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Peridynamic Modeling of the Dynamic Response of Heterogeneous Media

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Minisymposium on
Nonlocal and Scale Effects in Dynamic Shear Banding or in Dynamic Damage of Heterogeneous Media

International Symposium on Plasticity

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Outline

- Objective
- Theory
- EMU numerical method
- Examples
- Heterogeneity and nonlocality
- Fragmentation

Purposes of the peridynamic model

- To be able to apply the same equations on or off of 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.

PERGAMON

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Reformulation of elasticity theory for discontinuities and long-range forces

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Outline

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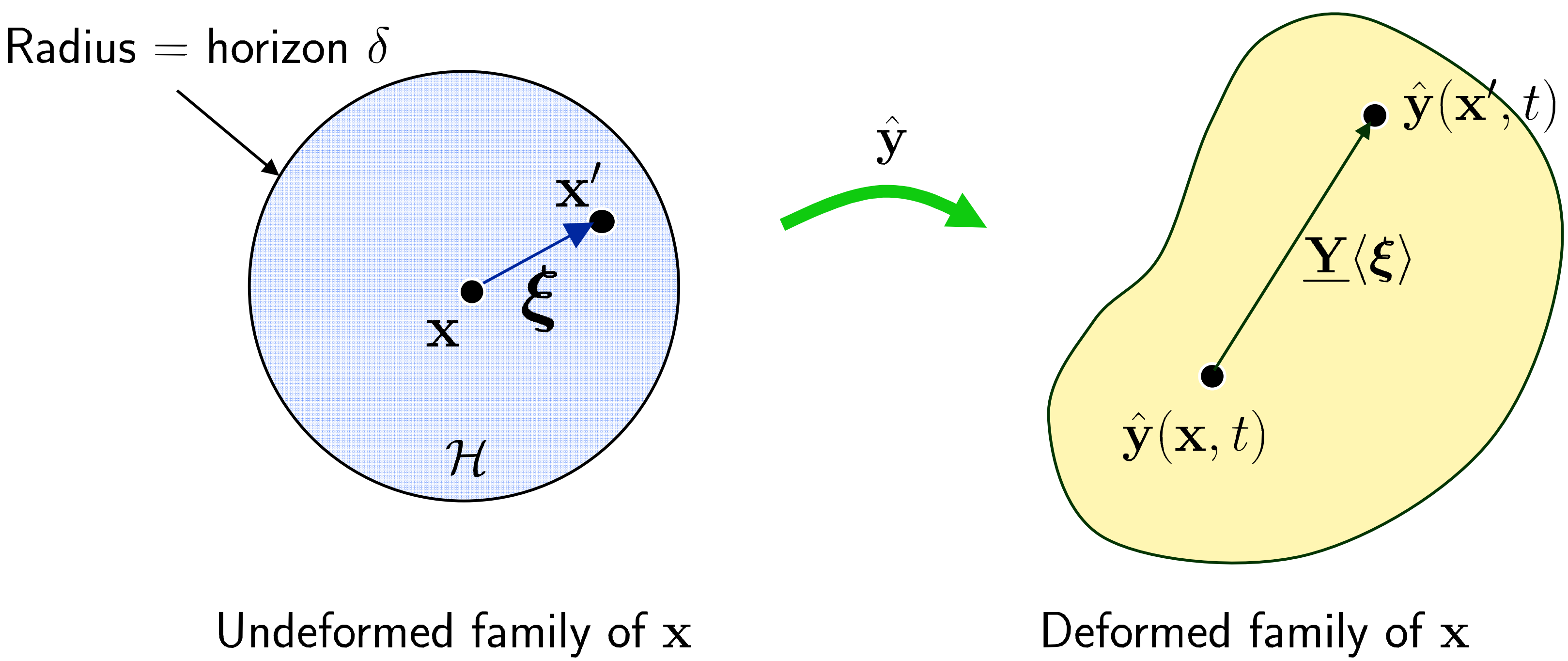
The basic assumption

The strain energy density at any point $\mathbf{x}$ depends on the deformation of a neighborhood $\mathcal{H}$ of $\mathbf{x}$.



Now need to introduce some tools ("peridynamic states") for keeping track of how these neighborhoods deform.

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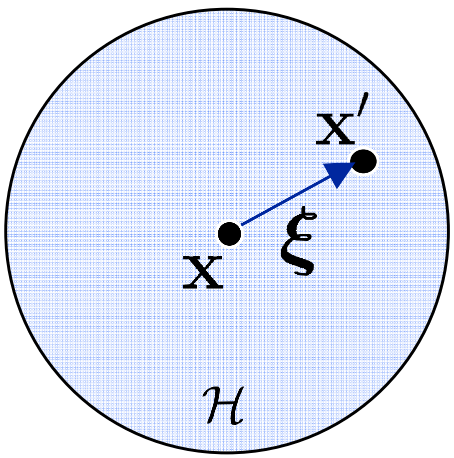
Peridynamic states: Mathematical tool for dealing with collections of bonds

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

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



$\mathcal{H}$= 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.

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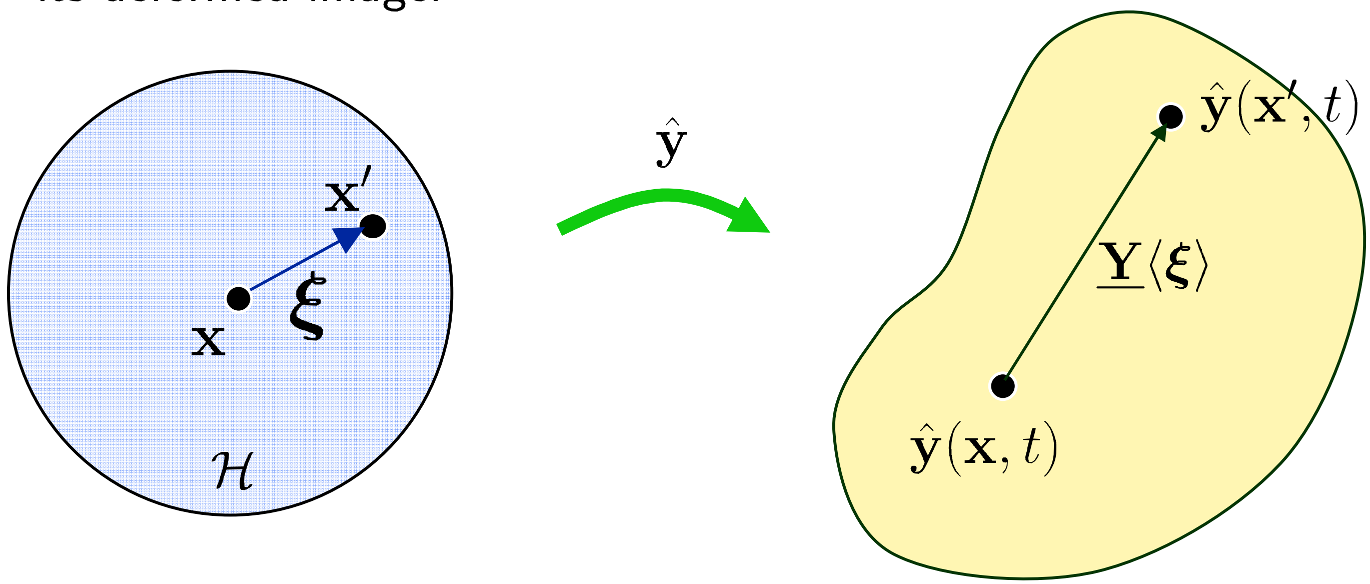
Deformation states

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



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

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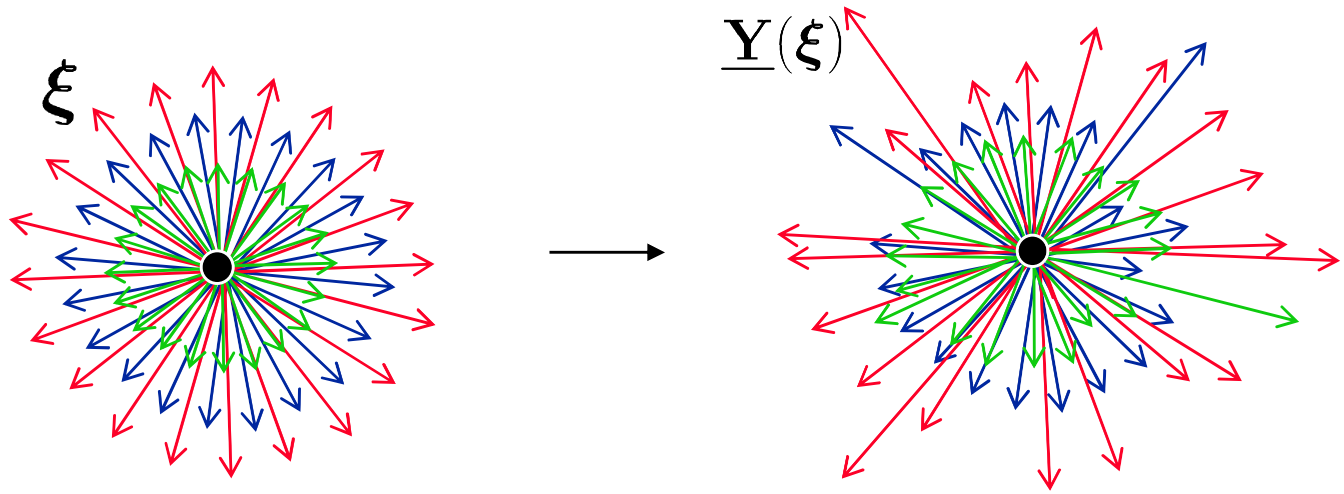
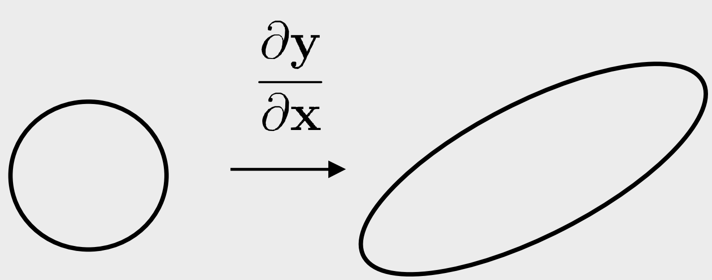
Deformation states contain a lot of kinematical complexity



Undeformed bonds connected to $\mathbf{x}$ Deformed bonds connected to $\mathbf{x}$



Compare this with standard theory in which small spheres are mapped into ellipsoids

Elastic materials

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

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

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

Potential energy statement leads to the peridynamic equation of equilibrium

Define the potential energy in a body $\mathcal{B}$ by

$$\Phi_{\mathbf{u}} = \int_{\mathcal{B}} W \, dV - \int_{\mathcal{B}} \mathbf{u} \cdot \mathbf{b} \, dV.$$

$\delta\Phi_{\mathbf{u}} = 0$ yields the Euler-Lagrange equation

$$\int_{\mathcal{H}} \Big(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \Big) \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}$$

for all $\mathbf{x} \in \mathcal{B}$, where $\underline{\mathbf{T}}[\mathbf{x}]$ is the *force state* at $\mathbf{x}$ defined by

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

where ∇ indicates the Frechet derivative.

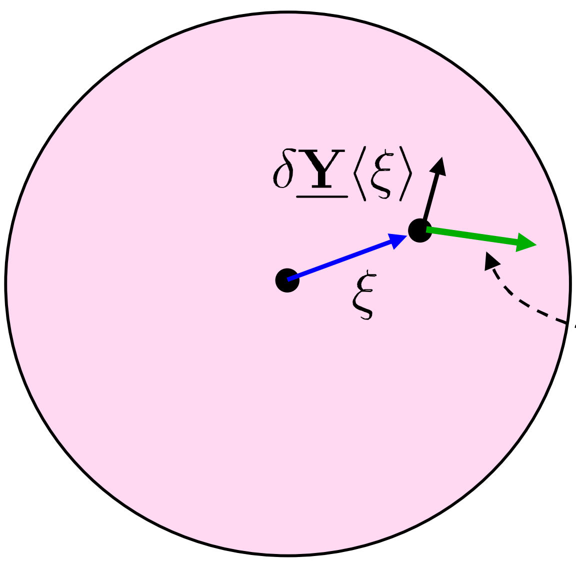
Meaning of the Frechet derivative

The force density $\underline{\mathbf{T}}\langle\xi\rangle$ in bond ξ is found by varying the bond displacement and evaluating the change in W.

$$\delta W(\xi) = \underline{\mathbf{T}}\langle\xi\rangle \cdot \delta\underline{\mathbf{Y}}\langle\xi\rangle$$

Thus the *force state* $\underline{\mathbf{T}}$ is the the work conjugate of $\underline{\mathbf{Y}}$:

$$\delta W = \int_{\mathcal{H}} \underline{\mathbf{T}}\langle\xi\rangle \cdot \delta\underline{\mathbf{Y}}\langle\xi\rangle \, dV_\xi$$



$\boxed{\text{Compare with standard theory: } \delta W = \sigma \cdot \delta\mathbf{F}}$

$\underline{\mathbf{T}}\langle\xi\rangle$=bond force density (dimensions force/volume^2)

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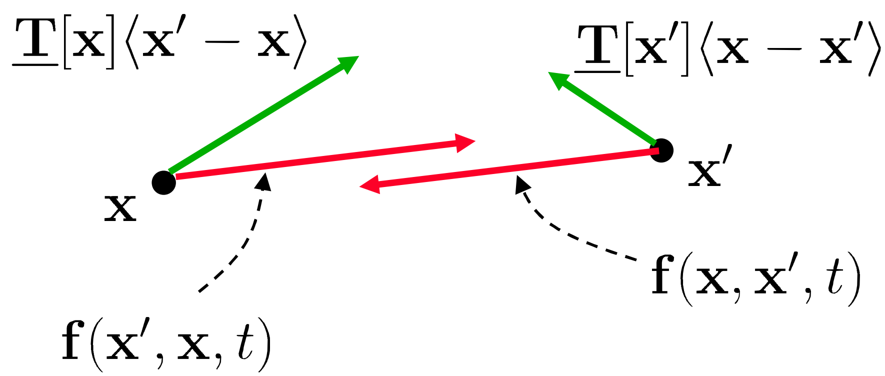
Force states and bond force

The total force density in bond $\mathbf{x}' - \mathbf{x}$ is composed of 2 parts:

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

The equation of motion is

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

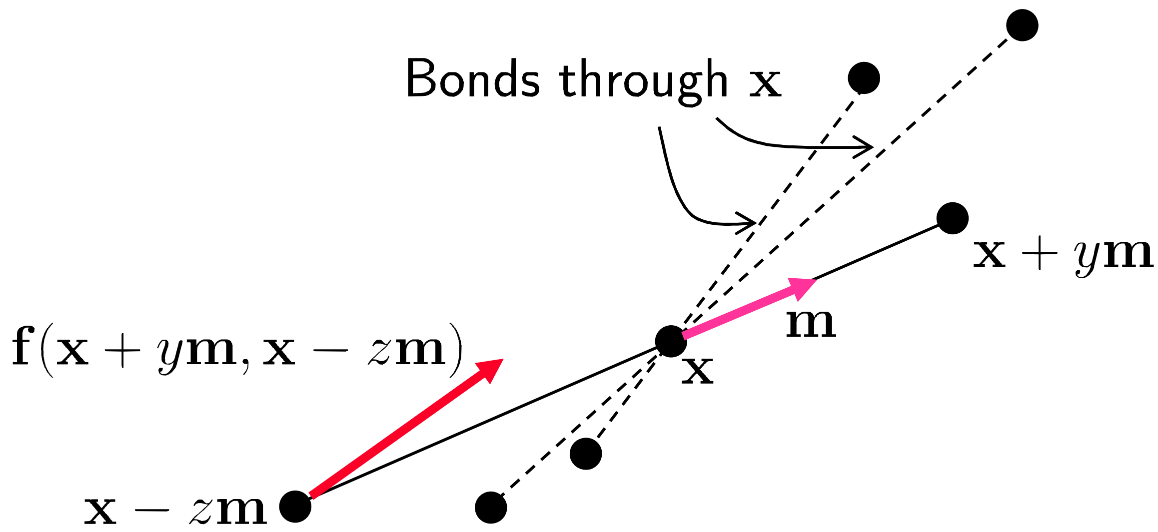


Peridynamic stress tensor

The peridynamic stress tensor is defined by

$$\boldsymbol{\nu}(\mathbf{x}) = \int_{\mathcal{S}} \int_0^\infty \int_0^\infty (y+z)^2 \mathbf{f}(\mathbf{x}+y\mathbf{m}, \mathbf{x}-z\mathbf{m}) \otimes \mathbf{m} \, dz \, dy \, d\Omega_{\mathbf{m}}$$

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



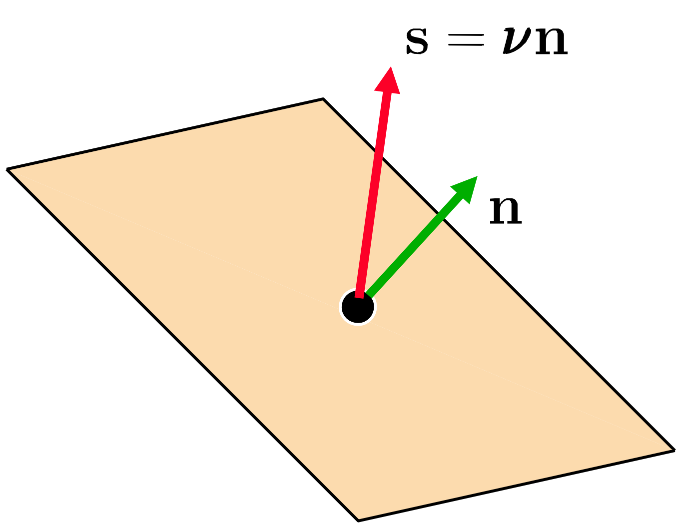
Properties of the peridynamic stress tensor

- The force per unit area at $\mathbf{x}$ through a plane with normal $\mathbf{n}$ is

$$\mathbf{s} = \boldsymbol{\nu}(\mathbf{x})\mathbf{n}$$

- The peridynamic equation of motion can be written as

$$\rho\ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\nu} + \mathbf{b}$$



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Force flux and the peridynamic stress tensor

R.B. Lehoucq[a,*,1], S.A. Silling[b,1]

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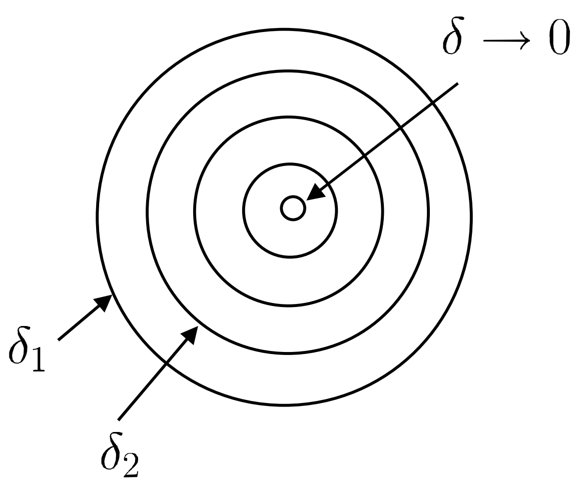
Convergence of peridynamics to the standard theory

- If the only requirement on a material model is that it reproduce bulk response under homogeneous deformation, then the horizon (length scale) is arbitrary.
- If we shrink the horizon to zero, the PD equations converge to the classical PDEs.
  - This result holds only if the deformation is smooth.



As $\delta \to 0$,

$$\nu(\underline{\mathbf{Y}}) \to \sigma(\mathbf{F}), \qquad \mathbf{F} = \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}}$$

hence

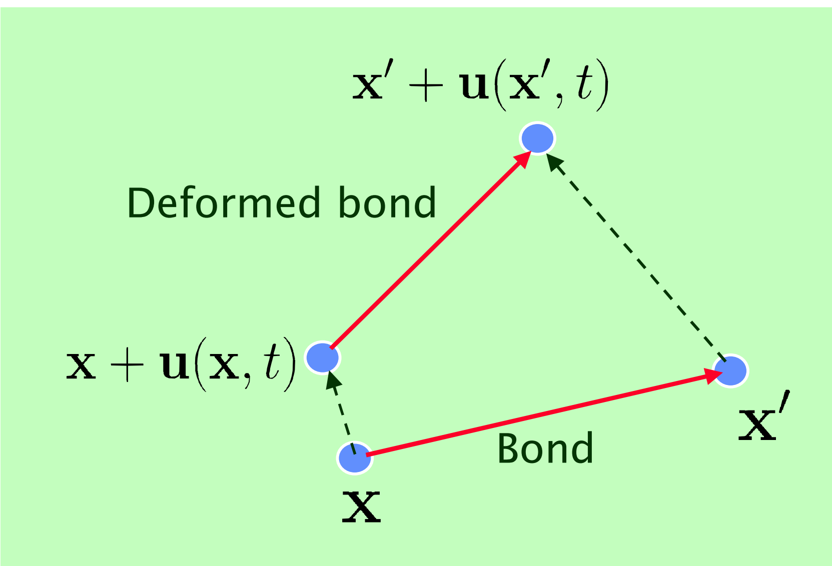
$$\int_{\mathcal{H}} \mathbf{f}\, dV \to \nabla \cdot \sigma$$

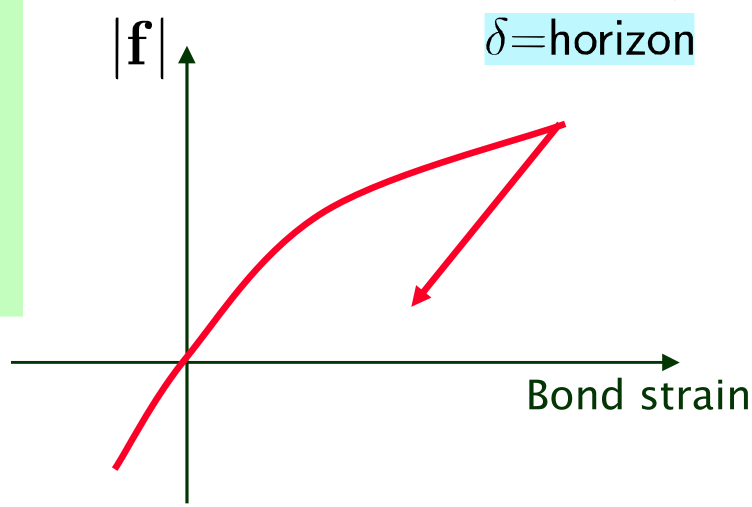
Bond-based peridynamic model

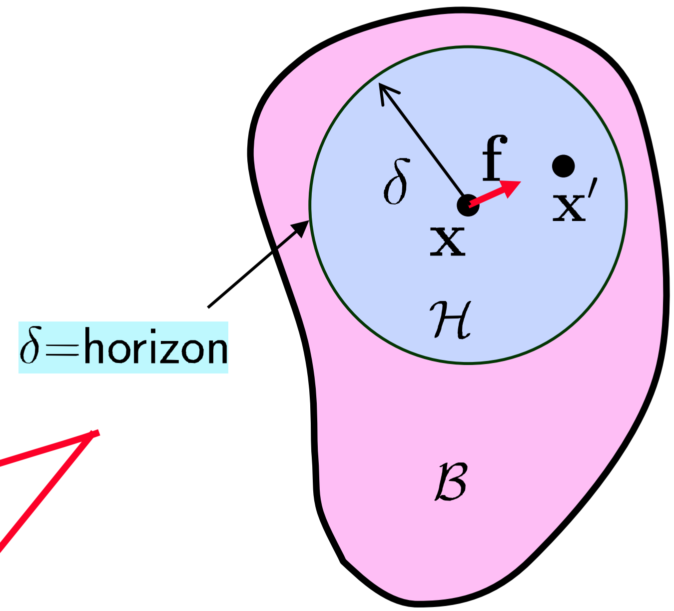
An important special case is when bonds respond independently of each other:

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

Unlike the general case, here each $\mathbf{f}$ depends only on the deformation of that particular bond.

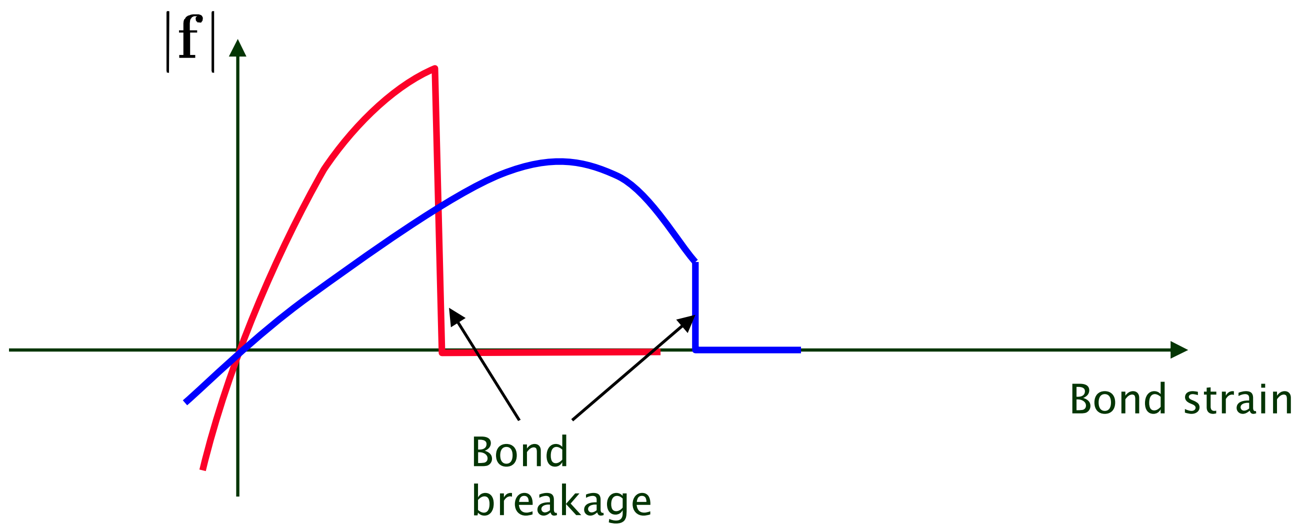






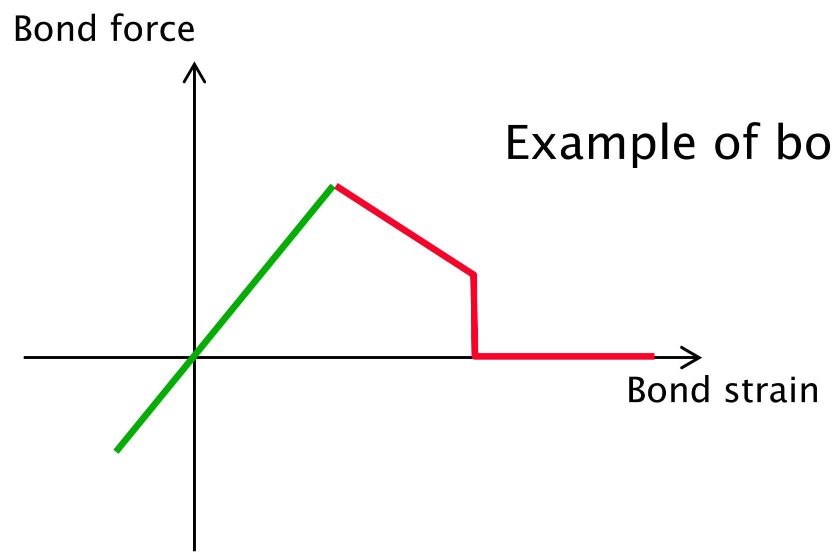
Damage is introduced through irreversible bond breakage

Two examples of material models that include damage:



How fracture occurs in a peridynamic body

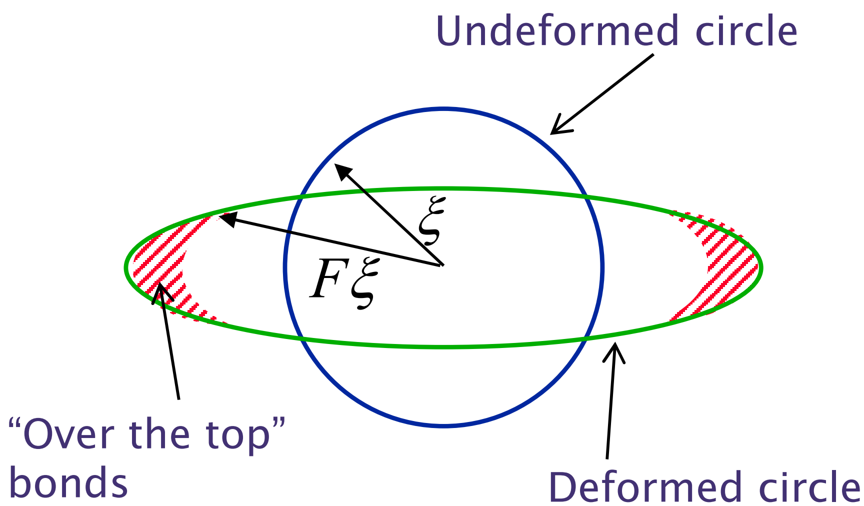
- As it stretches:
  - First it deforms continuously.
  - Then a material instability occurs, nucleating a crack.
  - Then the crack advances autonomously.

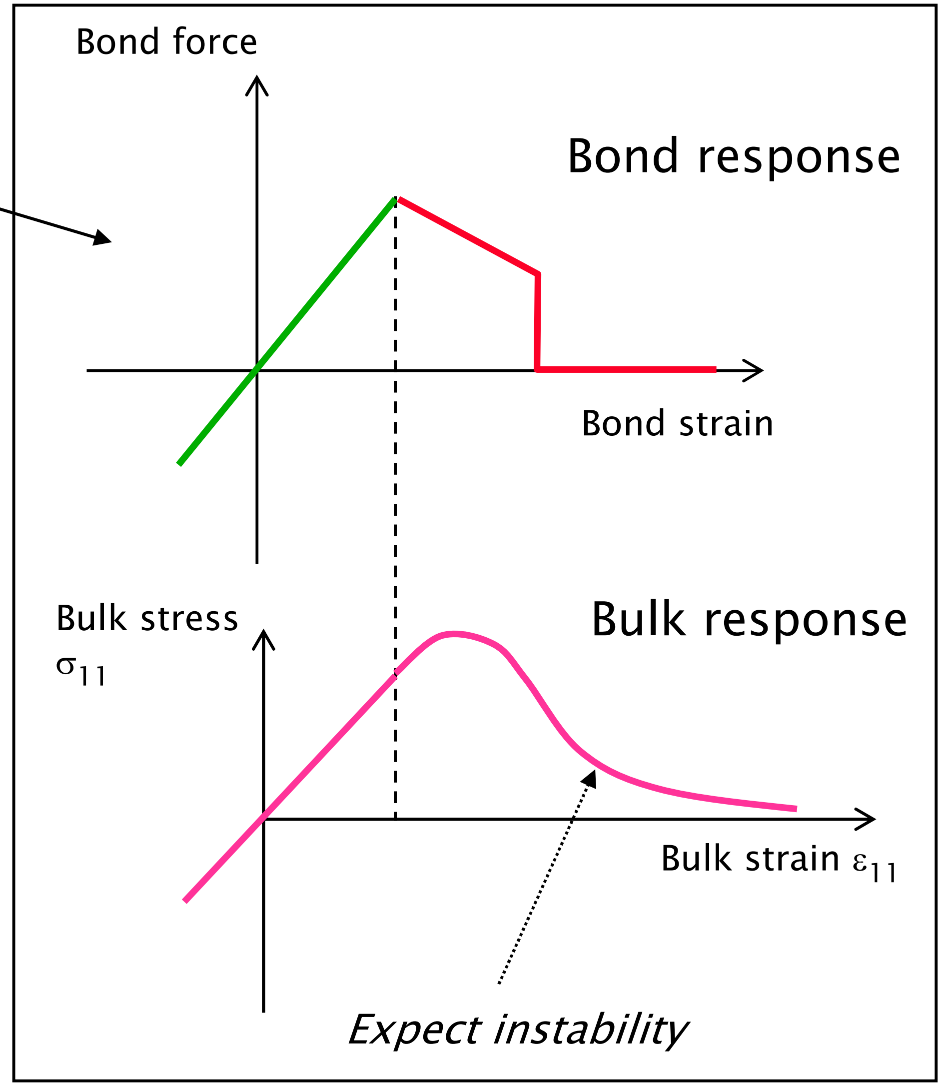


Example of bond response

Material instability and damage

- Assume a homogeneous deformation of this peridynamic material.
- When enough bonds stretch past the peak, material instability occurs.





Crack nucleation condition

- What material stability governs the spontaneous growth of a discontinuity in $\mathbf{u}$?
- Define a symmetric tensor field by

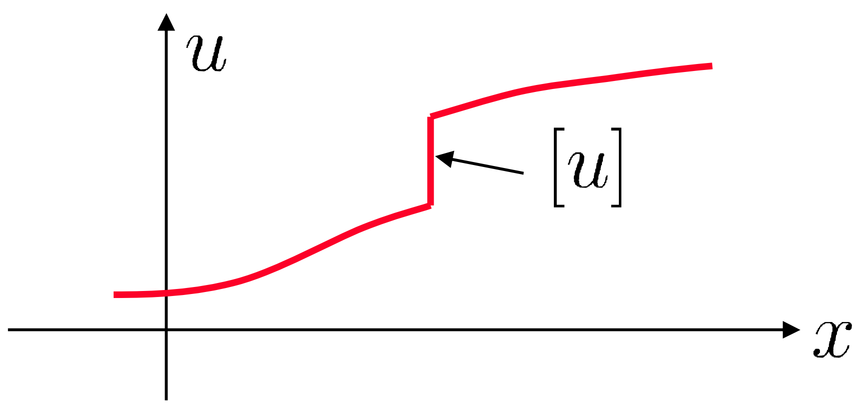
$$\mathbf{P}(\mathbf{x}) = \int \int \nabla\nabla W \langle \boldsymbol{\xi}, \boldsymbol{\zeta} \rangle \, dV_{\boldsymbol{\zeta}} \, dV_{\boldsymbol{\xi}}$$

2nd Frechet derivative

- Can show

$$\rho[\ddot{\mathbf{u}}] = -\mathbf{P}[\mathbf{u}]$$

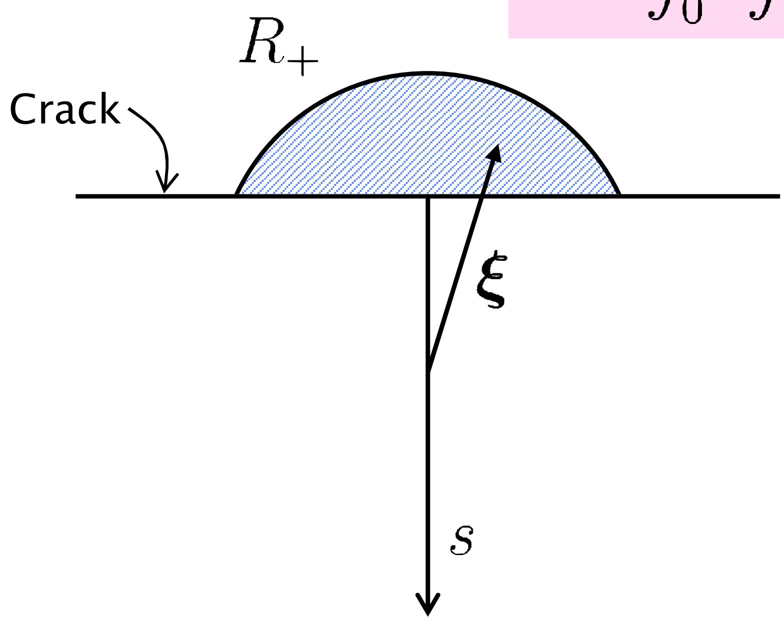
therefore $[\ddot{\mathbf{u}}] \cdot [\mathbf{u}] \geq 0$ if and only if $\mathbf{P}$ is *not* positive definite.

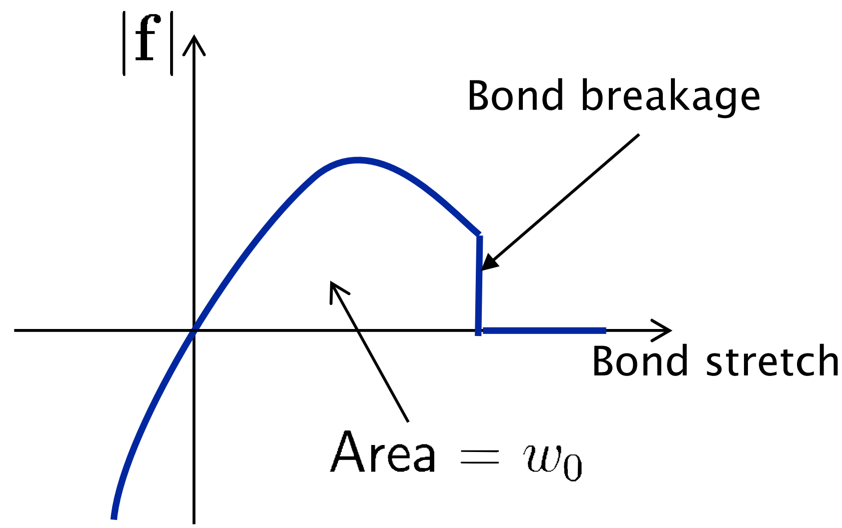


Energy required to advance a crack

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

$$G = \int_0^{\delta} \int_{R_+} w_0(\boldsymbol{\xi}) \, dV_{\boldsymbol{\xi}} \, ds$$





$w_0 =$ work (per unit volume^2) required to break one bond

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

Some nonlocal models and their relation to PD

- Navier (1820's, pre-Cauchy):
  - Solid as a collection of separated particles but linearized kinematics.
    - PD: nonlinear kinematics, not restricted to central potentials.
- Kroner, Edelen, Eringen, Kunin, Krumhansl, others (1960's on):
  - Continuum treatment of a lattice by averaging of strains over a volume.
  - Quasicontinuum formulated in terms of displacement.
    - PD: similar but nonlinear, allows damage, discontinuities.
- Bazant, Belytschko, others (1980's on):
  - Nonlocality in damage while retaining classical PDEs.
    - PD: damage included through constitutive treatment of bonds.
- Barenblatt, Dugdale, Hillerborg, Bazant, others (1960's on):
  - Cohesive crack models.
    - PD: cohesion across crack faces results from process of bond damage.
- Coleman, Aifantis, Hutchinson, Fleck, others (1950's on):
  - Gradient theories of elasticity and plasiticity ("weak nonlocality").
    - PD: strongly nonlocal, explicitly allows discontinuities.
- Lattice models, discrete elements, Cusatis model (1960's on):
    - PD is a continuum theory, but when discretized is similar to a lattice model.

Outline

- Objective
- Theory
- EMU numerical method
- Examples
- Heterogeneity and nonlocality
- Fragmentation

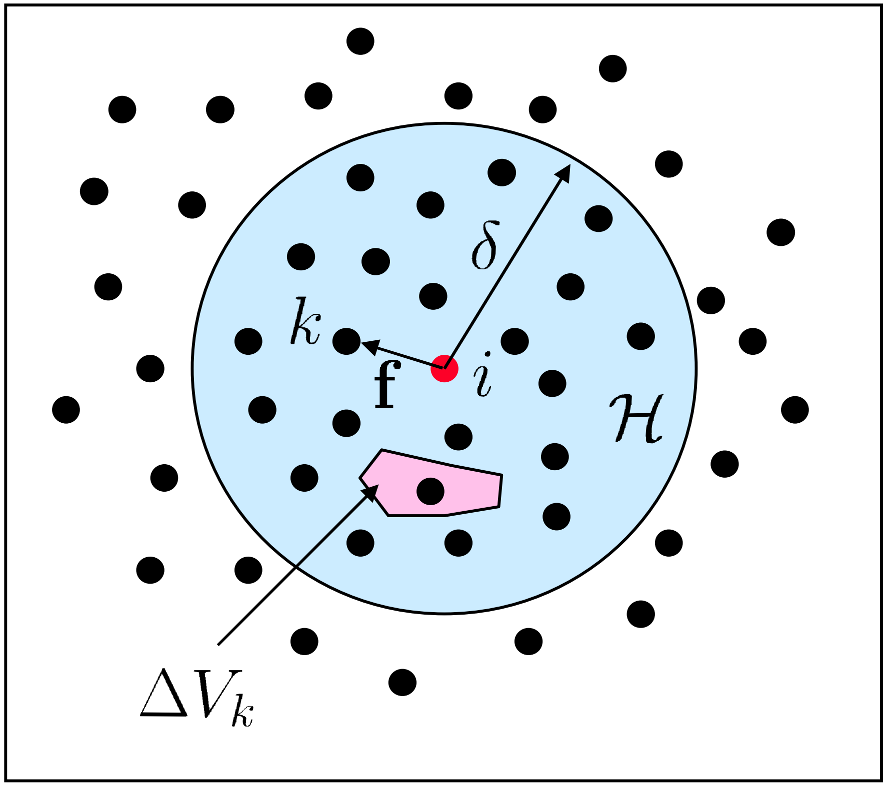
EMU numerical method

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

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

$$\downarrow$$

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



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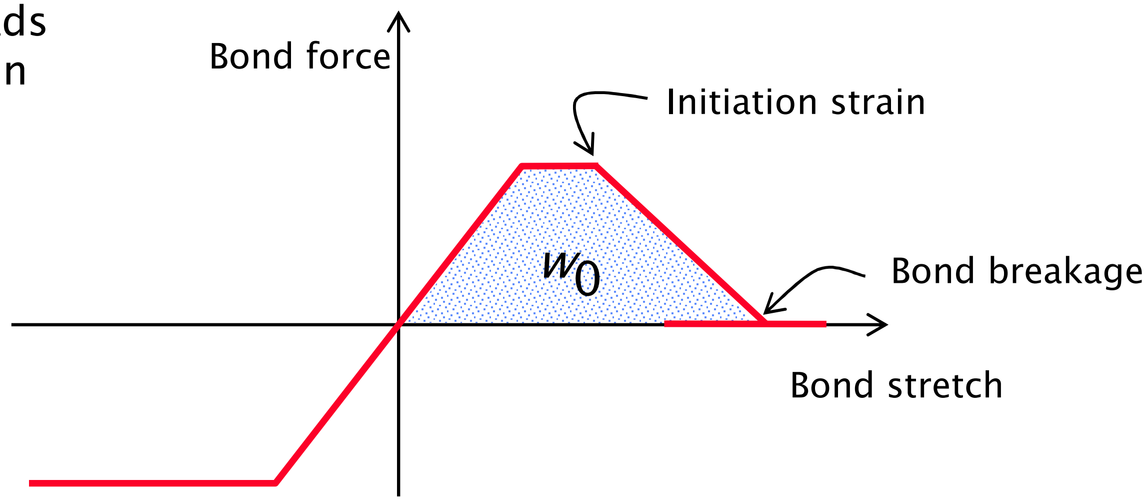
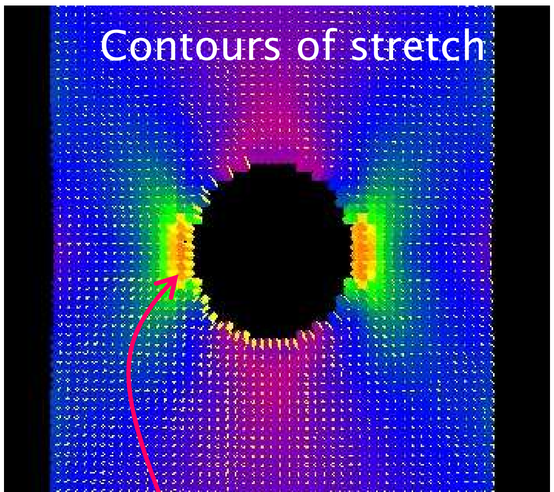
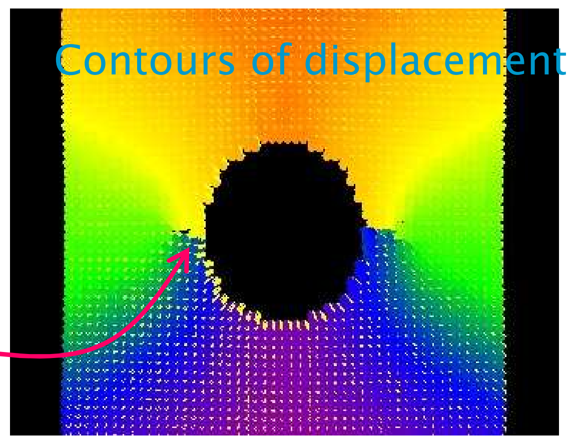
Crack nucleation

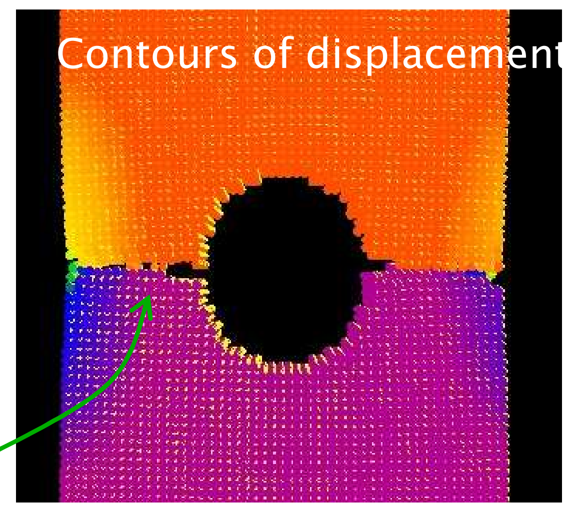
- A maximum in the bond force curve leads to crack nucleation at a prescribed strain independent of the breakage stretch.





Stretch > initiation strain leads to crack initiation



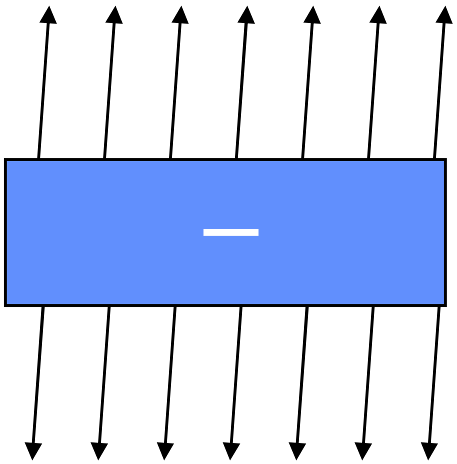


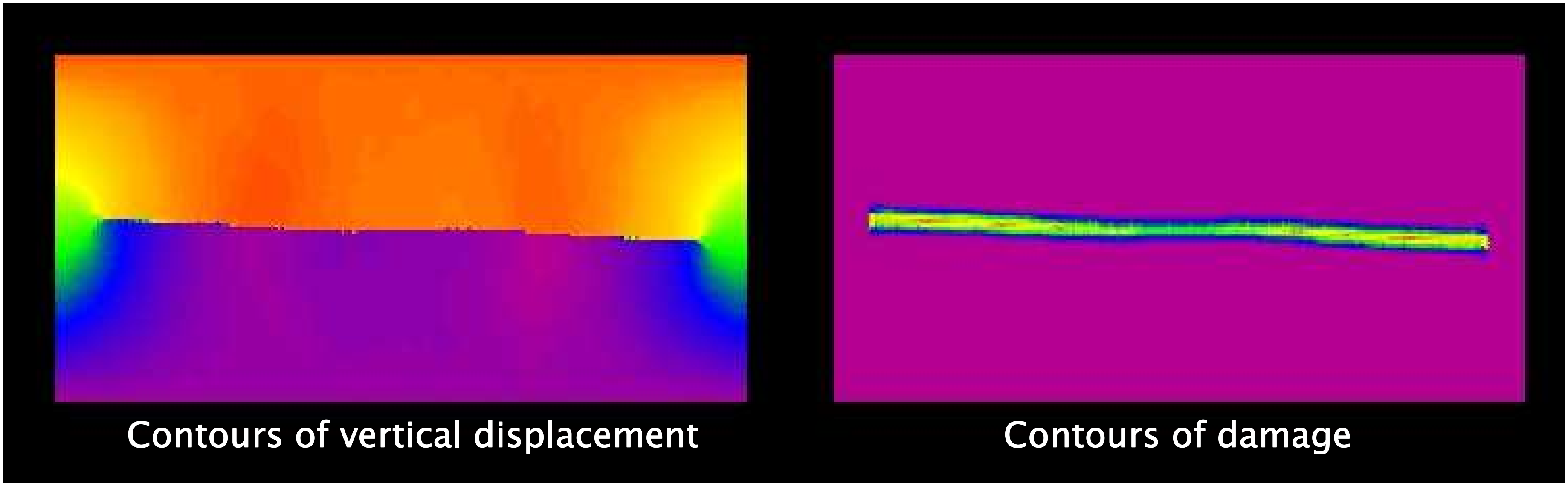
Crack initiation leads to dynamic fracture

Predicted crack growth direction depends continuously on loading direction

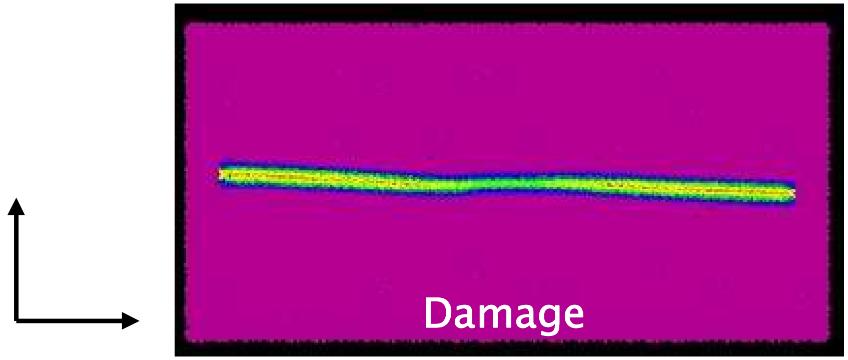
- Plate with a pre-existing defect is subjected to prescribed boundary velocities.
- These BC correspond to mostly Mode-I loading with a little Mode-II.

$$\dot{\varepsilon} = (0.25\mathrm{s}^{-1}) \begin{bmatrix} 0 & 0.1 \\ 0 & 1 \end{bmatrix}$$

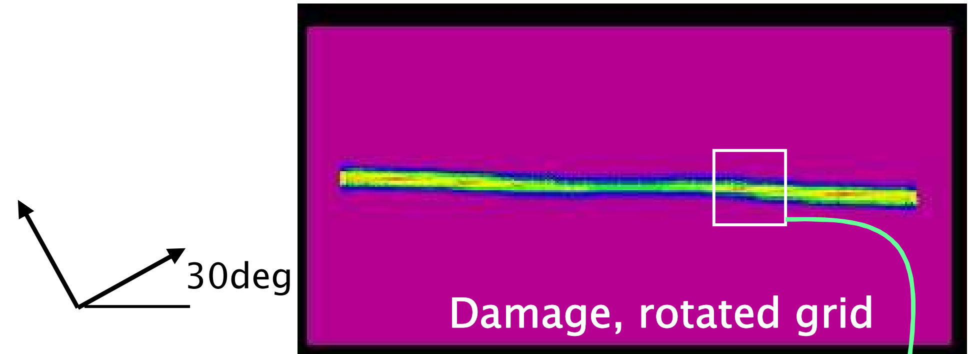




Effect of rotating the grid in the “mostly Mode-I” problem

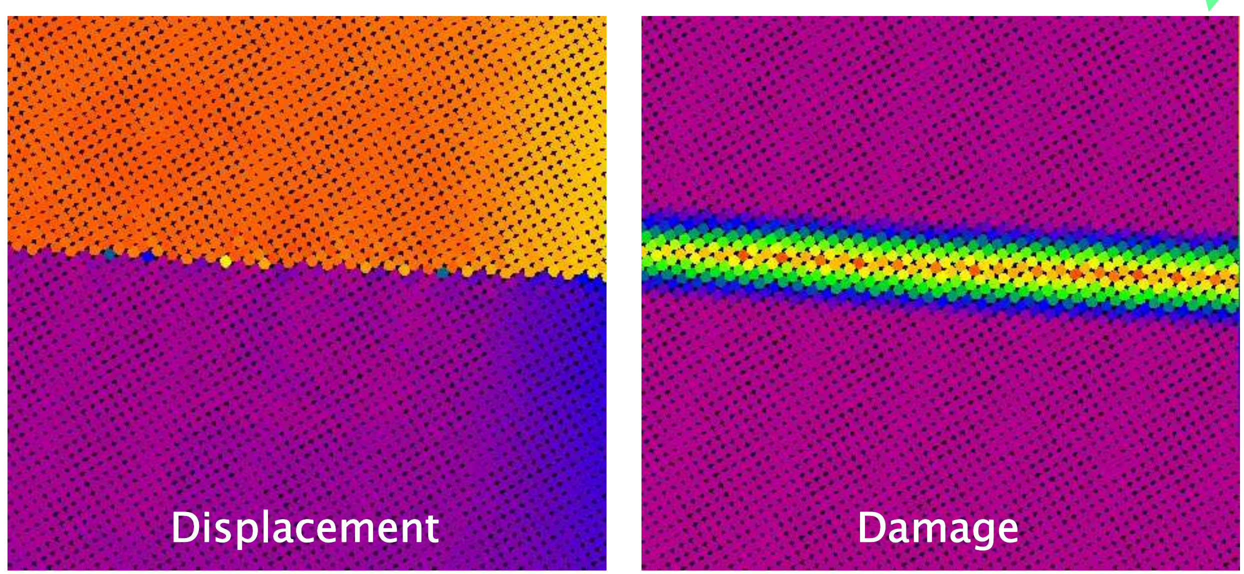


Original grid direction

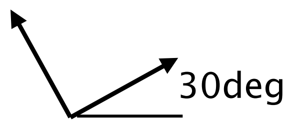


Rotated grid direction

Network of identical bonds in many directions allows cracks to grow in any direction.

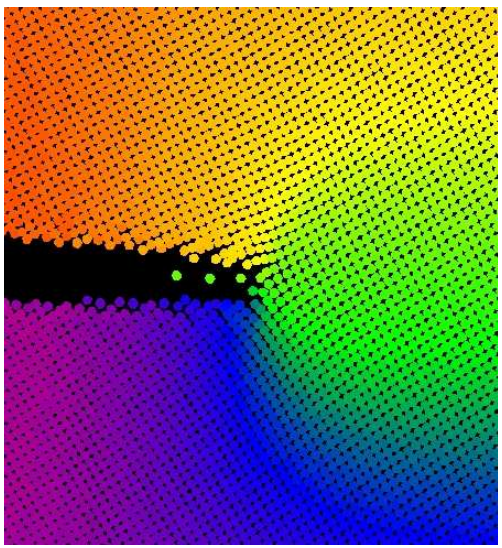


Crack tip fields in the "mostly Mode-I" problem

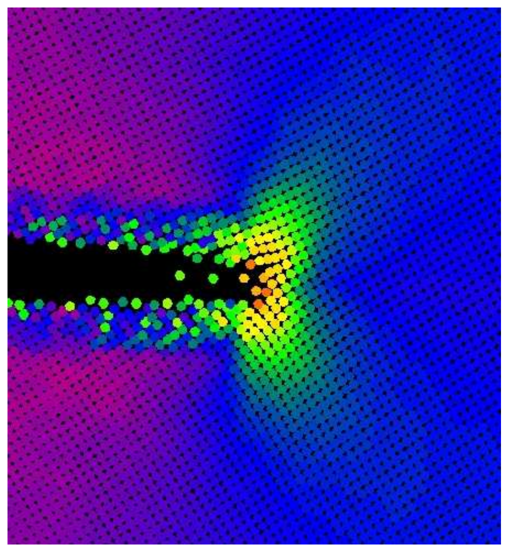


Rotated grid direction

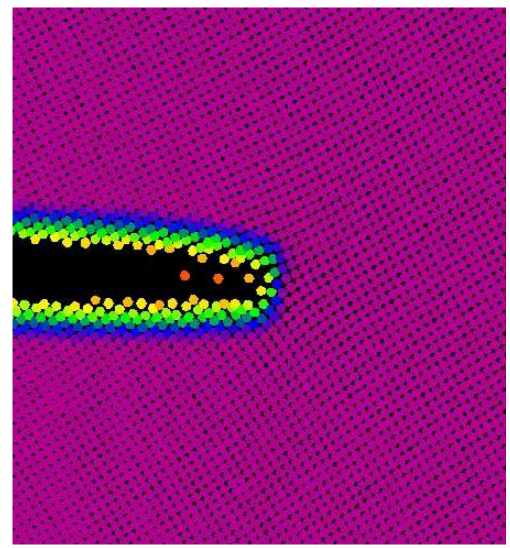
Nodal displacements shown below are x200.



Contours of vertical displacement



Contours of maximum bond stretch (similar to max principal strain)



Contours of damage

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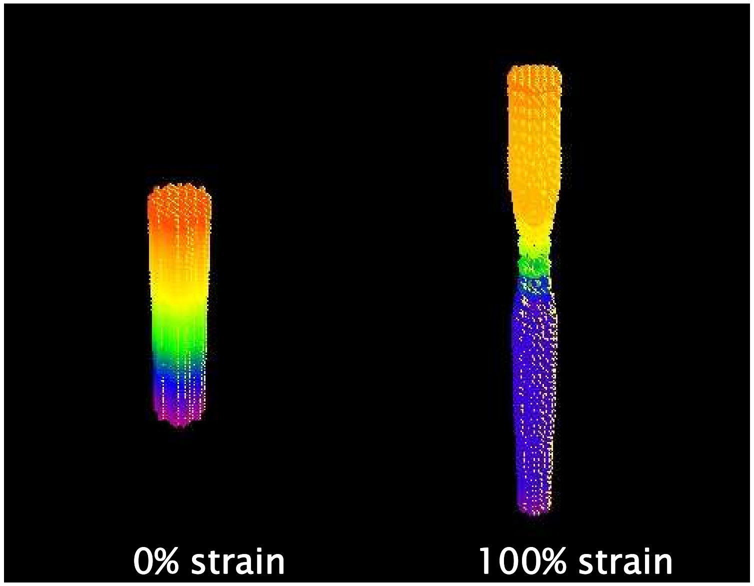
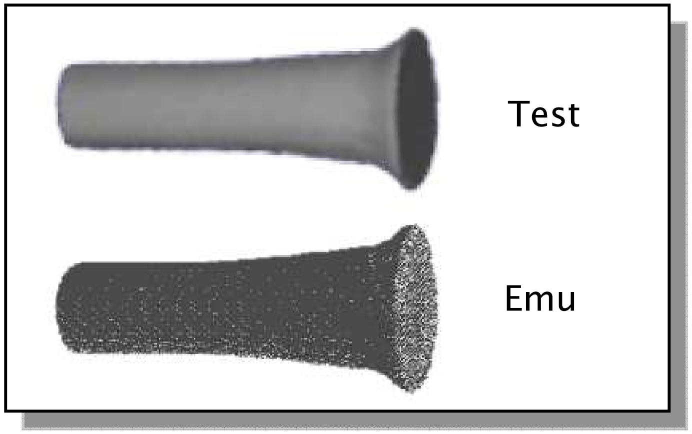
Peridynamic model of a 6061-aluminum bar

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



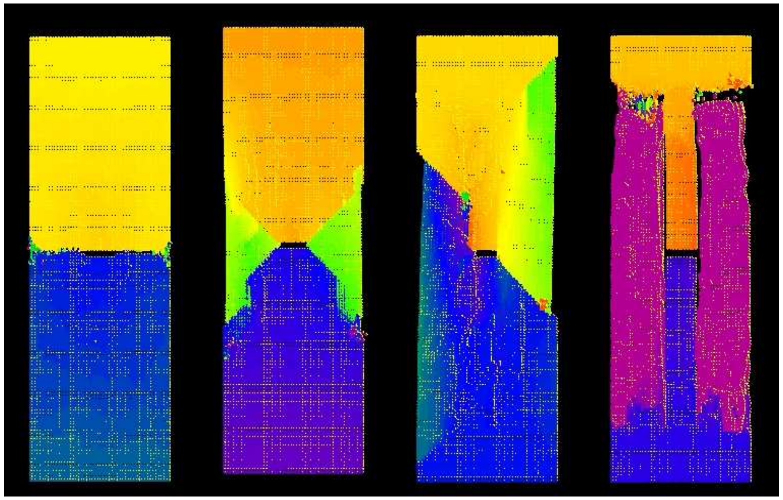
Necking under tension



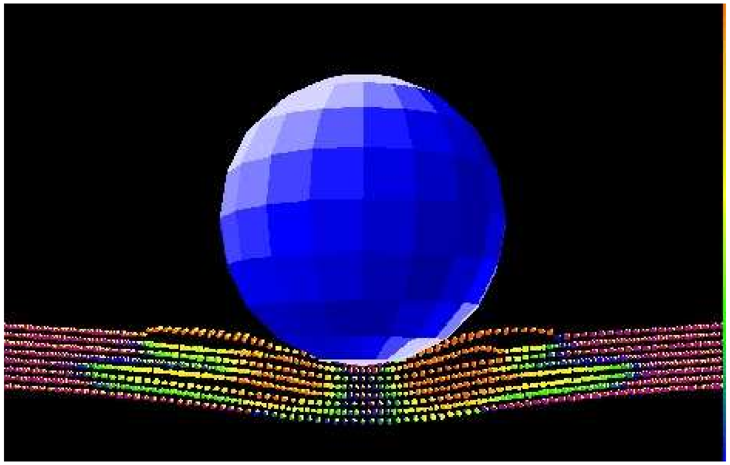
Taylor impact test
(J. Foster)

Bond based PD:
Damage in composites (Boeing)

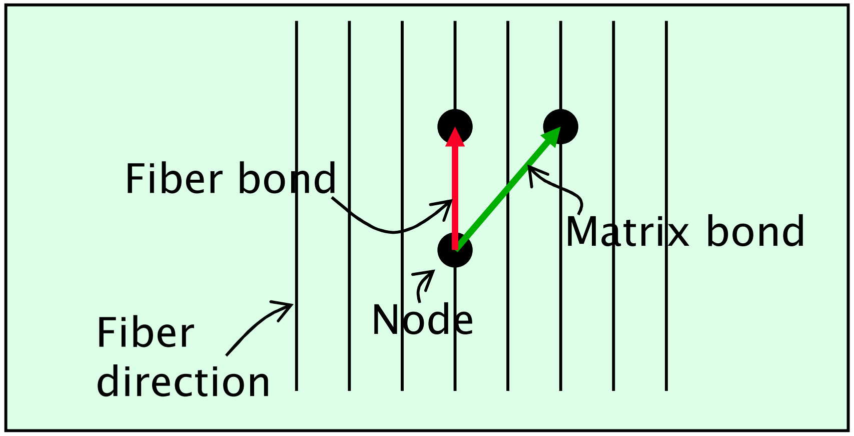
- How does the fraction of fibers in each direction affect the direction of crack growth?
- What damage occurs when a composite panel is struck by hail?



Crack growth in a notched panel

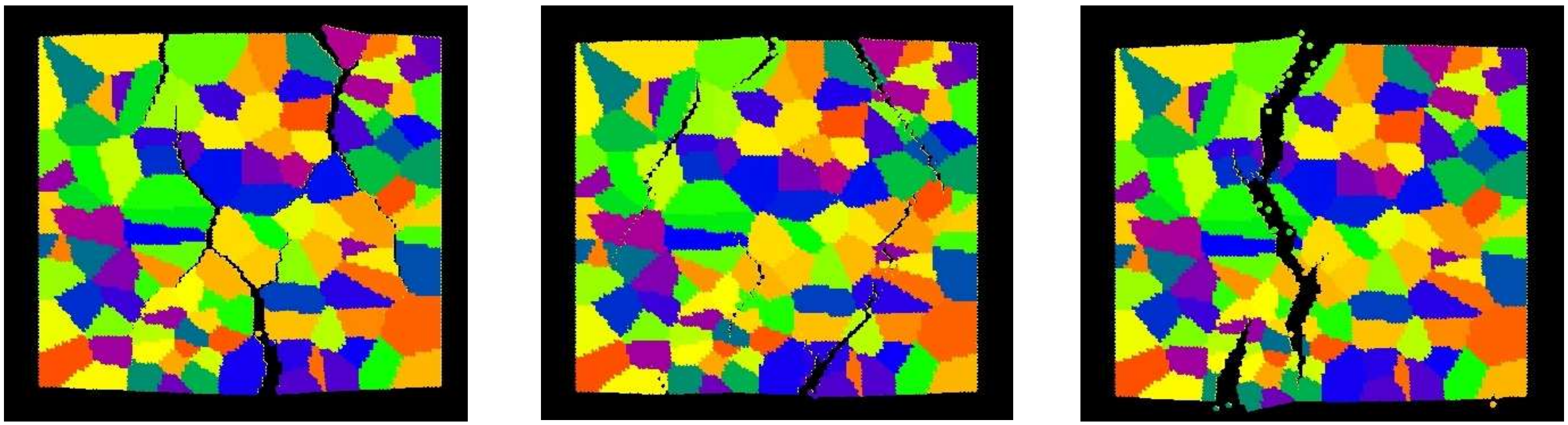


Delamination caused by impact



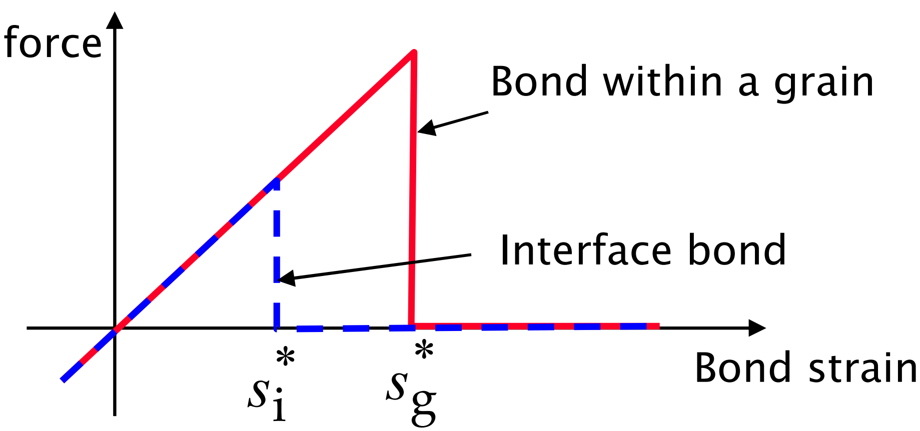
Polycrystals: Mesoscale model*

- What is the effect of grain boundaries on the fracture of a polycrystal?



β = 0.25   β = 1   β = 4

$$\boxed{\beta = \frac{s_{\mathrm{i}}^{*}}{s_{\mathrm{g}}^{*}}}$$



Large β favors intra(trans)-granular fracture.

* Work by F. Bobaru & students

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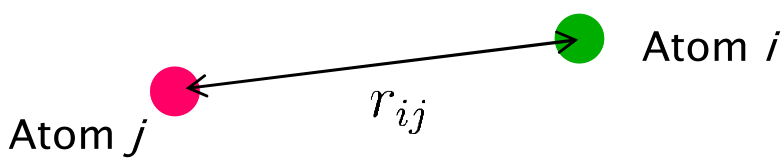
Nonlocality and length scales

- 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.



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

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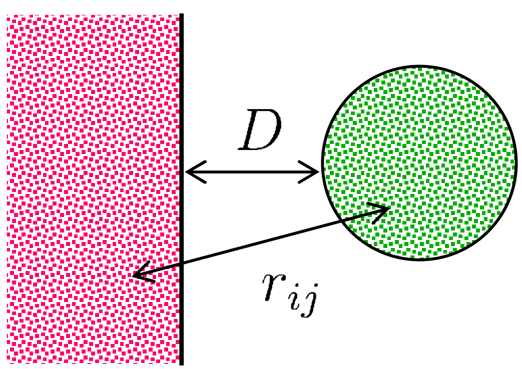
Nonlocality and length scales: surface forces

- 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:

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

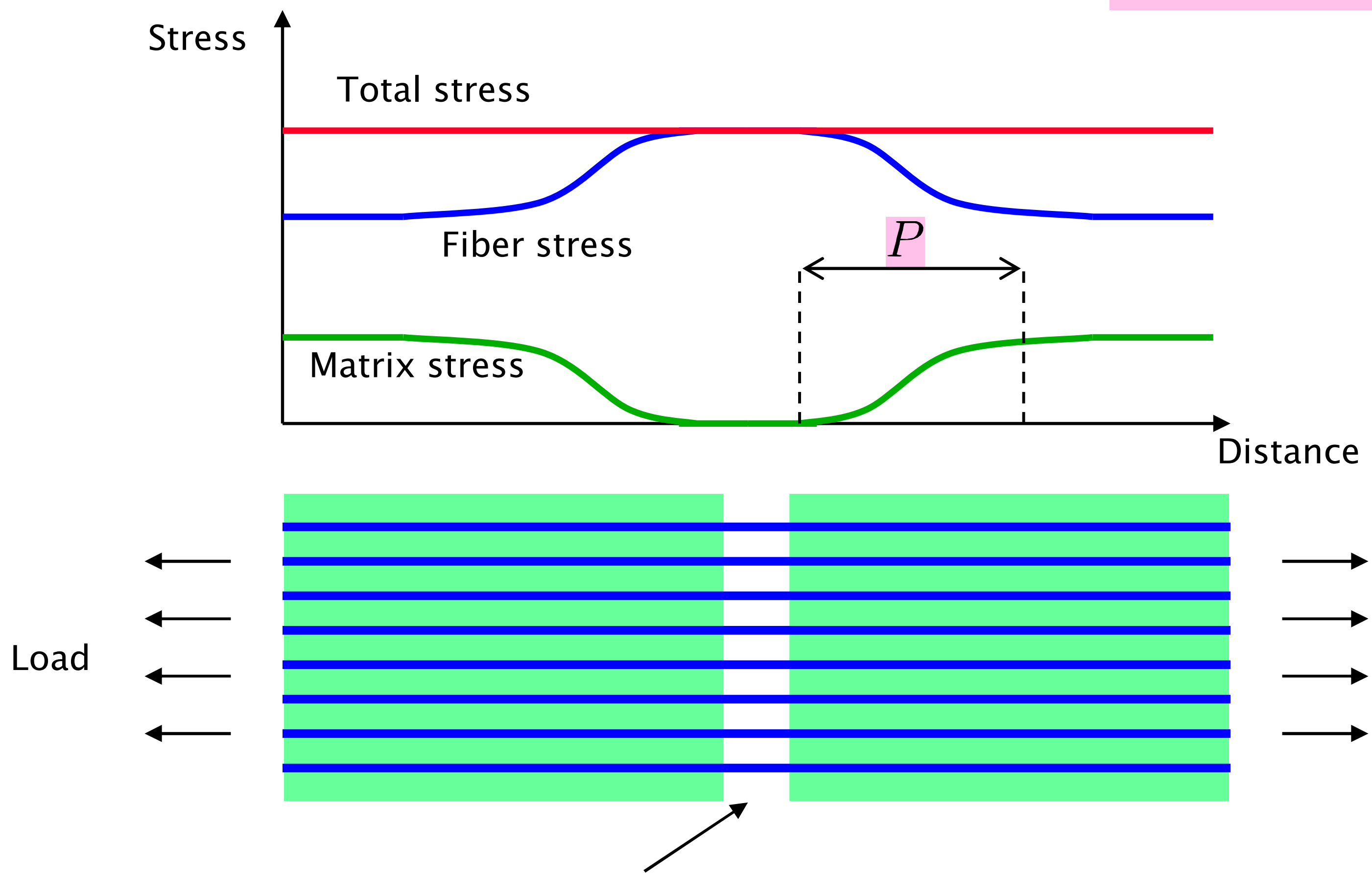


See J. Israelachvili, *Intermolecular and Surfaces Forces*, pp. 177.

Nonlocality and length scales: composites

- In a composite, the applicable length scale could be much greater than the fiber diameter or ply thickness.

$$P >> D_{\text{fiber}}$$



Fiber-reinforced composite with a gap in the matrix (“bridging”)

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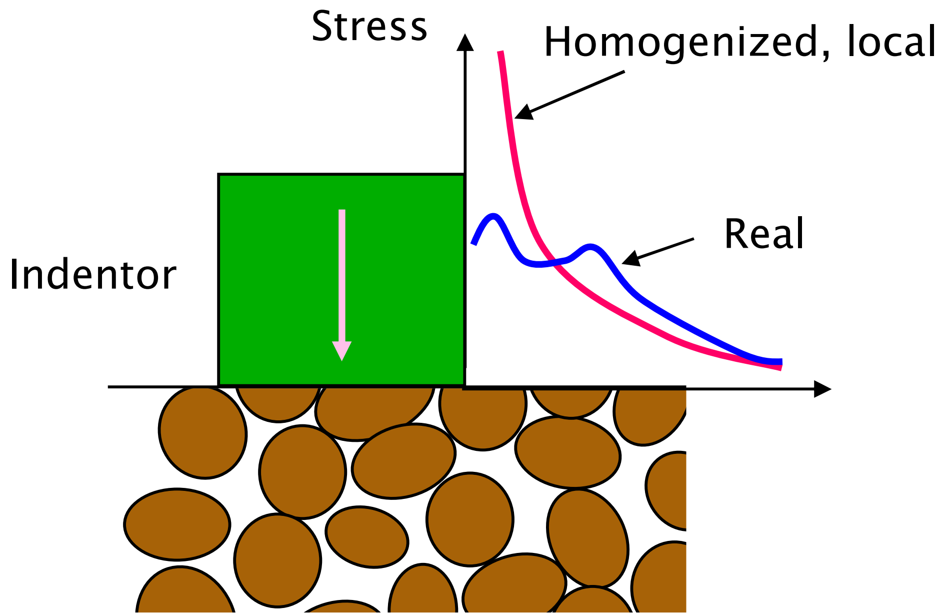
Nonlocality as a result of homogenization

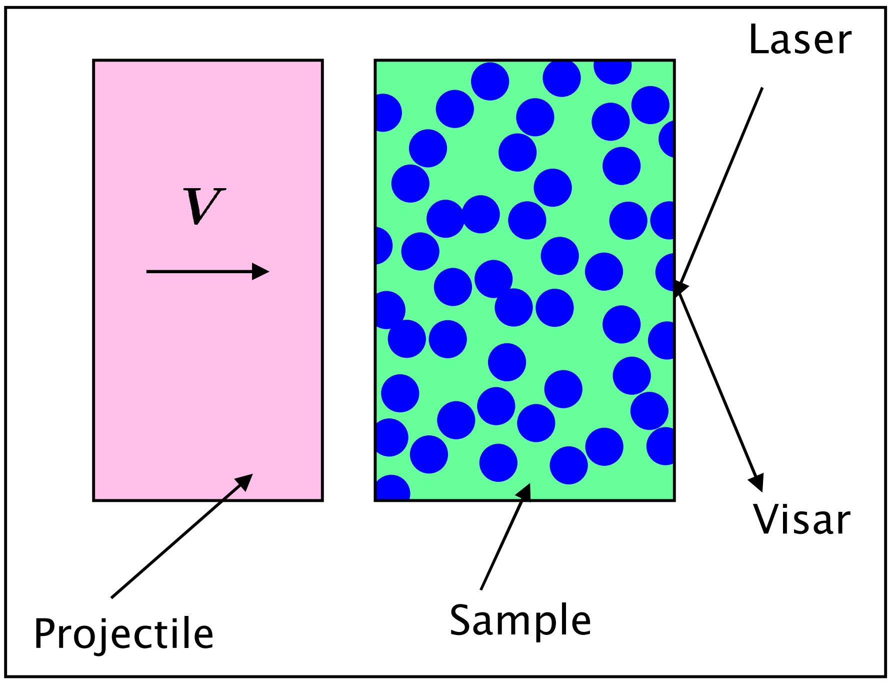
- Homogenization, neglecting the natural length scales of a system, often doesn't give good answers.

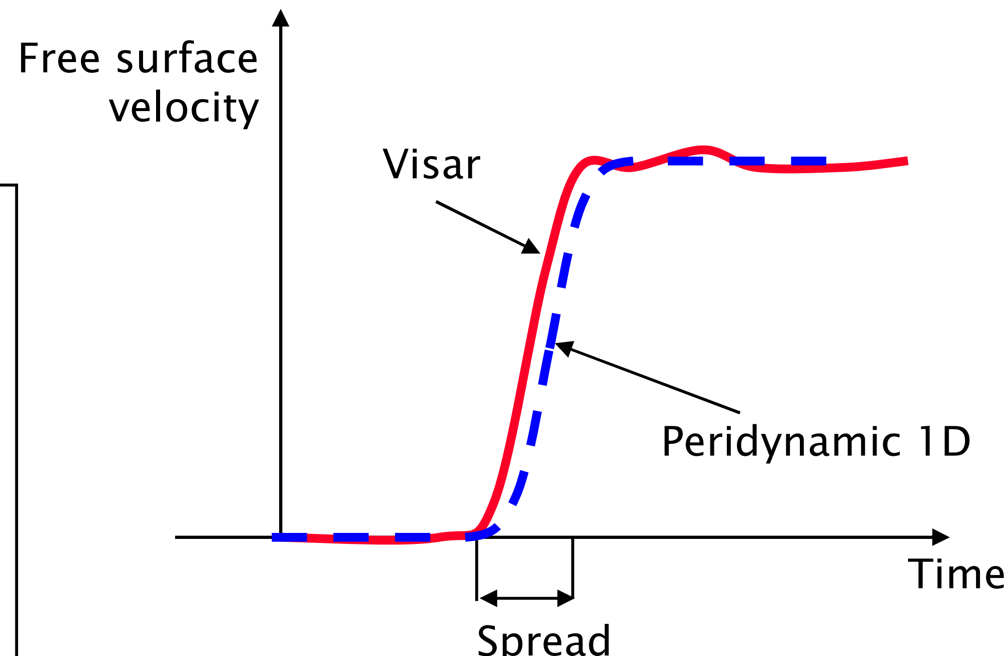


Claim: Nonlocality is an essential feature of a realistic homogenized model of a heterogeneous material.

Proposed experimental method for measuring the peridynamic horizon

- Measure how much a step wave spreads as it goes through a sample.
- Fit the horizon in a 1D peridynamic model to match the observed spread.





Local model would predict zero spread.

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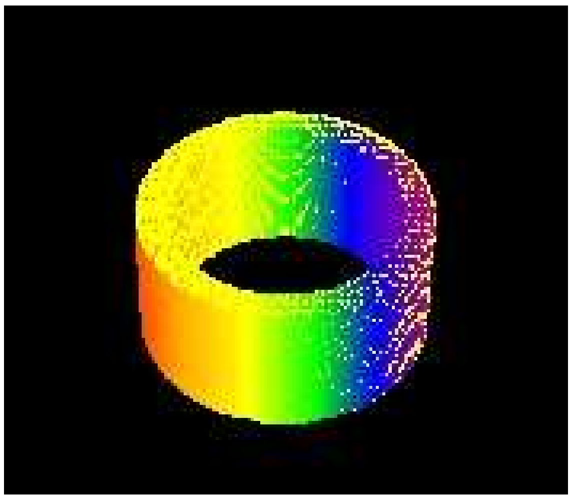
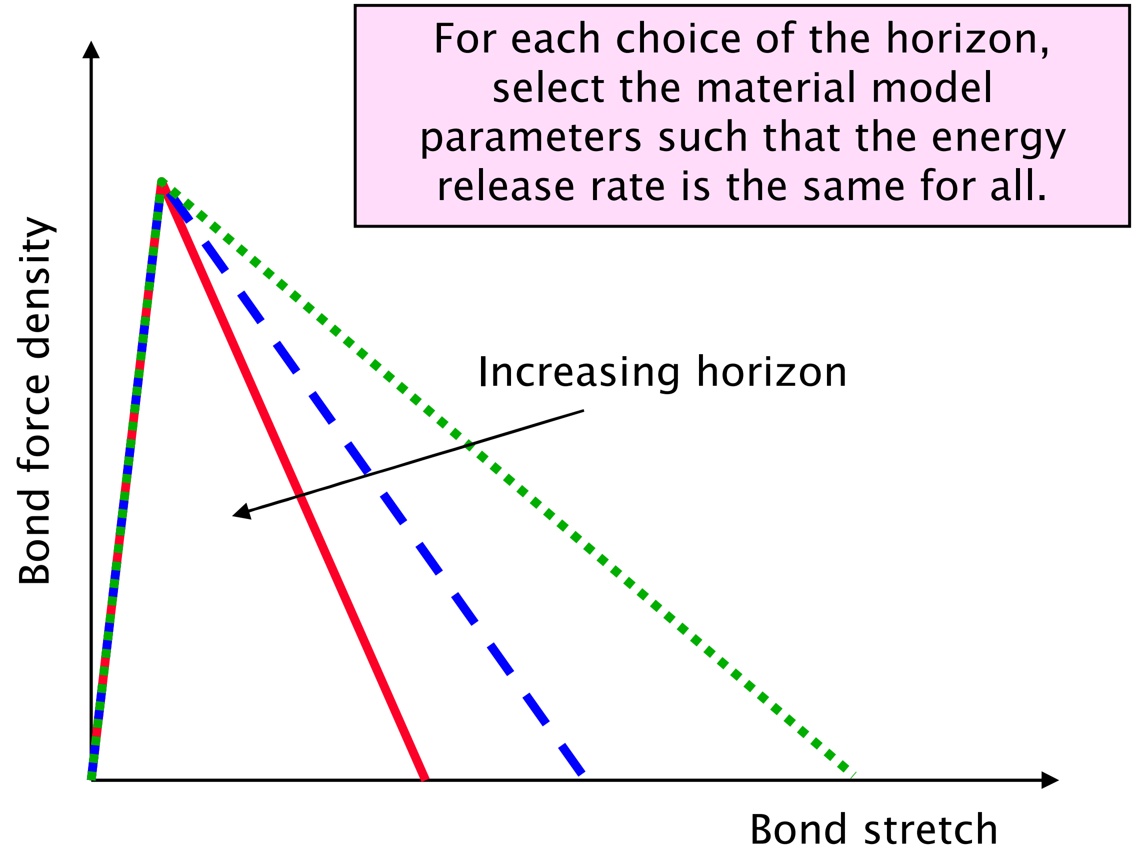
Outline

- Objective
- Theory
- EMU numerical method
- Examples
- Heterogeneity and nonlocality
- Fragmentation

Fragmentation example: Expanding brittle tube



- Outer radius = 100 mm
- Thickness = 10 mm
- Radial velocity = 600 m/s



- Grid contains 1% random perturbations to act as seed.

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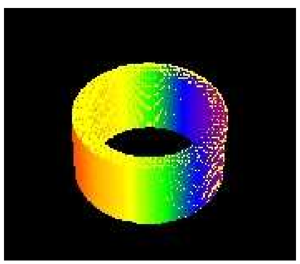
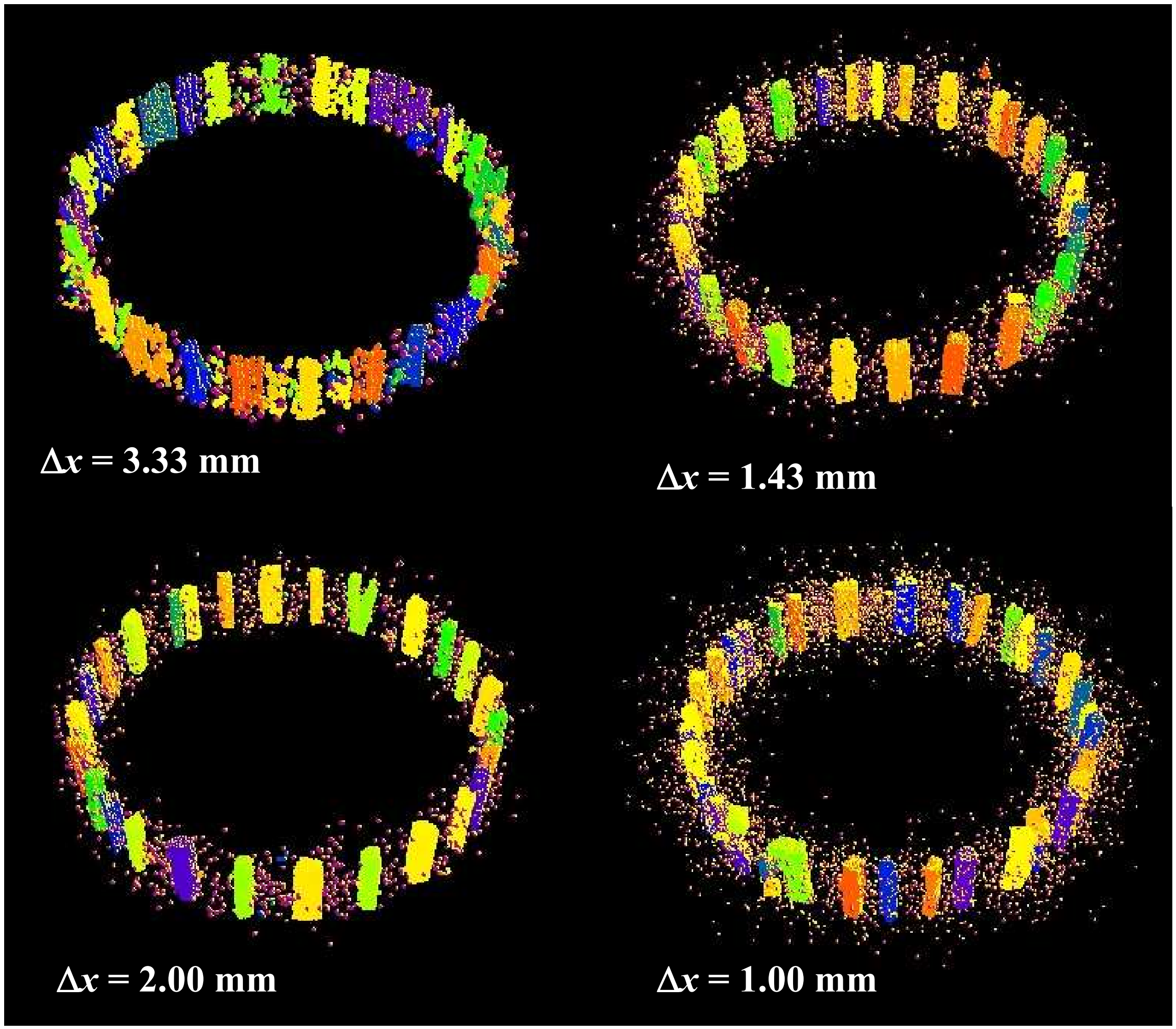
Fragmentation example: Same problem with 4 different grid spacings



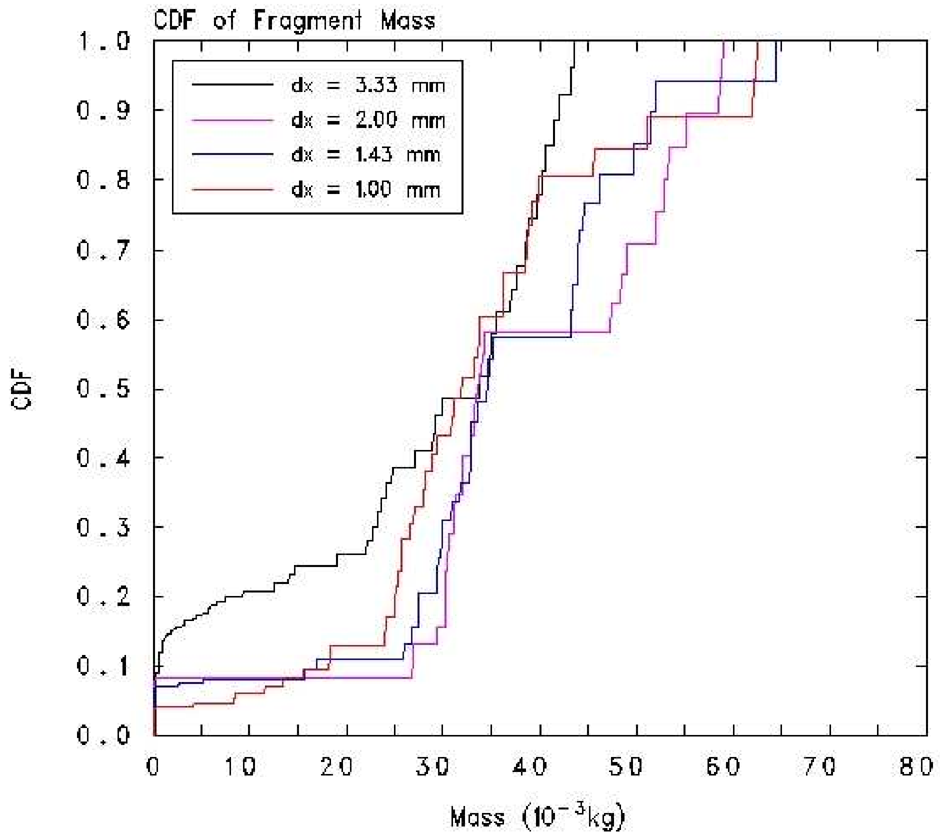
Colors are just for visualization



$$\boxed{\delta = 3\Delta x}$$

Fragmentation example: Fragment mass distribution

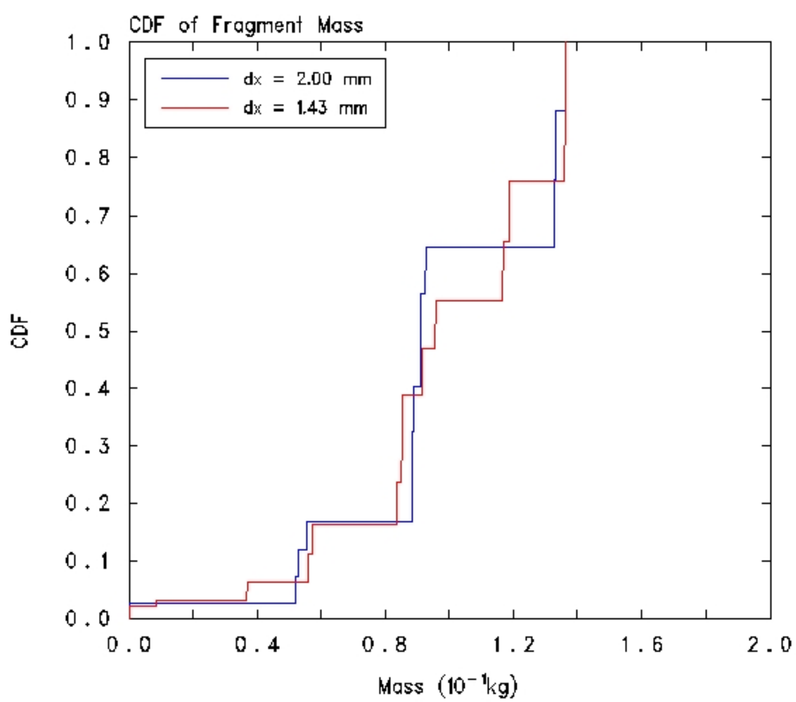
Cumulative distribution function for 4 grid spacings

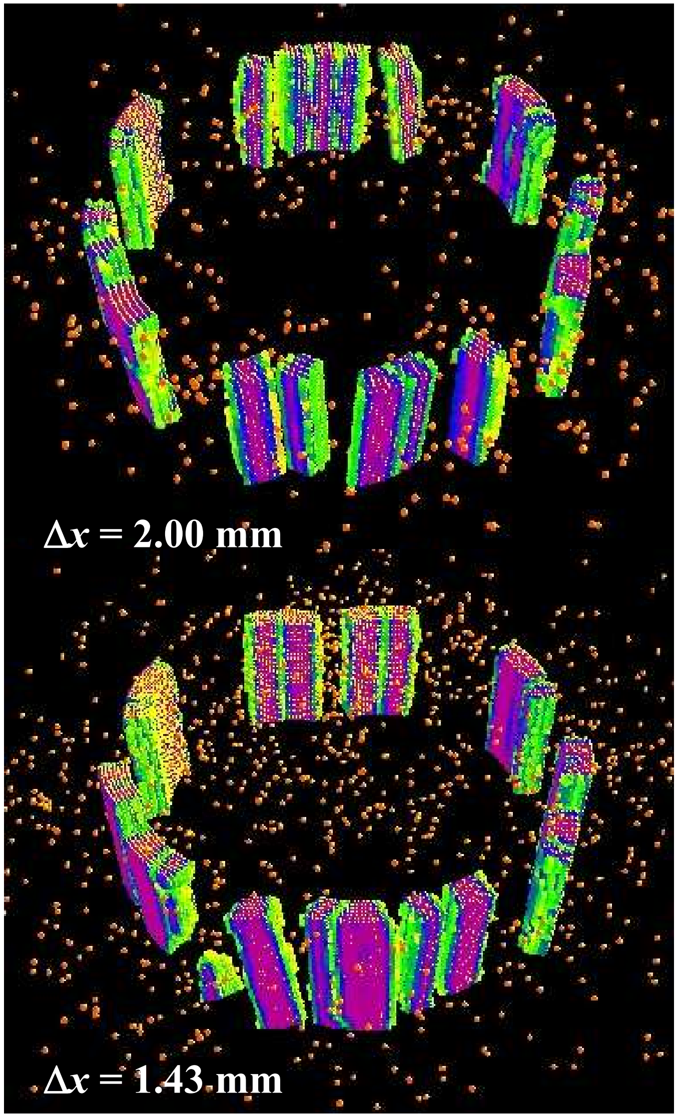


Δx (mm)	Mean fragment mass (g)
3.33	27.1
2.00	37.8
1.43	35.9
1.00	33.5

Fragmentation example: Lower initial velocity

- 200 m/s initial radial velocity.
- Not all cracks grow to completion.





Contours of damage

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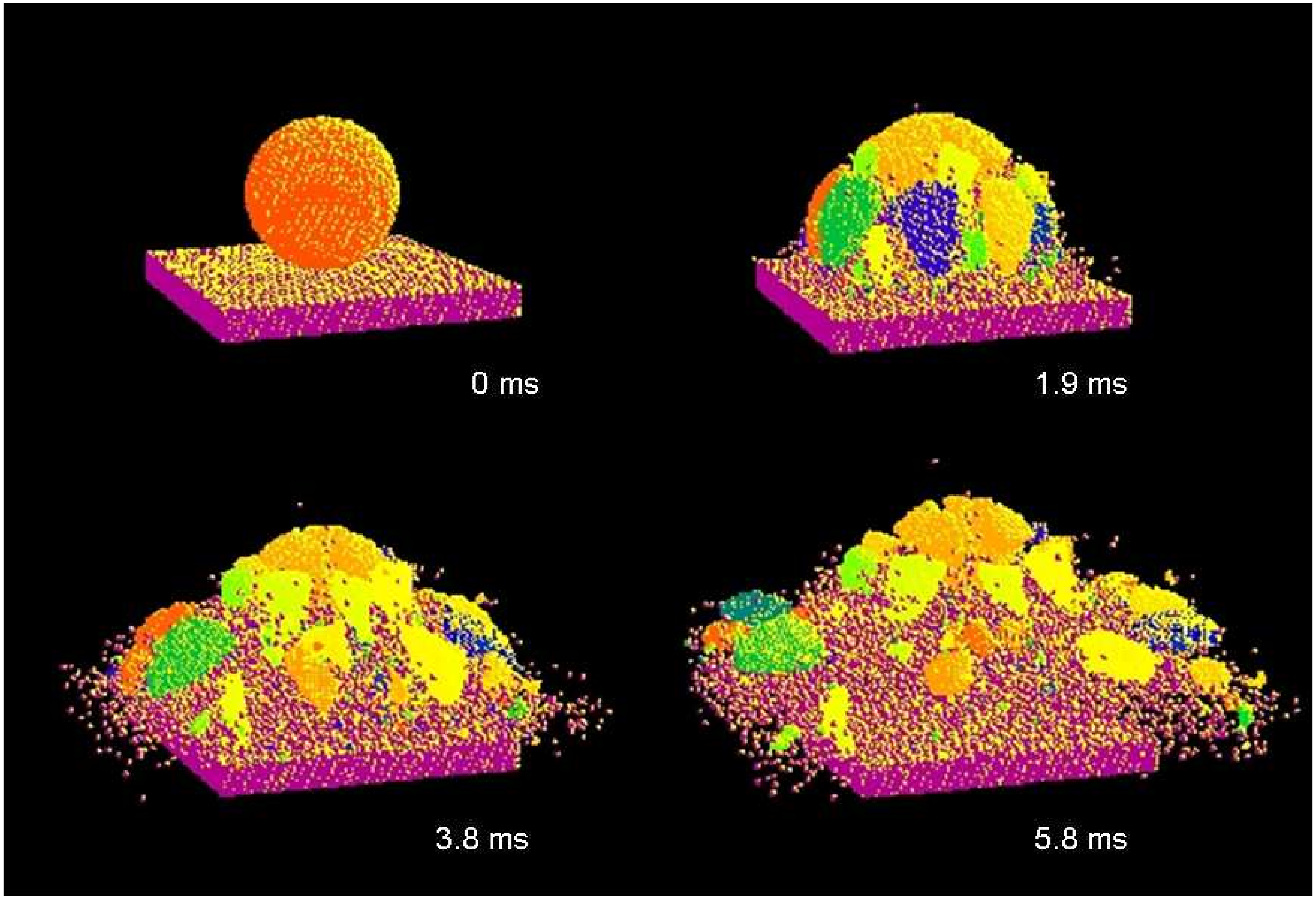
Applications: Fragmentation of a concrete sphere

- 15cm diameter concrete sphere against a rigid plate, 32.4 m/s.
  - Mean fragment size agrees well with experimental data of Tomas.



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Conclusions

- The ability to apply exactly the same equations everywhere yields practical benefits:
  - Cracks nucleate spontaneously.
  - Cracks advance "autonomously" – no need for supplemental equations.
  - Dynamic fracture/fragmentation examples appear to have good convergence properties.

- The theory converges to the classical theory in the limit of small interaction distance.
  - Yet nonlocality seems to be an essential feature of heterogeneous media.