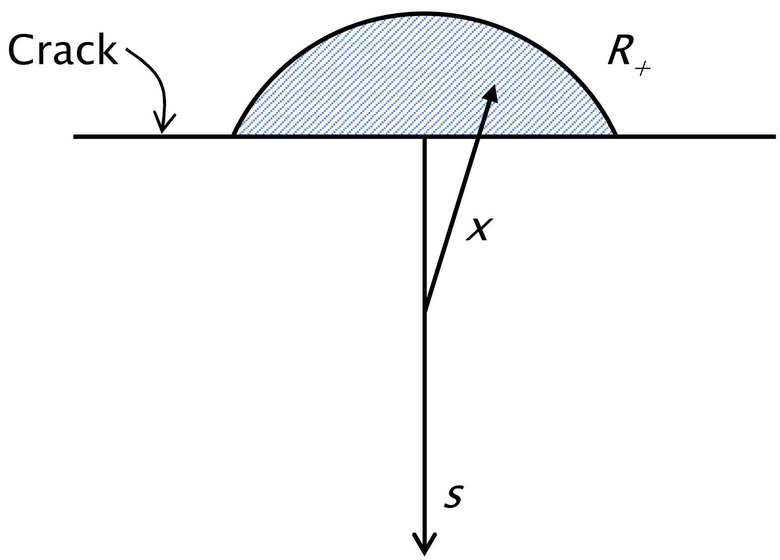
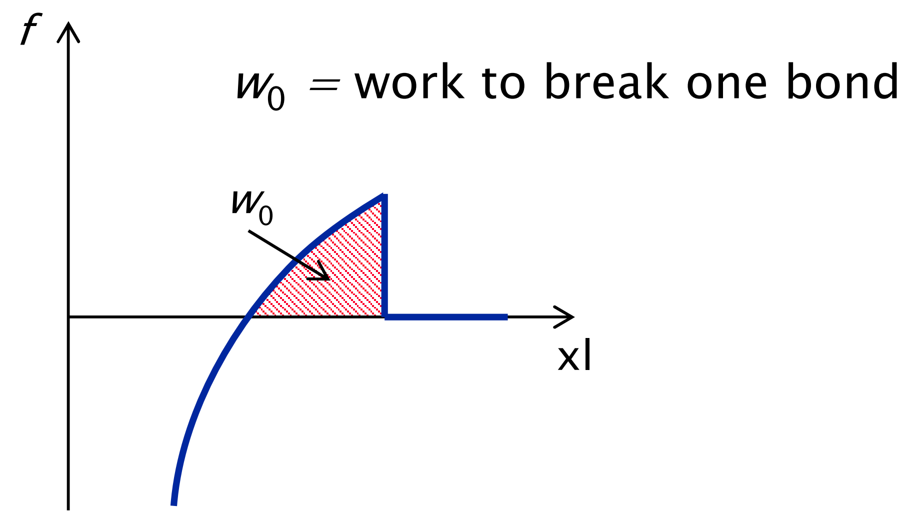
Peridynamic theory:
Energy required to advance a crack

- Adding up the work needed to break all bonds across a line yields the energy release rate:

$$G = 2h\int_0^{\delta}\int_{R_+} w_0 \, dV ds$$





There is also a version of the J-integral that applies in this theory.

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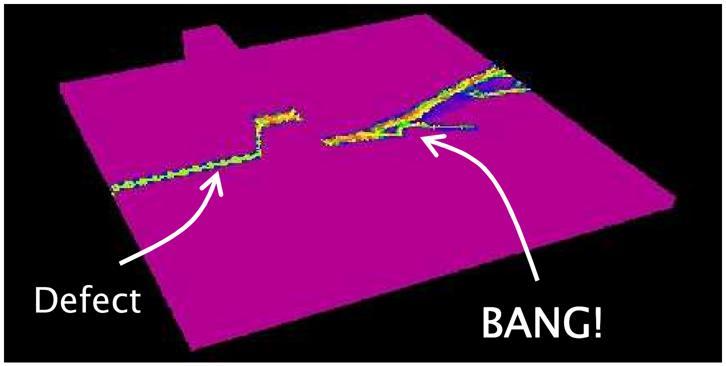
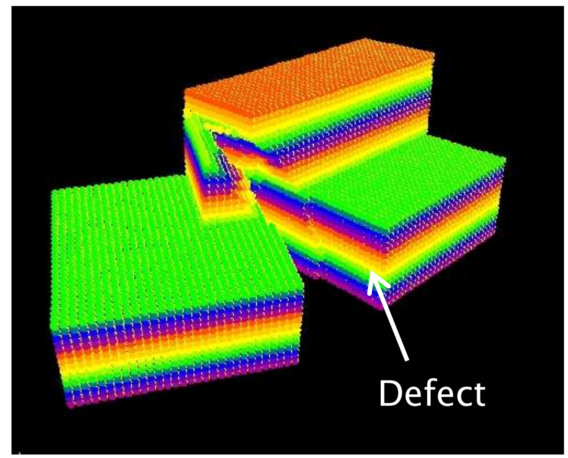
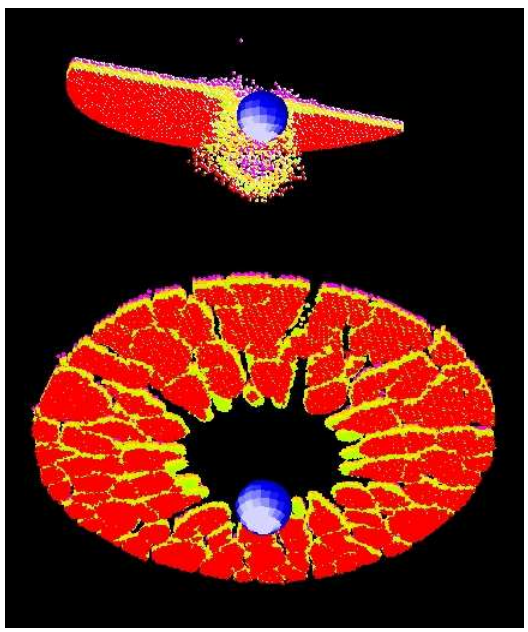
Bond based PD:
Fracture and fragmentation



Transition to unstable crack growth



Crack turning in a 3D feature



Impact and fragmentation

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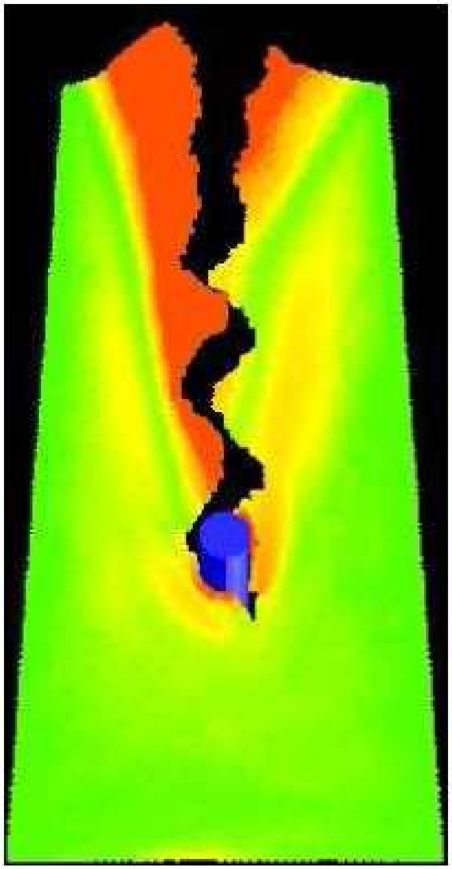
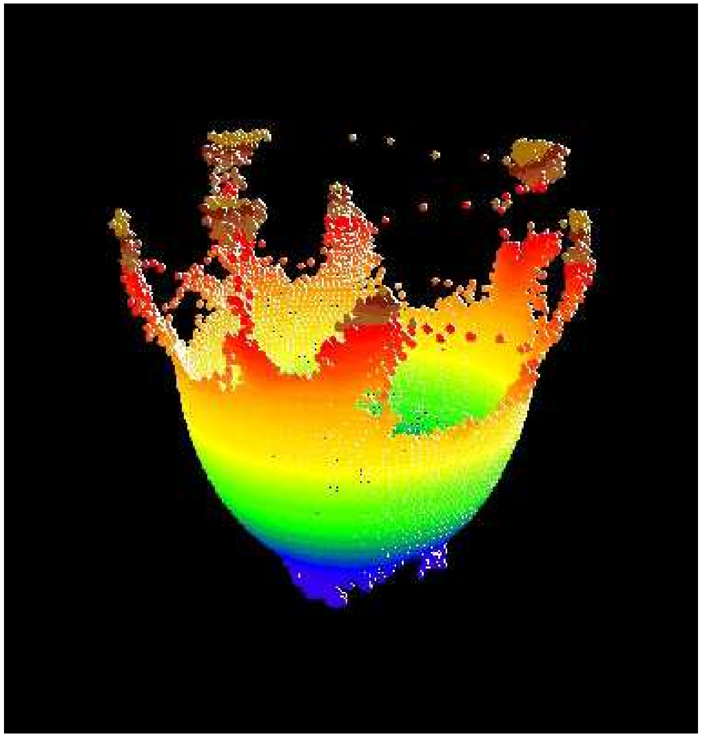
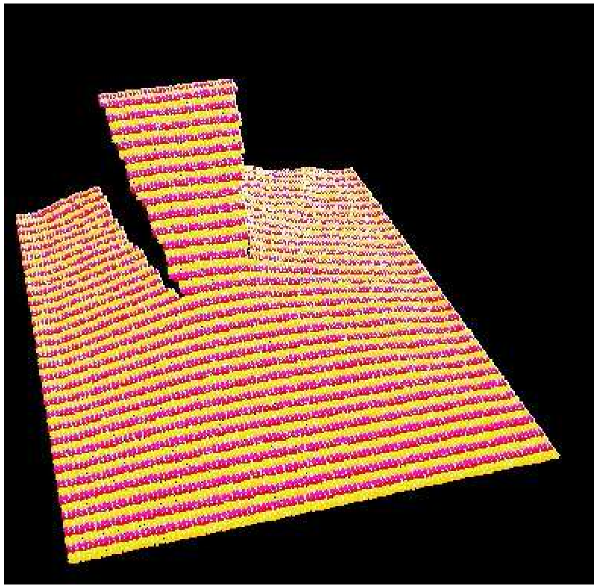
Bond based PD:
Elastic membranes


Tearing instability


Balloon pop


Peeling

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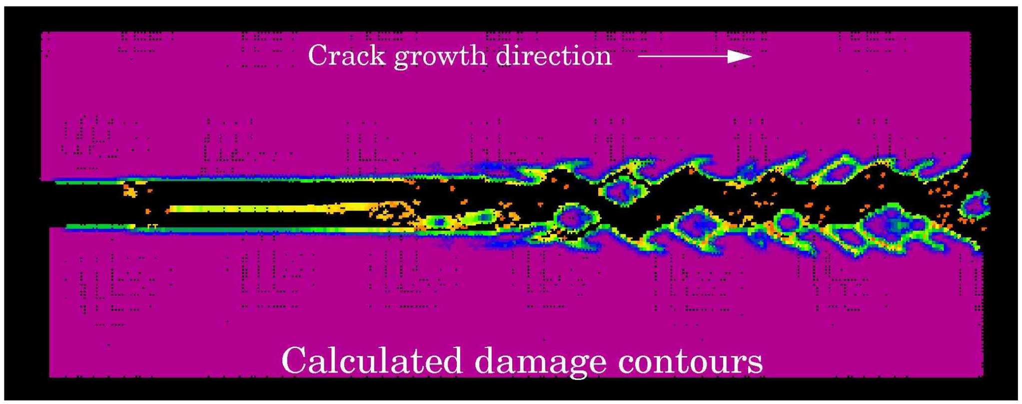
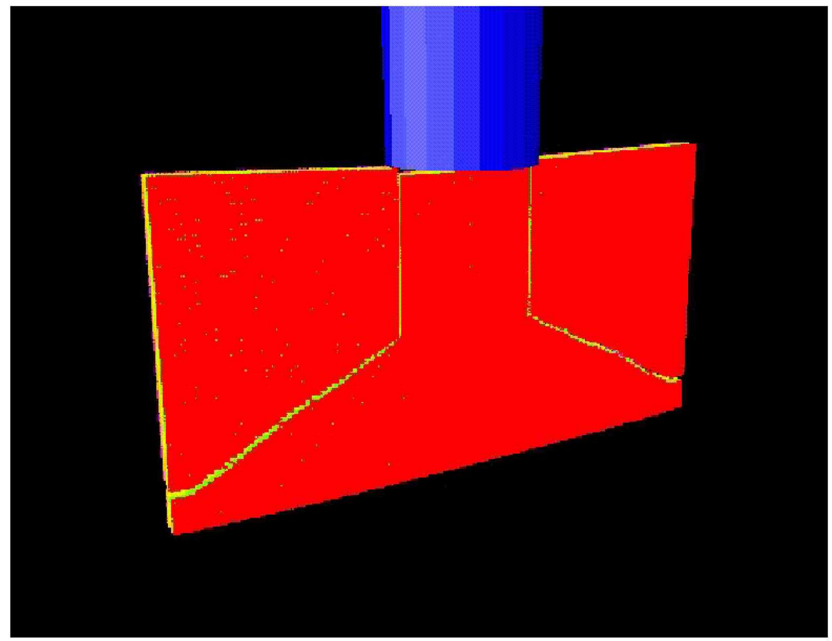
Bond based PD:
Dynamic fracture



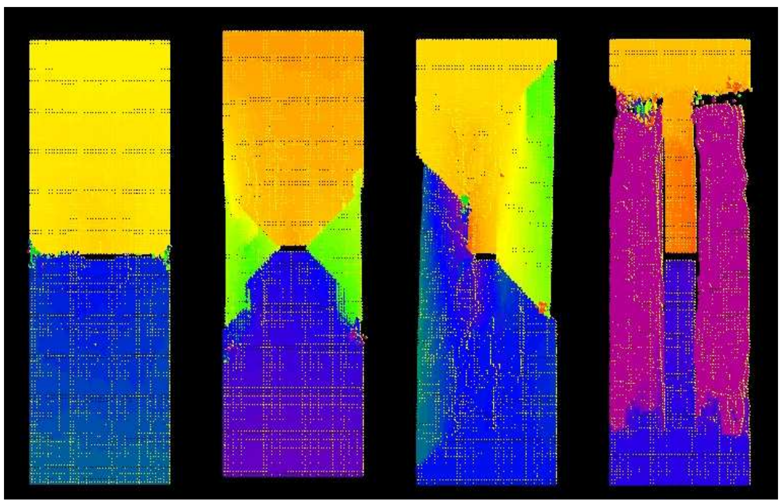
Crack instability in PMMA
(Fineberg & Marder, 1999)



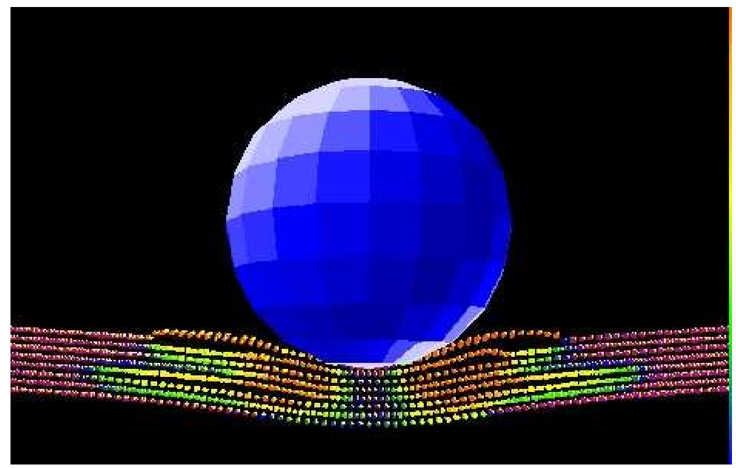
Dynamic fracture in steel
(Kalthoff & Winkler, 1988)

Bond based PD: Damage in composites (Boeing)

- How does the fraction of fibers in each direction affect the direction of crack growth?
- What damage occurs when a composite panel is struck by hail?



Crack growth in a notched panel



Delamination caused by impact

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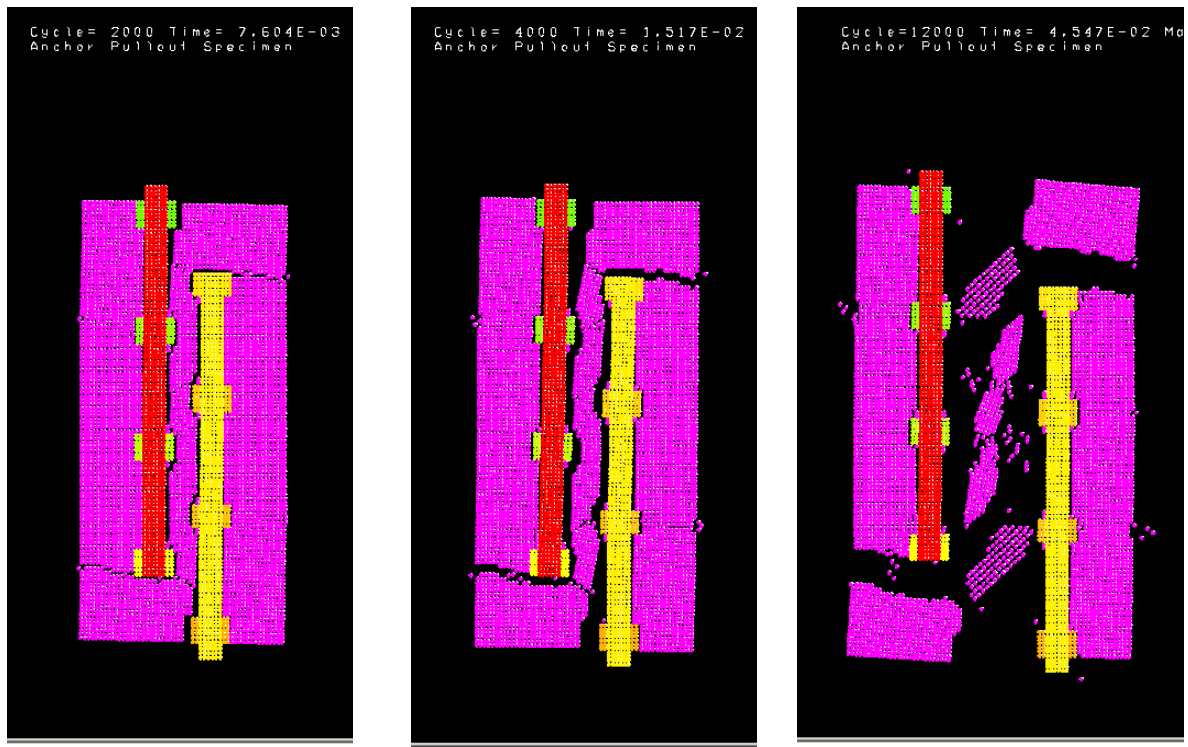
Splice of ribbed reinforcing bars

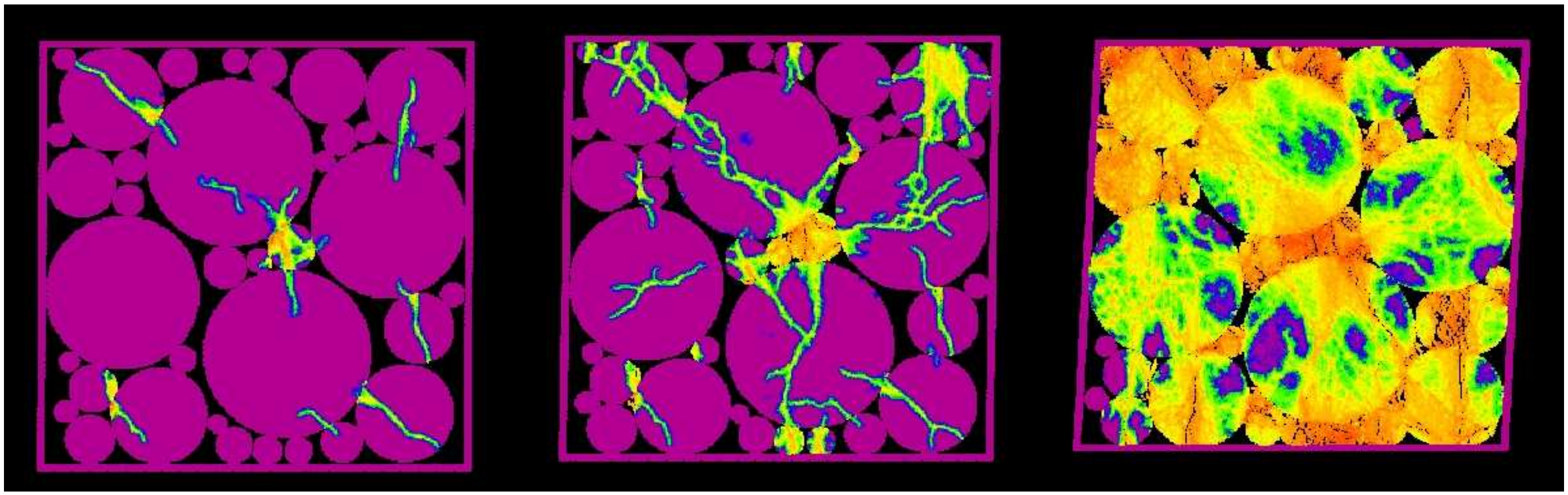


Magnified deformed shapes of splice of reinforcing bars in concrete at three stages
(fine discretization – grid spacing is 0.03 m)

Courtesy Prof. Walter Gerstle, University of New Mexico

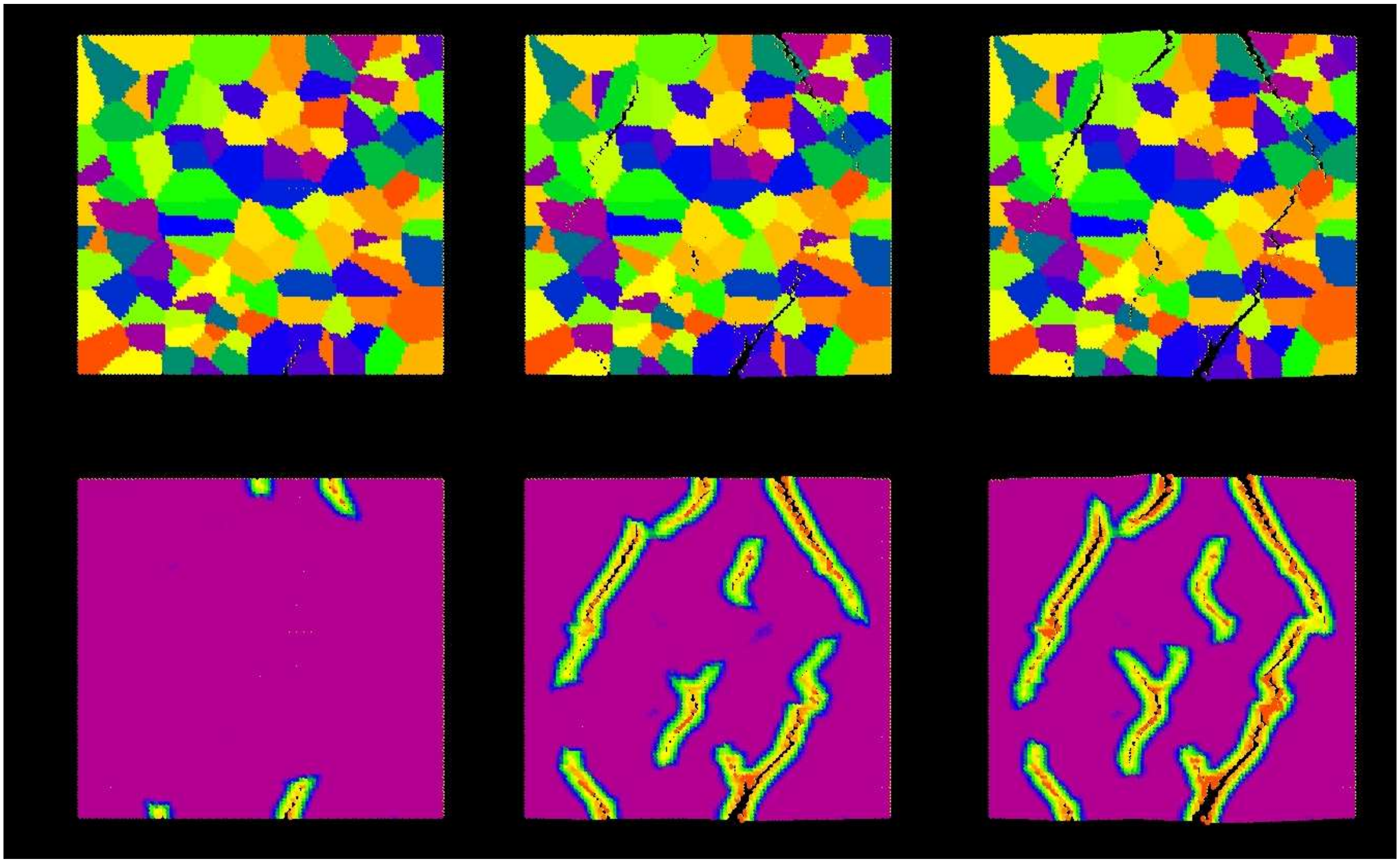
Multiscale high-rate material modeling

- Grain-scale model includes all relevant physics.
- Statistical treatment leads to macroscale material model.



Combined compression and shear loading at boundaries

Fracture in a polycrystal



20.5 ms　　21.3 ms　　22.1 ms

Images courtesy of Prof. Florin Bobaru, University of Nebraska

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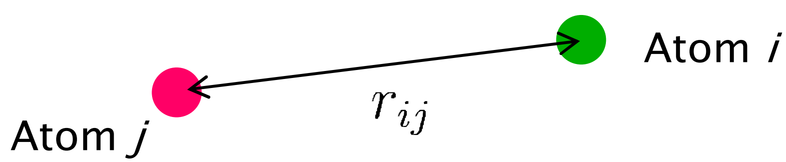
Nonlocality and length scales

- Many physical problems have some natural length scale.
  - Sometimes the length scale is obvious, e.g.,
    - Interatomic forces
    - Molecular dynamics cannot be done without nonlocality.



$$F_{ij} \sim \left(\frac{a}{r_{ij}}\right)^{12} - \left(\frac{a}{r_{ij}}\right)^{6}$$

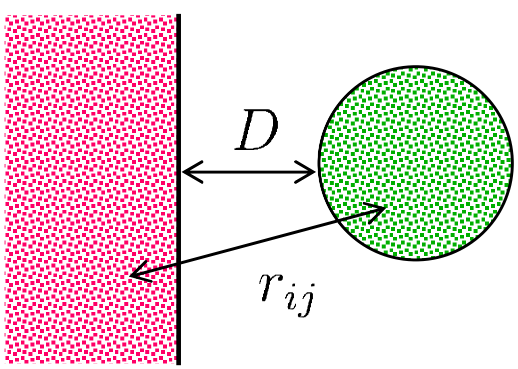
Nonlocality and length scales

- Sometimes the length scale is a little less obvious, e.g.
  - van der Waals forces that lead to longer-range surface forces.
  - Force between a pair of atoms as they are separated:

$$F_{ij} \sim 1/r_{ij}^6$$

  - Net force between halfspace and a sphere made of many of these atoms* occurs over a much larger length scale:

$$F_{\text{sphere}} \sim 1/D$$



See J. Israelachvili, *Intermolecular and Surfaces Forces*, pp. 177.

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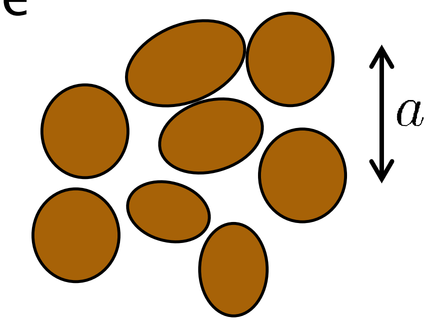
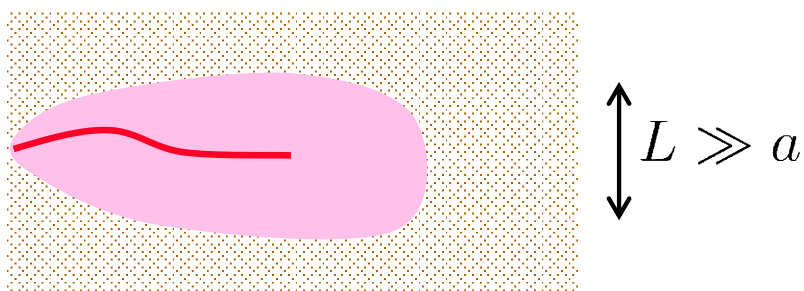
Nonlocality and length scales

- Macroscale: sometimes a length scale is determined by heterogeneity, e.g., concrete aggregate size



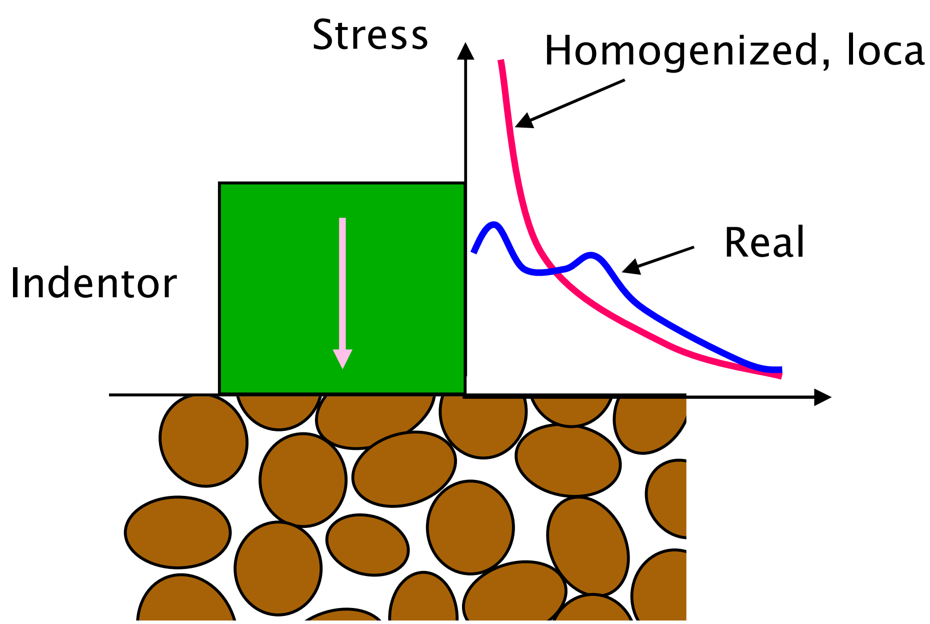
  - Yet damage can occur in a much larger process zone



See Bazant, ….

Nonlocality and length scales

- Homogenization, neglecting the natural length scales of a system, often doesn't give good answers.



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Bond-based peridynamic model: Observations

- Good things:
  - Now have a mathematically consistent way to treat material with cracks.
  - No additional equations are needed to tell cracks what to do.
- Bad things:
  - Independent bonds imply Poisson ratio = 1/4.
  - Can have permanent deformation in bonds, but can't enforce plastic incompressibility.
  - Can't use material models from the standard theory.

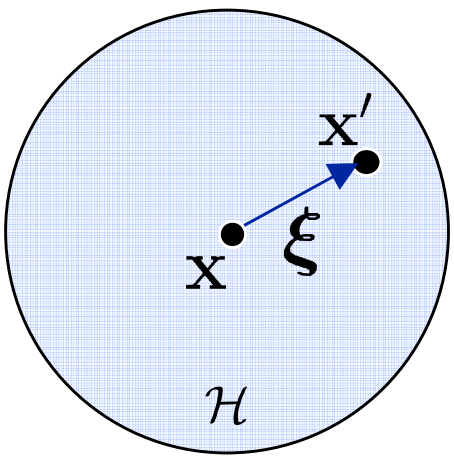
Can overcome these limitations by allowing bonds to interact with each other.

Peridynamic states: Mathematical tool for dealing with collections of bonds

A vector state $\underline{\mathbf{A}}$ is a mapping from $\mathcal{H}$ to $\mathbb{R}^3$.

A scalar state $\underline{a}$ is a mapping from $\mathcal{H}$ to $\mathbb{R}$.

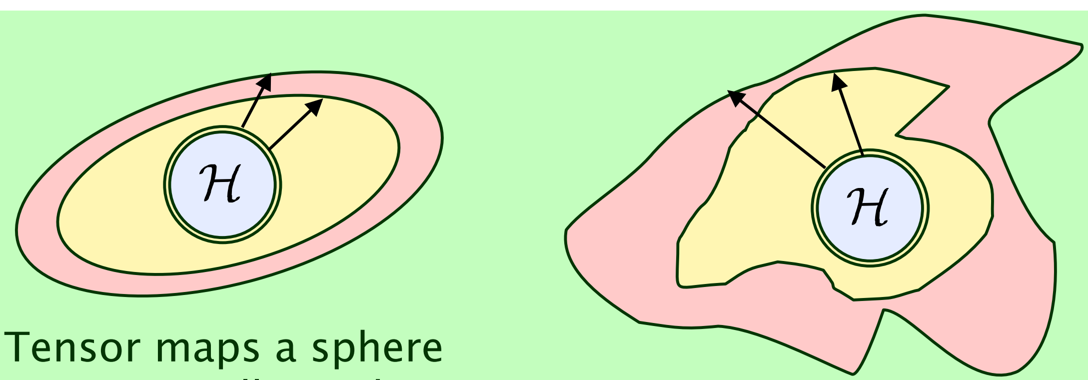
$\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ is a bond. $\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle$ is a vector. $\underline{a}\langle\boldsymbol{\xi}\rangle$ is a scalar.



$\mathcal{H}$= set of all bonds connected to $\mathbf{x}$

A vector state is like a 2nd order tensor, except:

- A vector state can be nonlinear.
- A vector state can be discontinuous.



Tensor maps a sphere onto an ellipsoid. **(boring !)**

Vector state maps a sphere onto anything.

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Dot product of two vector states

Suppose $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ are two vector states. Define the dot product of $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ by

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

The set of all vector states $\mathcal{V}$ is an inner product space (even though each $\underline{\mathbf{A}} \in \mathcal{V}$ is a nonlinear mapping.)

Functions of states and Frechet derivatives

Suppose $\Psi(\cdot)$ is a scalar-valued function of a vector state $\underline{\mathbf{A}}$. For any differential $d\underline{\mathbf{A}}$ let

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

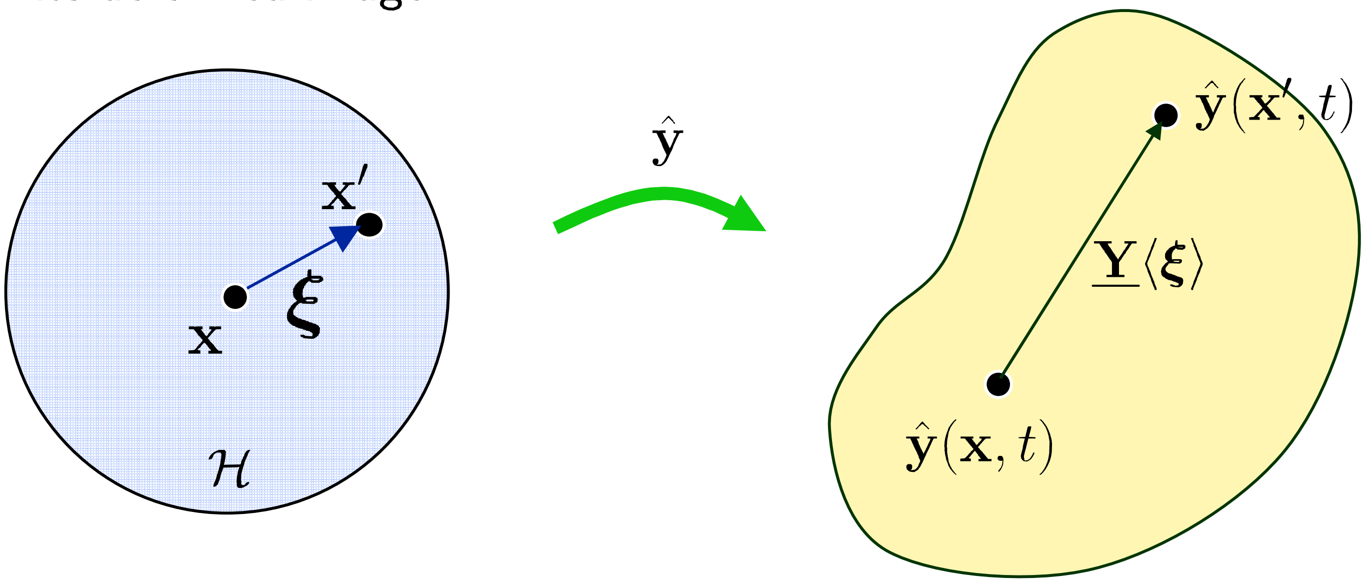
If there is a vector state $\nabla\Psi$ such that

$$d\Psi = \nabla\Psi \bullet d\underline{\mathbf{A}}$$

for any $d\underline{\mathbf{A}}$ then $\nabla\Psi$ is the Frechet derivative of Ψ at $\underline{\mathbf{A}}$.

Deformation states

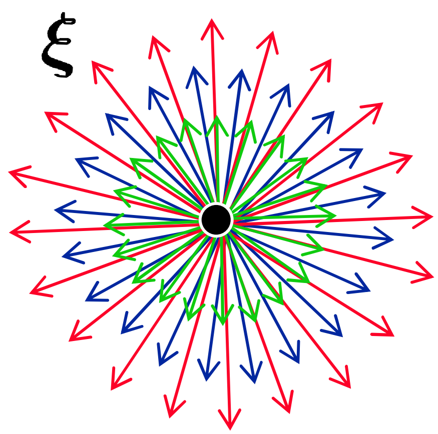
The deformation state $\underline{\mathbf{Y}}[\mathbf{x}, t]$ maps any bond connected to $\mathbf{x}$ into its deformed image.



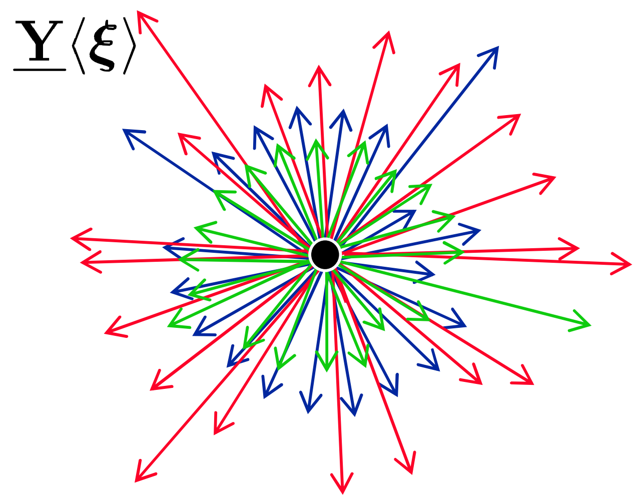
$$\underline{\mathbf{Y}}[\mathbf{x}, t]\langle\mathbf{x}' - \mathbf{x}\rangle = \hat{\mathbf{y}}(\mathbf{x}', t) - \hat{\mathbf{y}}(\mathbf{x}, t)$$

Deformation states contain a lot of kinematical complexity

$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ is the deformed image of any bond $\boldsymbol{\xi}$.



Undeformed bonds connected to $\mathbf{x}$



Deformed bonds connected to $\mathbf{x}$

Elastic materials

Strain energy density at $\mathbf{x}$ depends only on the deformation state there:

$$W(\mathbf{x}, t) = \hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t]) \tag{1}$$

Is this really so different from the standard theory?

Standard:

$$\hat{W}\left(\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}}\right)$$

Energy depends on a linear transformation

Peridynamic:

$$\hat{W}(\underline{\mathbf{Y}})$$

Energy depends on a nonlinear transformation

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Equation of motion from Hamilton's principle

Hamiltonian:

$$H = \int_0^\infty \int_{\mathcal{R}} \left\{ W - \frac{\rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}}}{2} - \mathbf{b} \right\} dV_{\mathbf{x}}\, dt$$

Euler-Lagrange equation (equation of motion):

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}' \rangle \right\} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

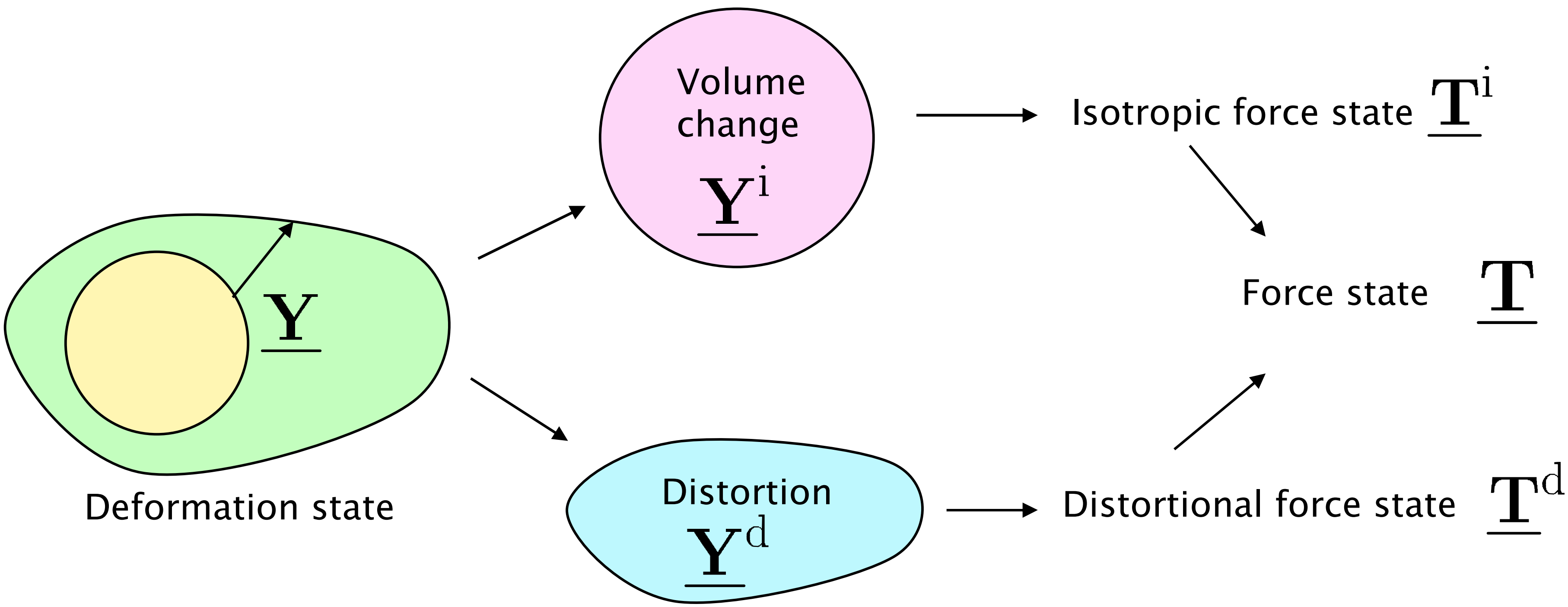
where $\underline{\mathbf{T}}$ is the *force state*:

$$\underline{\mathbf{T}}(\underline{\mathbf{Y}}) = \nabla \hat{W}(\underline{\mathbf{Y}})$$

i.e.,

$$dW = \int_{\mathcal{H}} \underline{\mathbf{T}}(\underline{\mathbf{Y}})\langle \boldsymbol{\xi} \rangle \cdot d\underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle\, dV_{\boldsymbol{\xi}}$$

Can now treat pressure–volume response as decoupled from distortional response



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PD material from a conventional model

Define an approximate deformation gradient tensor by

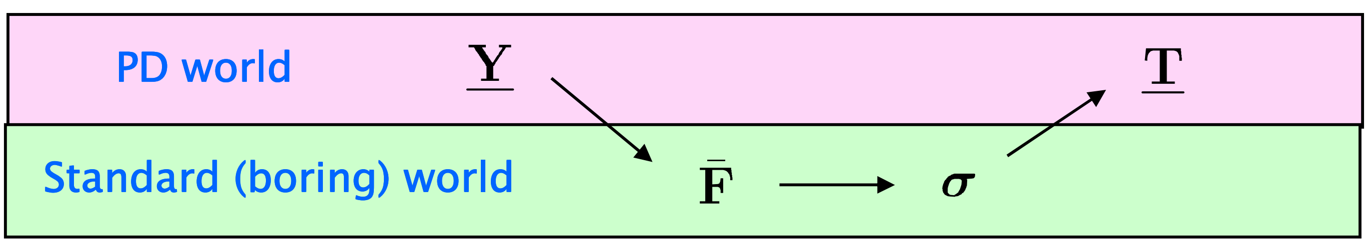
$$\bar{\mathbf{F}}(\underline{\mathbf{Y}}) = m \int_{\mathcal{H}} \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \otimes \boldsymbol{\xi} \; dV_{\boldsymbol{\xi}} \qquad \forall \underline{\mathbf{Y}}$$

Now take any hyperelastic strain energy density function from the standard theory $\Omega(\mathbf{F})$ and set

$$\hat{W}(\underline{\mathbf{Y}}) = \Omega(\bar{\mathbf{F}}(\underline{\mathbf{Y}})) \qquad \forall \underline{\mathbf{Y}}$$

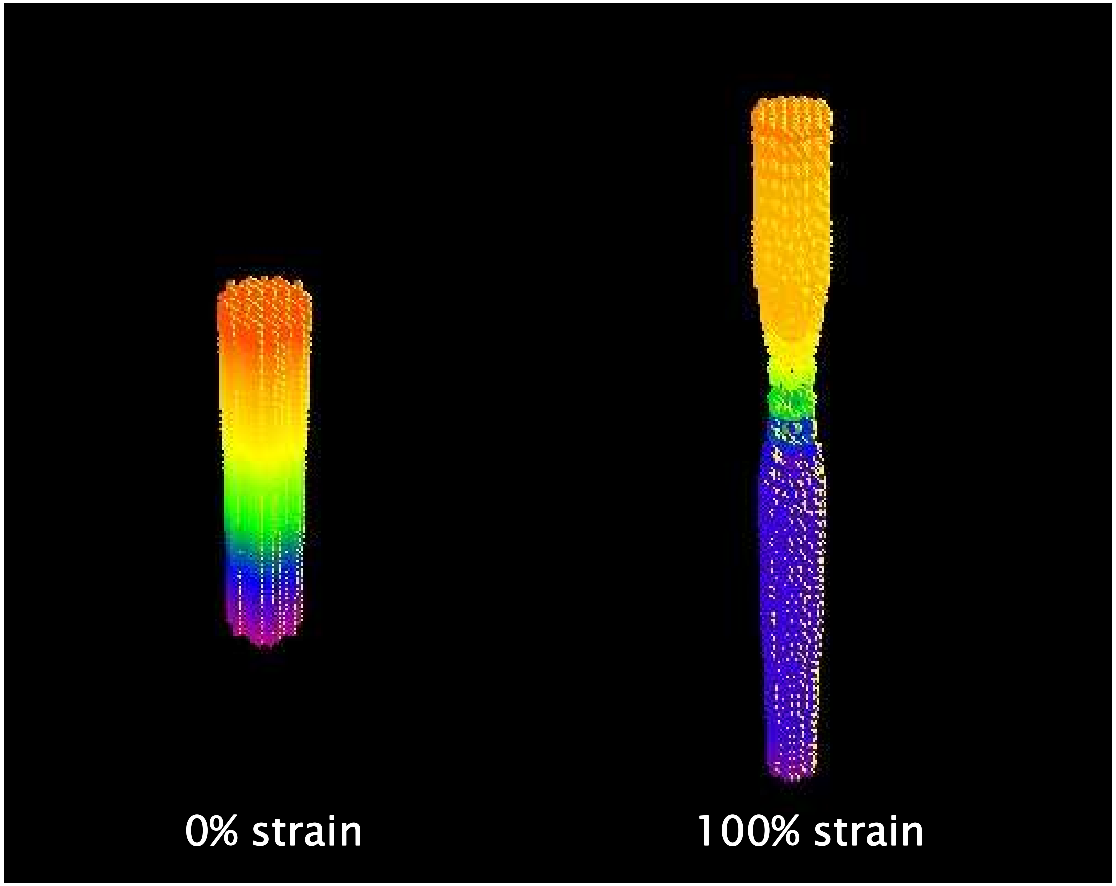
Find that the force state is related to the PK stress by

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \frac{1}{m}\boldsymbol{\sigma}\boldsymbol{\xi}, \qquad \boldsymbol{\sigma} = \frac{\partial\Omega}{\partial\mathbf{F}}(\bar{\mathbf{F}})$$



Necking in a 6061-Aluminum Bar

- EMU simulation with state-based peridynamic implementation of large-deformation, strain-hardening, rate-dependent material model.
  - Material model implementation by J. Foster, SNL 5431.

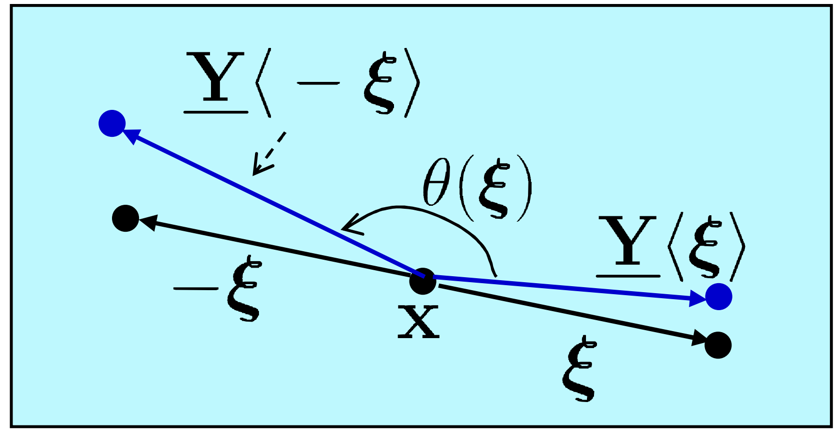


Contours of axial velocity

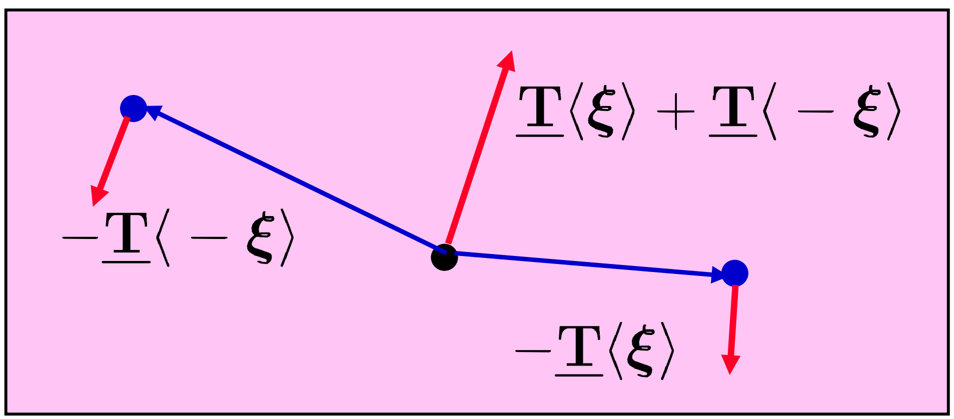
PD states can model interesting collective behavior

Consider a material that responds to angle changes between bonds at $\pm 180°$.

$$\hat{W}(\underline{\mathbf{Y}}) = \int_{\mathcal{H}} \left(\theta(\boldsymbol{\xi}) - \pi\right)^2 \, dV_{\boldsymbol{\xi}}$$



After evaluating the Frechet derivative, find that the force state resists these angle changes.



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Discrete particles and PD states

$N-$body potential:

$$U(\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N),$$

$\mathbf{y}_1, \ldots, \mathbf{y}_N =$ deformed positions, $\mathbf{x}_1, \ldots, \mathbf{x}_N =$ reference positions.
Define a PD body by

$$\hat{W}(\underline{\mathbf{Y}}, \mathbf{x}) = \delta_d(\mathbf{x}-\mathbf{x}_0) U(\underline{\mathbf{Y}}\langle\mathbf{x}_1-\mathbf{x}_0\rangle, \underline{\mathbf{Y}}\langle\mathbf{x}_2-\mathbf{x}_0\rangle, \ldots, \underline{\mathbf{Y}}\langle\mathbf{x}_N-\mathbf{x}_0\rangle),$$

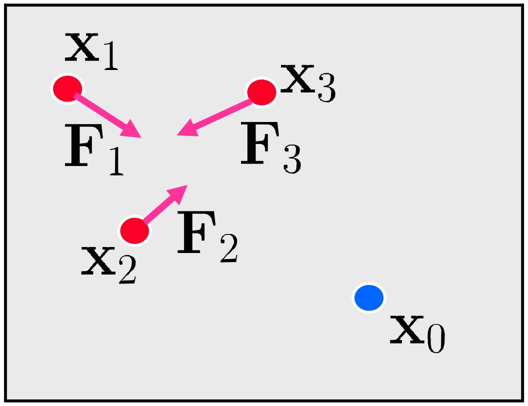
$$\rho(\mathbf{x}) = \sum_i \delta_d(\mathbf{x}-\mathbf{x}_i) M_i$$

Dirac delta

Particle mass

where $\mathbf{x}_0$ is an arbitrary point. Can show the PD equation of motion implies

$$M_i \ddot{\mathbf{u}}(\mathbf{x}_i, t) = -\frac{\partial U}{\partial \mathbf{y}_i}, \qquad i = 1, \ldots, N$$



Have represented discrete particles as a continuum

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Convergence of peridynamics to the standard theory

- Suppose we change the horizon while holding the bulk properties (e.g., bulk modulus) fixed.
- If the deformation is continuous, the kinematical approximation

$$\mathbf{y}(\mathbf{x}+\boldsymbol{\xi})-\mathbf{y}(\mathbf{x})=\mathbf{F}(\mathbf{x})\boldsymbol{\xi}+o(|\boldsymbol{\xi}|^2)$$

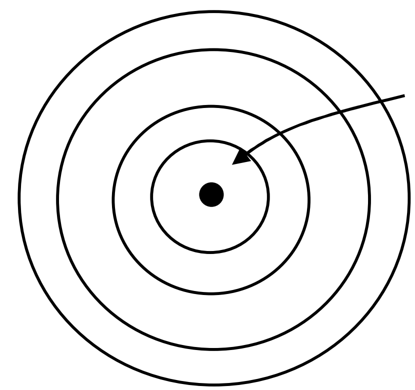
becomes more and more accurate.
- Therefore

$$W(\underline{\mathbf{Y}})\approx\hat{W}(\mathbf{F})$$

also becomes more accurate.
- The peridynamic force density is closely approximated by

$$\mathbf{L}(\mathbf{x})\approx\nabla\cdot\boldsymbol{\sigma},\qquad \boldsymbol{\sigma}=\frac{\partial\hat{W}}{\partial\mathbf{F}}$$

Sequence of horizons



Conclusions

- The peridynamic approach offers a consistent mathematical framework for discontinuous problems.
  - Basic equations can be applied directly on cracks.
  - Nonlocality is inherent in the method, length scale is variable.
  - Discrete particles are treated with the same equations as a continuum.

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