SAND2007-3464C

Peridynamic Simulation of High-Rate Material Failure

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2007 ASME Applied Mechanics and Materials Conference, Austin, TX
June 6, 2007

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

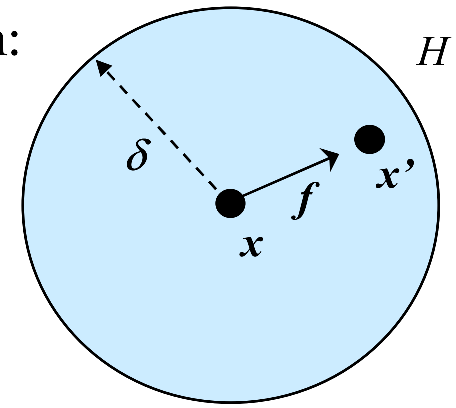
Background:
A better way to model cracks

- Problem
  - Develop a general tool for modeling material and structural failure due to cracks.
- Motivation
  - Standard mathematical theory for modeling deformation cannot handle cracks.
    - PDE's break down if a crack is present.
    - Finite elements and similar methods inherit this problem.
- Approach
  - Develop a mathematical theory in which:
    - The same equations apply on or off of a crack.
    - Cracks are treated like any other type of deformation.
    - Cracks are self-guided: no need for supplemental equations.
  - Implement the theory in a meshless Lagrangian code called **EMU**.

Peridynamic theory – the basic idea

- PDEs are replaced by the following integral equation:

$$\rho\, \ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_H \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{x}',t) - \boldsymbol{u}(\boldsymbol{x},t), \boldsymbol{x}' - \boldsymbol{x})\, dV' - \boldsymbol{b}(\boldsymbol{x},t)$$



- Compare classical PDE:

$$\rho\, \ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \nabla \bullet \boldsymbol{\sigma}(\boldsymbol{x},t) - \boldsymbol{b}(\boldsymbol{x},t)$$

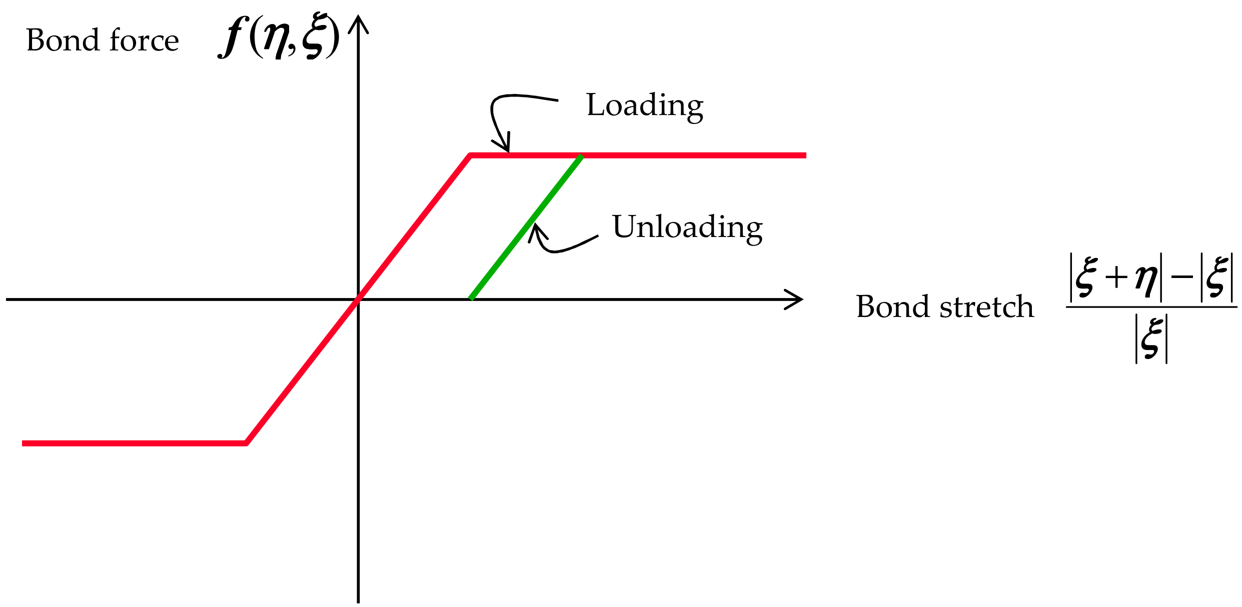
where

u = displacement; ***f*** = force density that ***x'*** exerts on ***x;***

b = prescribed external force density; *H* = neighborhood of ***x*** with fixed radius δ.

Material models

- A peridynamic material model gives bond force density as a function of bond stretch.
- Can include dependence on rate and history of stretch.
- Notation: $\eta = u' - u$ $\xi = x' - x$

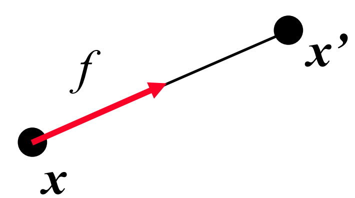


Microelastic materials

- A body is microelastic if f is derivable from a scalar **micropotential** w, i.e.,

$$f(\eta,\xi) = \frac{\partial w}{\partial \eta}(\eta,\xi) \qquad \eta = u' - u \qquad \xi = x' - x$$

- Interactions ("bonds") can be thought of as elastic (possibly nonlinear) springs.



- Strain energy density at $\boldsymbol{x}$ is found by summing the energies of all springs connected to $\boldsymbol{x}'$:

$$W(x) = \frac{1}{2}\int_R w(u'-u, x'-x)\,dV'$$

What if you really want a stress tensor?

- Stress tensors (and strain tensors) play no role in the theory so far.
- However, define the peridynamic stress tensor field by

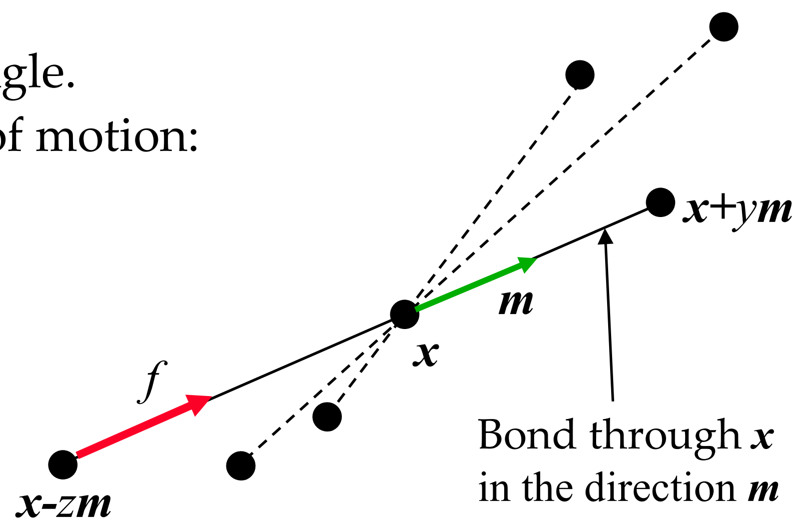
$$\sigma_{ij}(\mathbf{x}) = \frac{1}{2}\int_S \int_0^\infty \int_0^\infty (y+z)^2 \hat{f}_i(\mathbf{x}+y\mathbf{m}, \mathbf{x}-z\mathbf{m}) m_j \, dz\, dy\, d\Omega_m$$

$$\hat{f}_i(\mathbf{p},\mathbf{q}) = f_i(\mathbf{u}(\mathbf{p})-\mathbf{u}(\mathbf{q}), \mathbf{p}-\mathbf{q})$$

where S is the unit sphere and Ω is solid angle.

- This field satisfies the **classical** equation of motion:

$$\rho \ddot{u}_i = \sigma_{ij,j} + b_i$$



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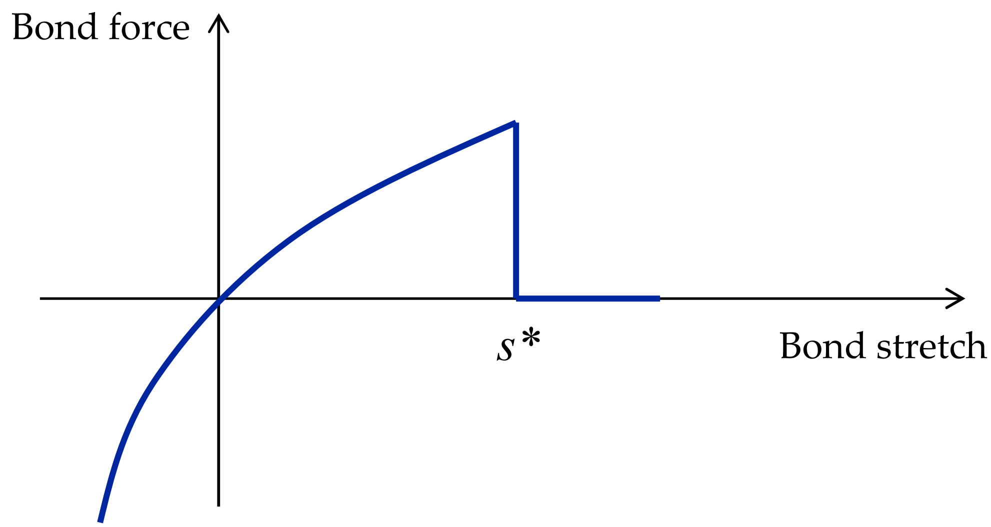
Material modeling: Damage

- Damage is introduced at the bond level.
- Bond breakage occurs irreversibly according to some criterion such as exceeding a prescribed critical stretch.
- In practice, bond breakages tend to occur along 2D surfaces (cracks).



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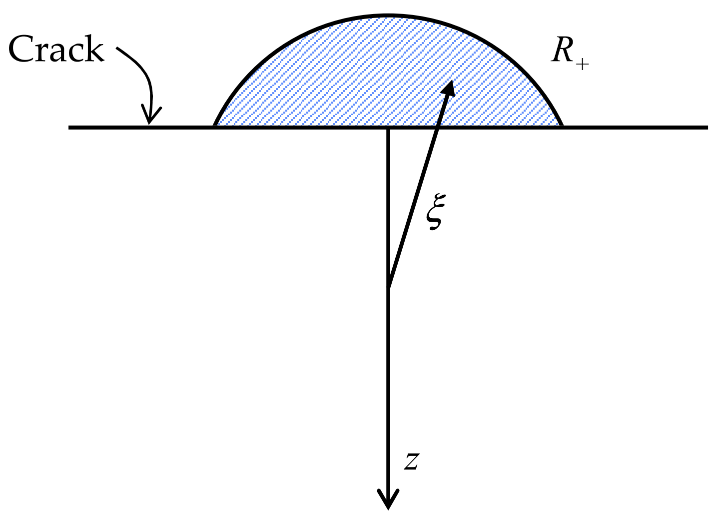
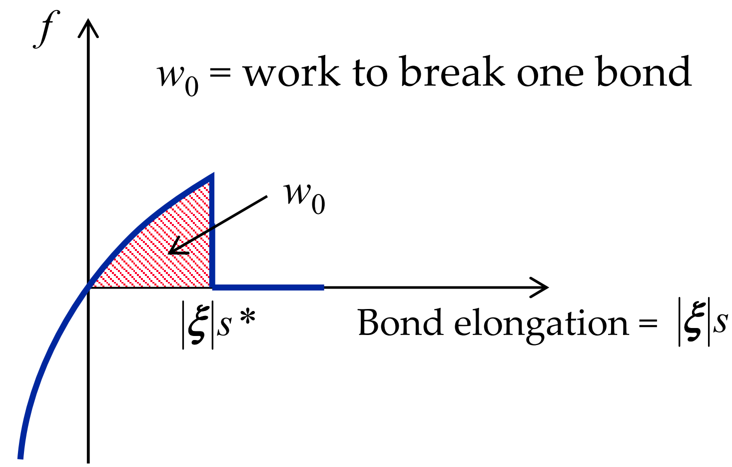
Energy required to advance a crack determines the bond breakage stretch

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

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





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

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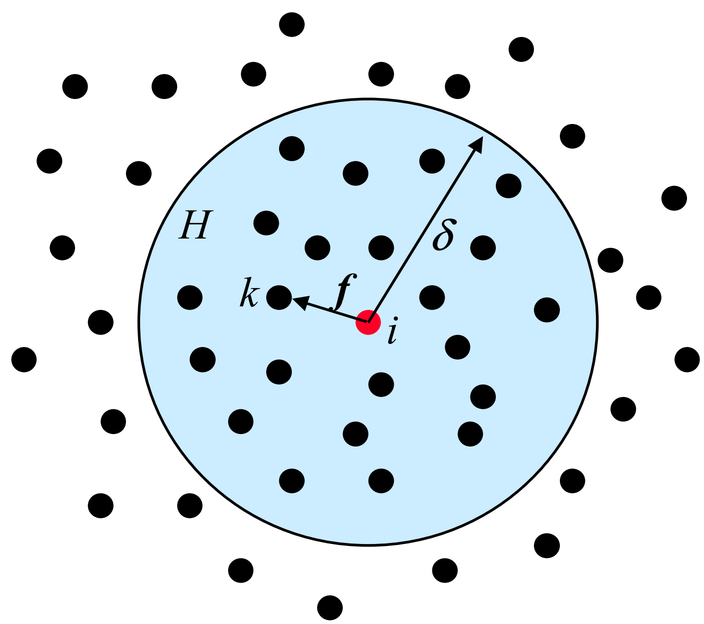
EMU numerical method

- Integral is replaced by a finite sum.

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

- Resulting method is meshless and Lagrangian.



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EMU numerical method: Relation to SPH

SPH

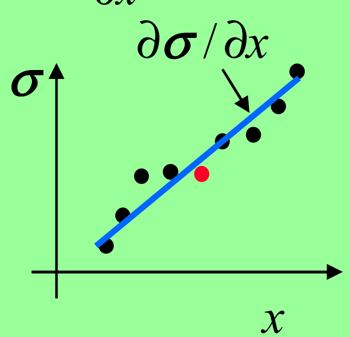
$$\frac{\partial v}{\partial x} = \int v(x')K(x')dV'$$

$$\dot{\varepsilon} = \frac{1}{2}\left(\left(\frac{\partial v}{\partial x}\right) + \left(\frac{\partial v}{\partial x}\right)^T\right)$$

$$\sigma = \sigma(\varepsilon)$$

$$\frac{\partial \sigma}{\partial x} = \int \sigma(x')K(x')dV'$$

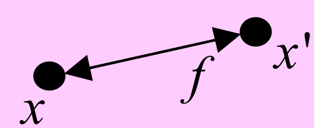
$$\rho\ddot{u} = \frac{\partial \sigma}{\partial x} + b$$



- Both are meshless Lagrangian methods.
- Both involve integrals.
- But the basic equations are fundamentally different:
  - SPH relies on curve fitting to approximate derivatives that appear in the classical PDEs.
  - Peridynamics does not use these PDEs, relies on pair interactions.

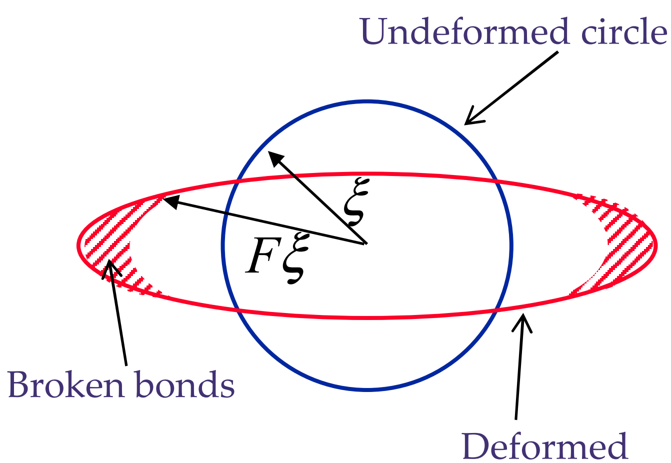
Emu

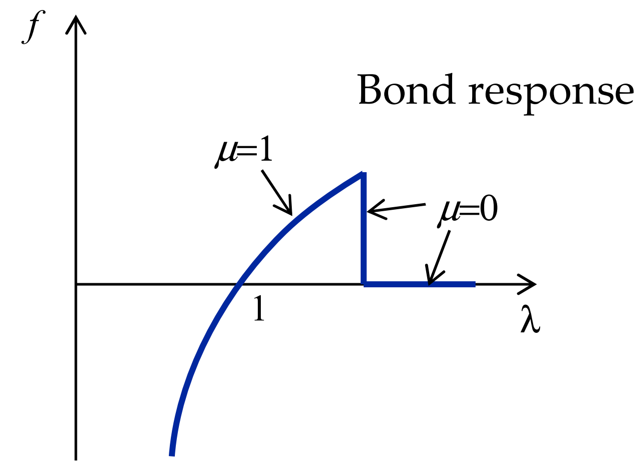
$$\rho\ddot{u}(x) = \int f\left(u(x') - u(x), x' - x\right)dV' + b(x)$$

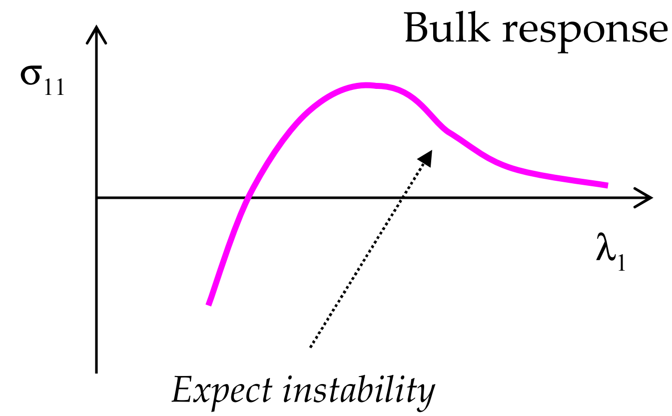


Bulk response with damage

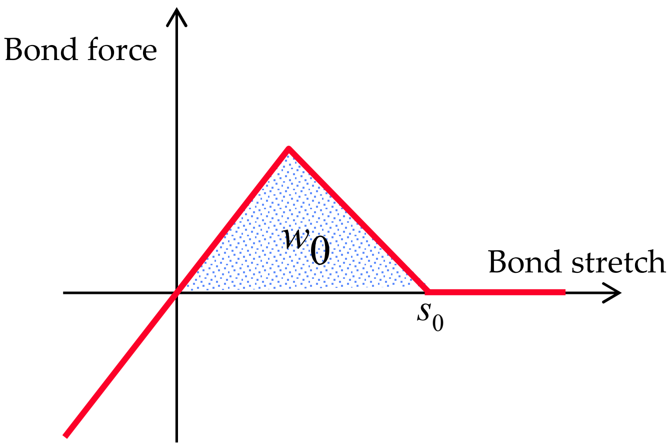
- Assume a homogeneous deformation.

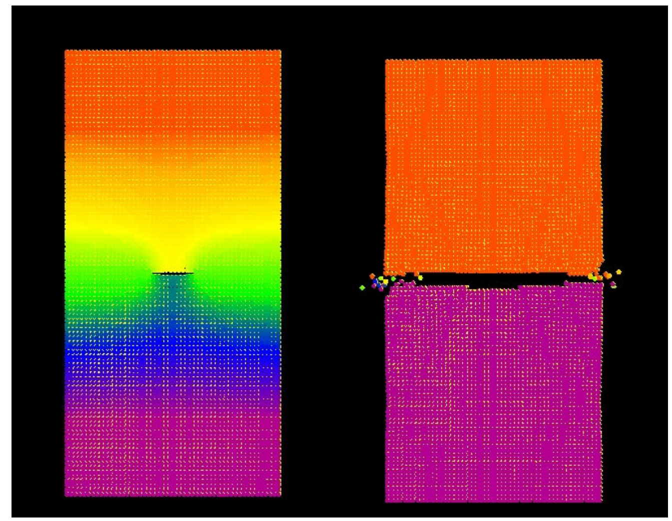






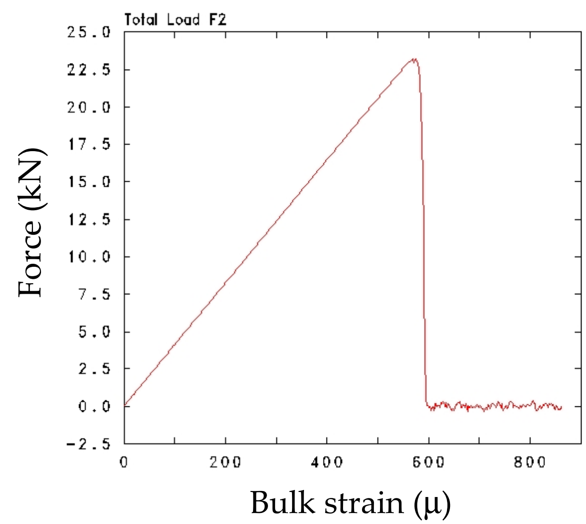
A validation problem:
Center crack in a brittle panel (3D)





Based on s_0=0.002, find ***G*=384 J/m²**.
Full 3D calculation shows crack growth
when σ=46.4 MPa. Use this in

$$G = \frac{\pi\sigma^2 a}{E} = 371\,\mathrm{J/m^2}$$



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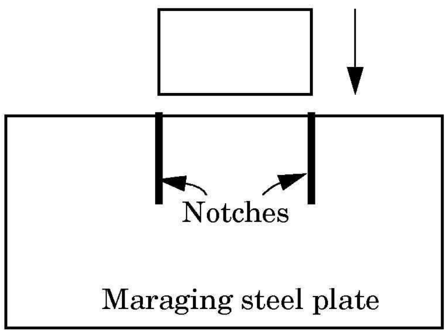
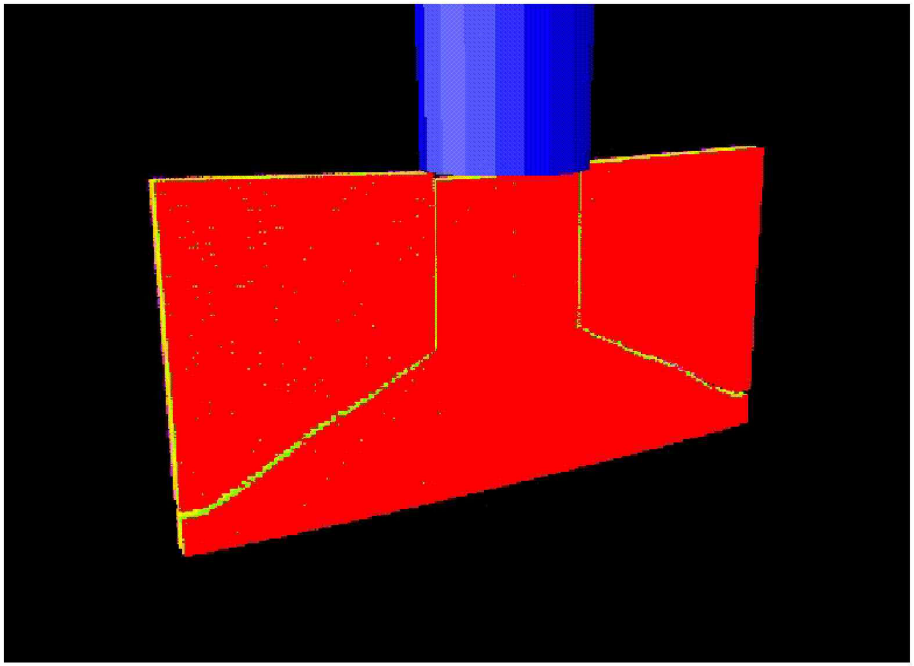
Example: dynamic fracture in steel

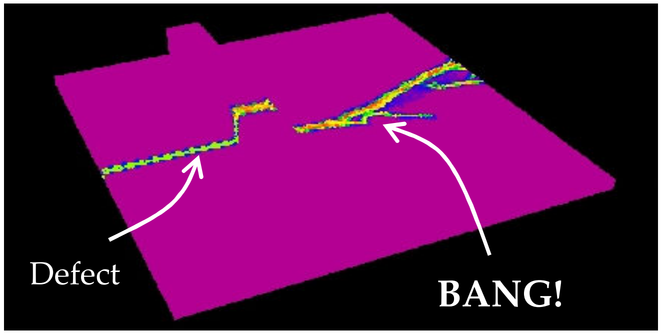


- Code predicts correct crack angles*.
- Crack velocity ~ 900 m/s.

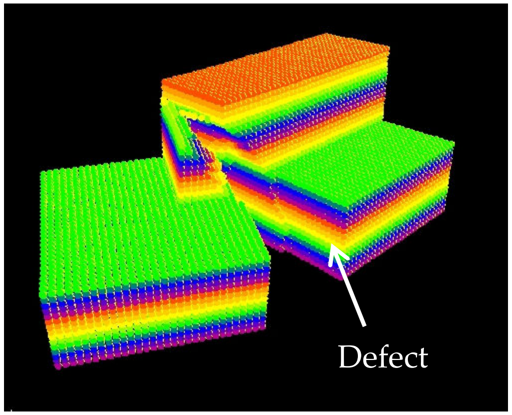


*J. F. Kalthoff & S. Winkler, in *Impact Loading and Dynamic Behavior of Materials*, C. Y. Chiem, ed. (1988)

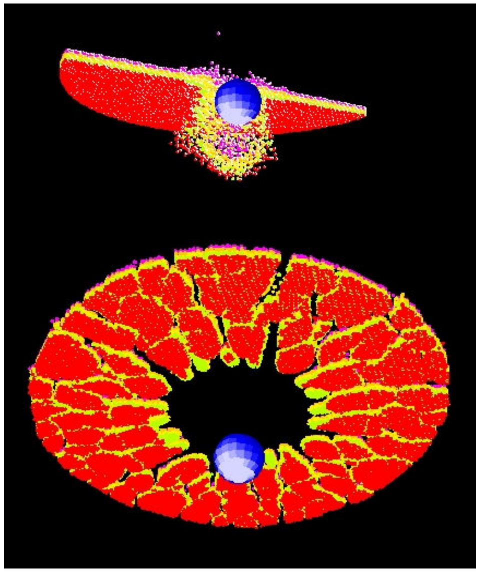
Isotropic materials: Other examples



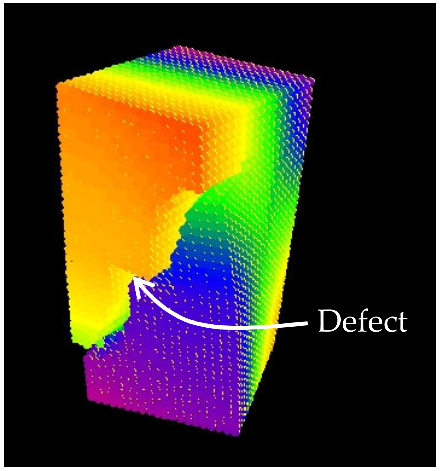
Transition to unstable crack growth



Crack turning in a 3D feature



Impact and fragmentation



Spiral crack due to torsion

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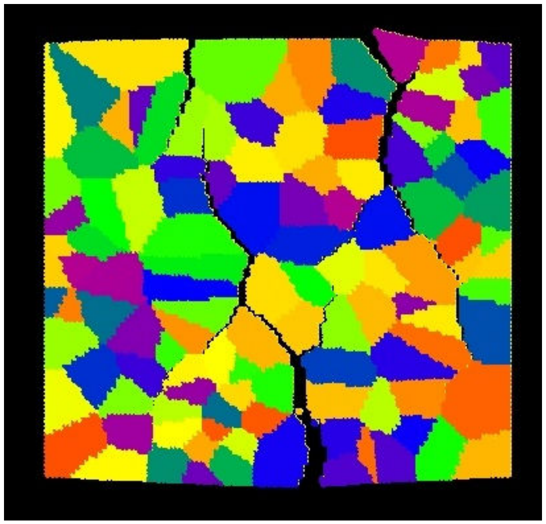
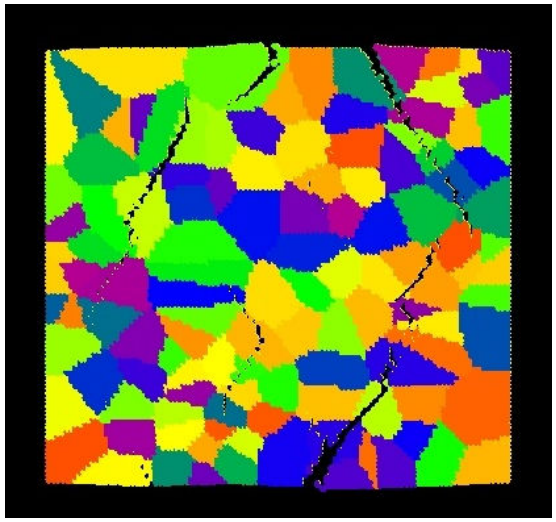
Polycrystals: Mesoscale model

(courtesy F. Bobaru, University of Nebraska)

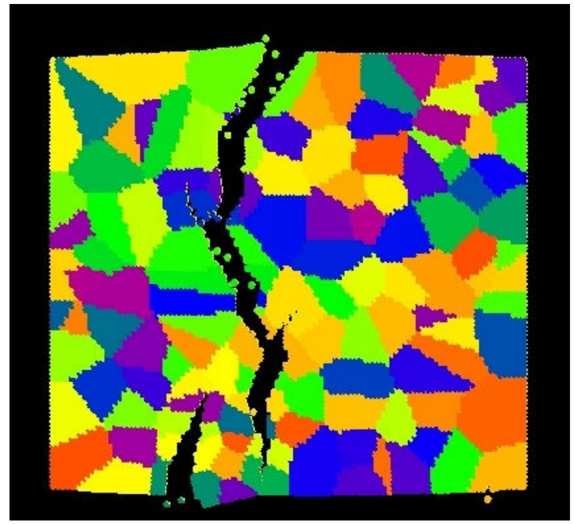
- What is the effect of grain boundaries on the fracture of a polycrystal?



$\beta = 0.25$



$\beta = 1$



$\beta = 4$

$$\beta = \frac{s^*_{\text{interface}}}{s^*_{\text{grain}}}$$

Large β favors intra(trans)-granular fracture.

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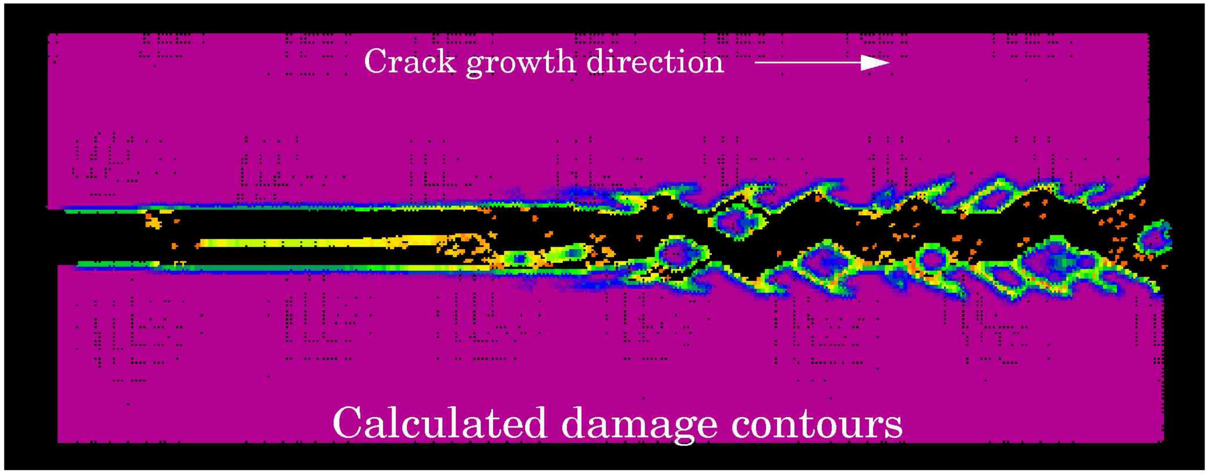
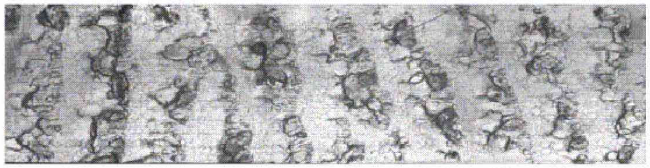
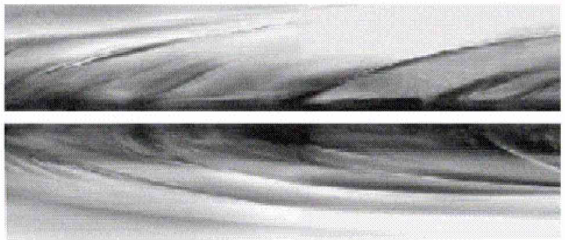
Example: dynamic fracture in PMMA

- Plate is stretched vertically.
- Code predicts stable-unstable transition.





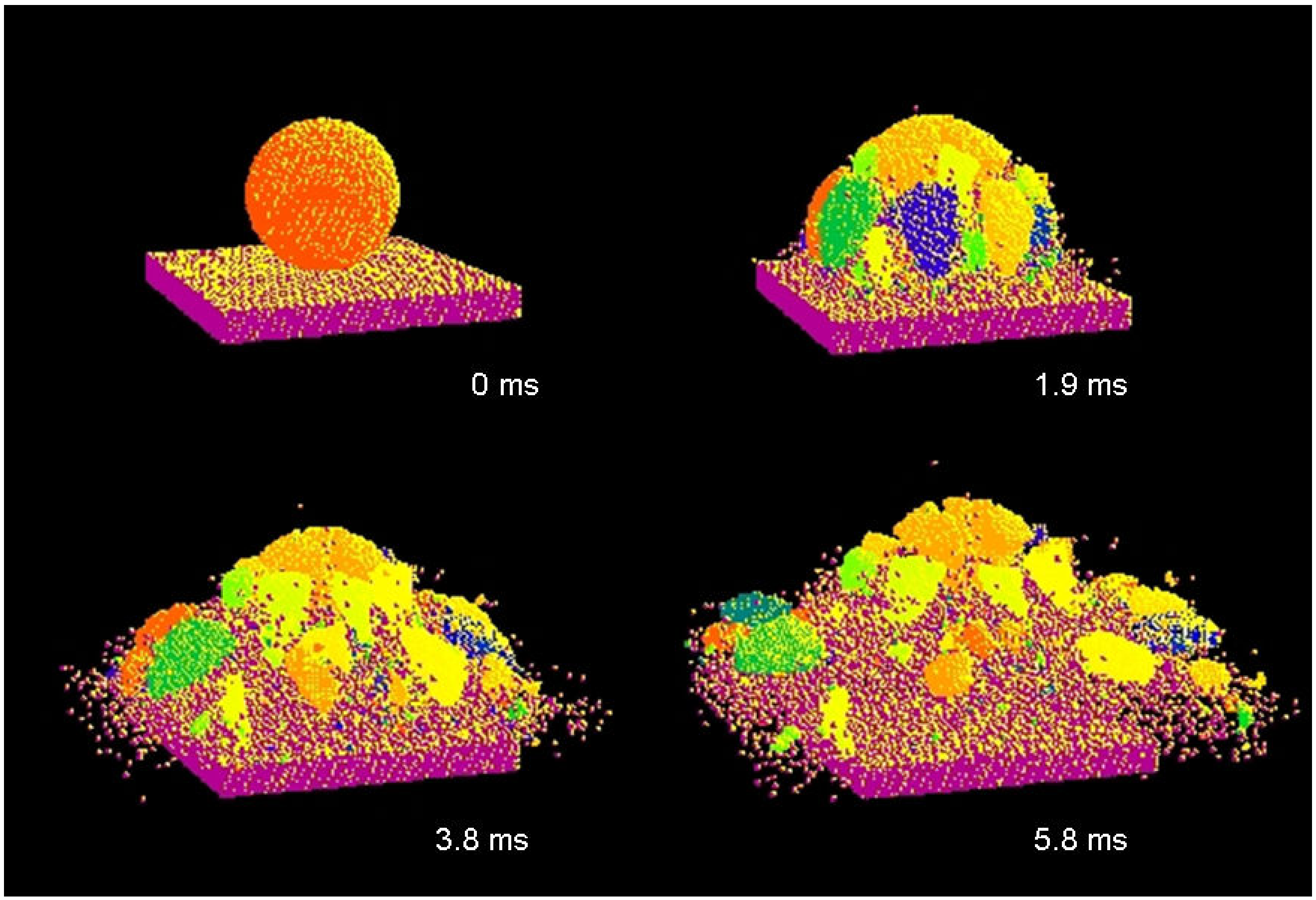


Experiment*

*J. Fineberg & M. Marder, *Physics Reports* **313** (1999) 1-108

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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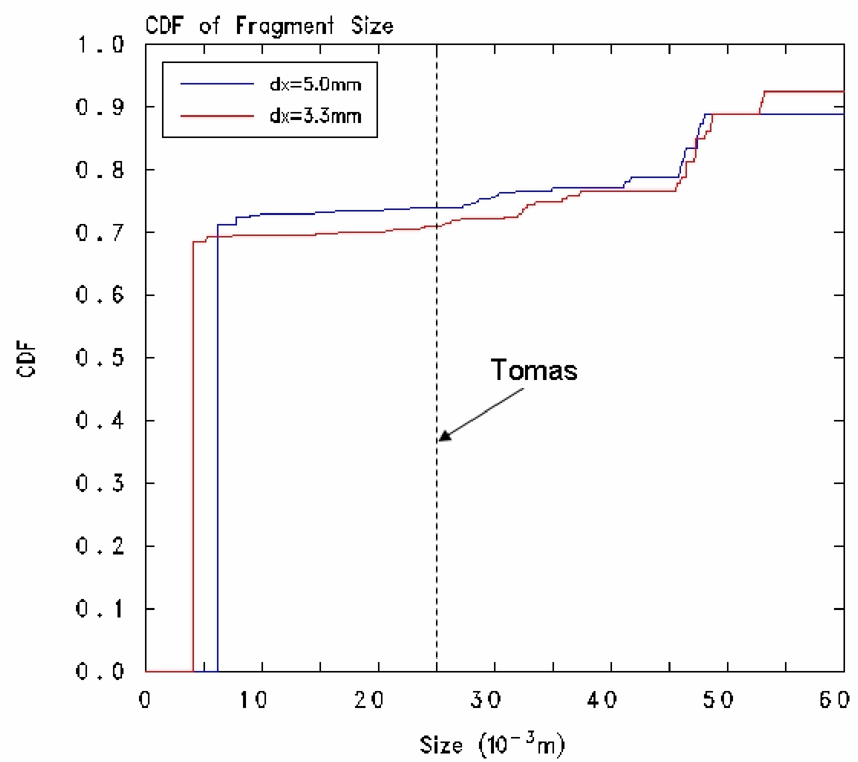
Example:
Concrete sphere drop, ctd.

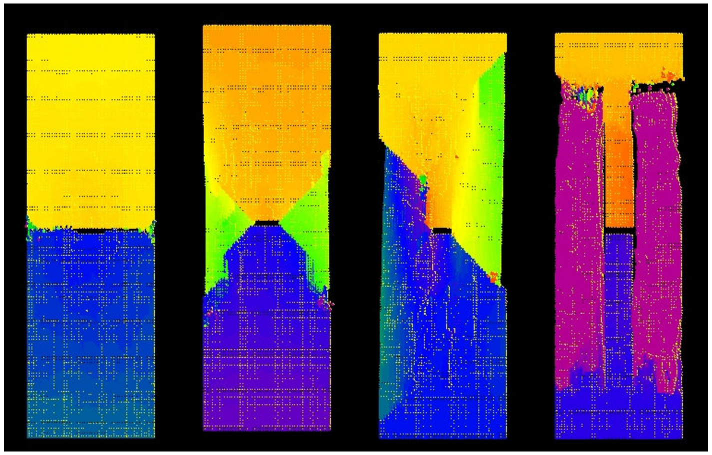
- Cumulative distribution function of fragment size (for 2 grid spacings):
  - Also shows measured mean fragment size*



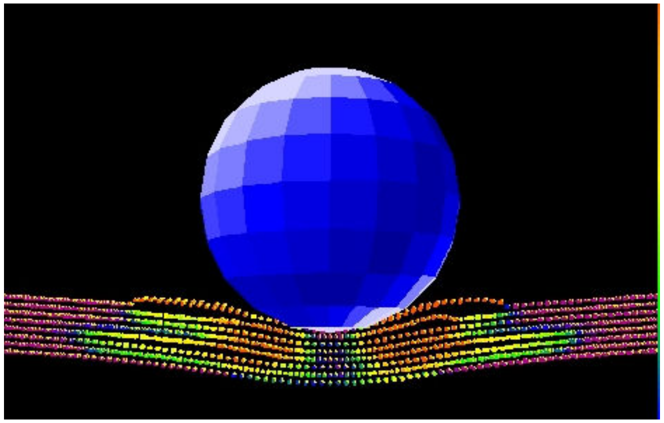
*J. Tomas et. al., *Powder Technology* **105** (1999) 39-51.

Complex materials: Prediction of composite material fracture

- Bonds in different directions can have different properties
  - Can use this principle to model anisotropic materials and their failure.



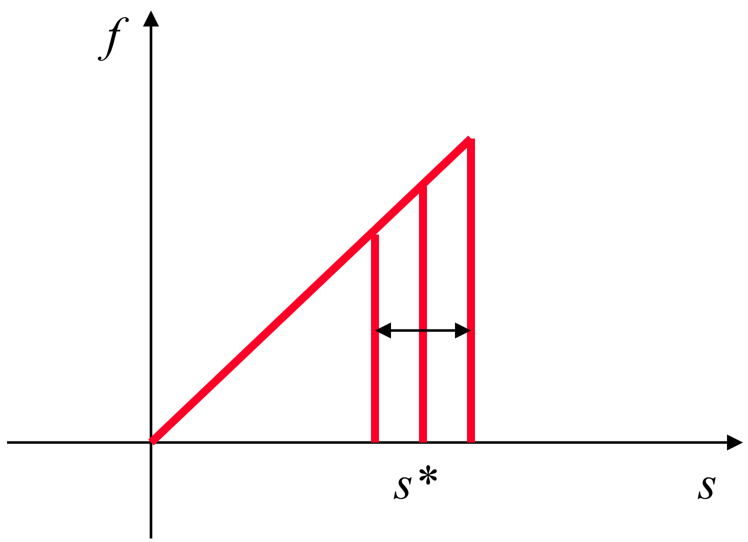
Crack growth in a notched panel

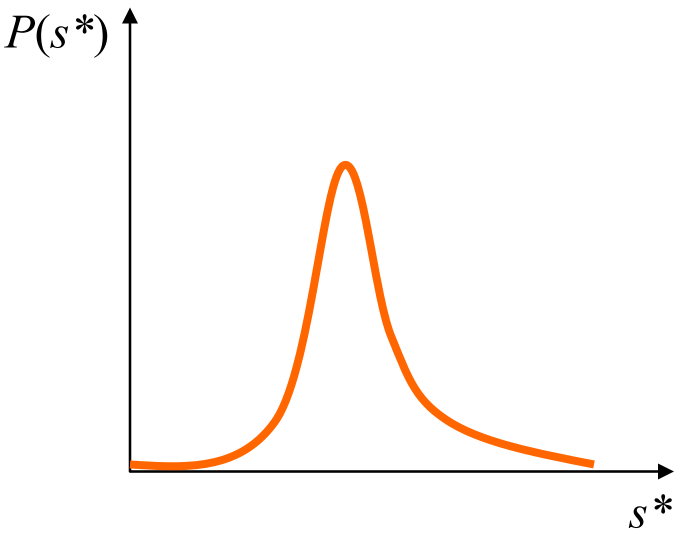


Delamination caused by impact

Statistical distribution of critical stretches

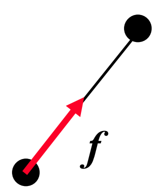
- We can introduce fluctuations in s^* as a function of position and bond orientation according to Weibull or other distribution.
- This is one way of incorporating the statistical nature of damage evolution.



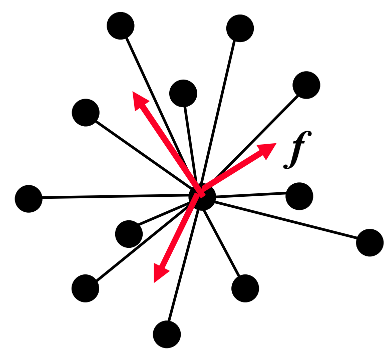


Peridynamic states:
A more general theory

- Limitations of theory described so far:
  - Poisson ratio = 1/4.
  - Can't enforce plastic incompressibility (can't decouple deviatoric and isotropic response).
  - Can't reuse material models from the classical theory.
- More general approach: **peridynamic states**.
  - Force in ***each*** bond connected to a point is determined collectively by the deformation of ***all*** the bonds connected to that point.



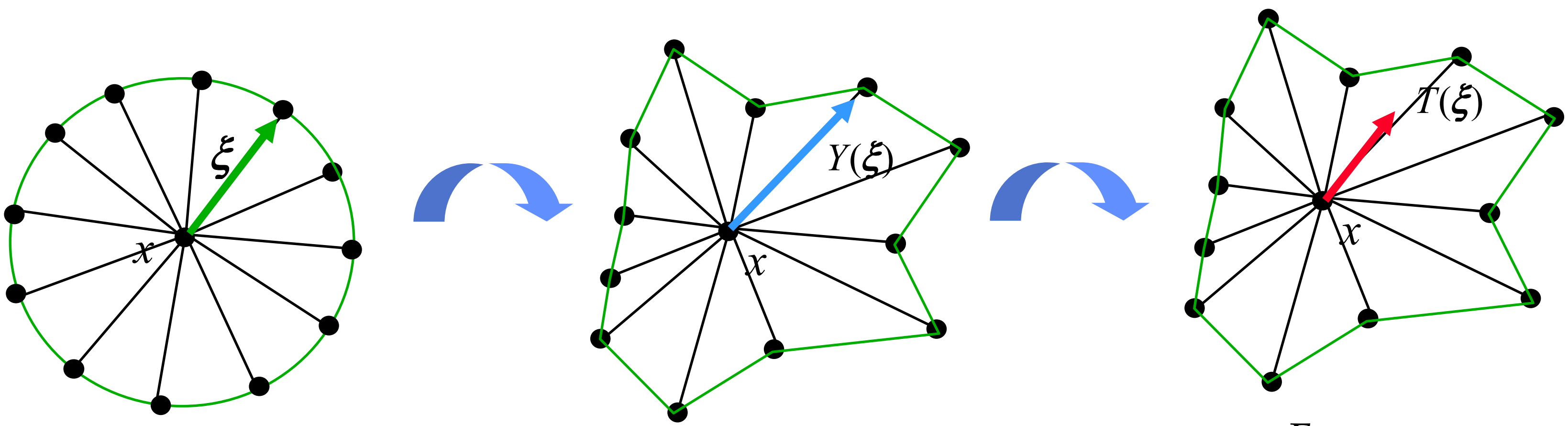
Bond



State

Peridynamic deformation states and force states

- A <u>deformation state</u> maps any bond ξ into its deformed image $\boldsymbol{Y}(\xi)$.
- A <u>force state</u> maps any bond ξ into its force density $\boldsymbol{T}(\xi)$.
- Constitutive model: relation between $\boldsymbol{T}$ and $\boldsymbol{Y}$.



Deformation state

Force state

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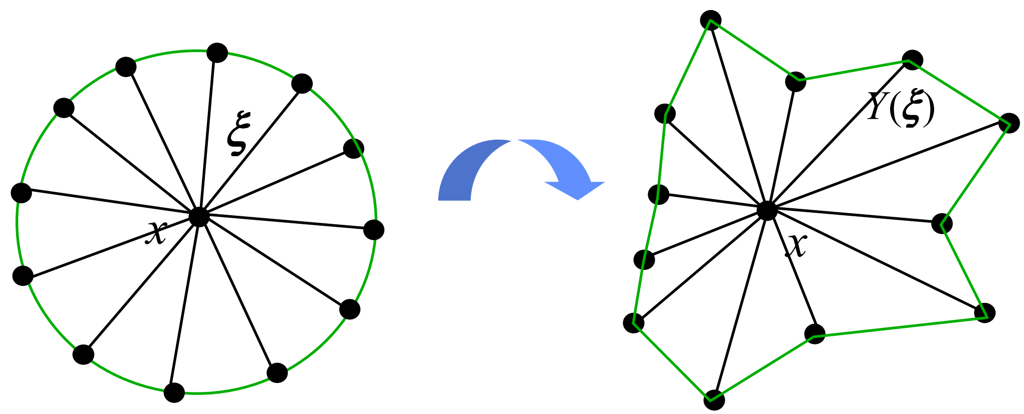
Peridynamic states: Volume term in strain energy

- One thing we can now do is explicitly include a volume-dependent term in the strain energy density… can get any Poisson ratio.

Dilatation: $$\vartheta = \int \frac{|Y(\xi)| - |\xi|}{|\xi|} dV$$

Strain energy density: $$W(x) = \int w(\eta, \xi) dV + \psi(\vartheta)$$

or: $$W(x) = \int \tilde{w}(\eta, \xi, \vartheta) dV$$



Undeformed state

Deformed state

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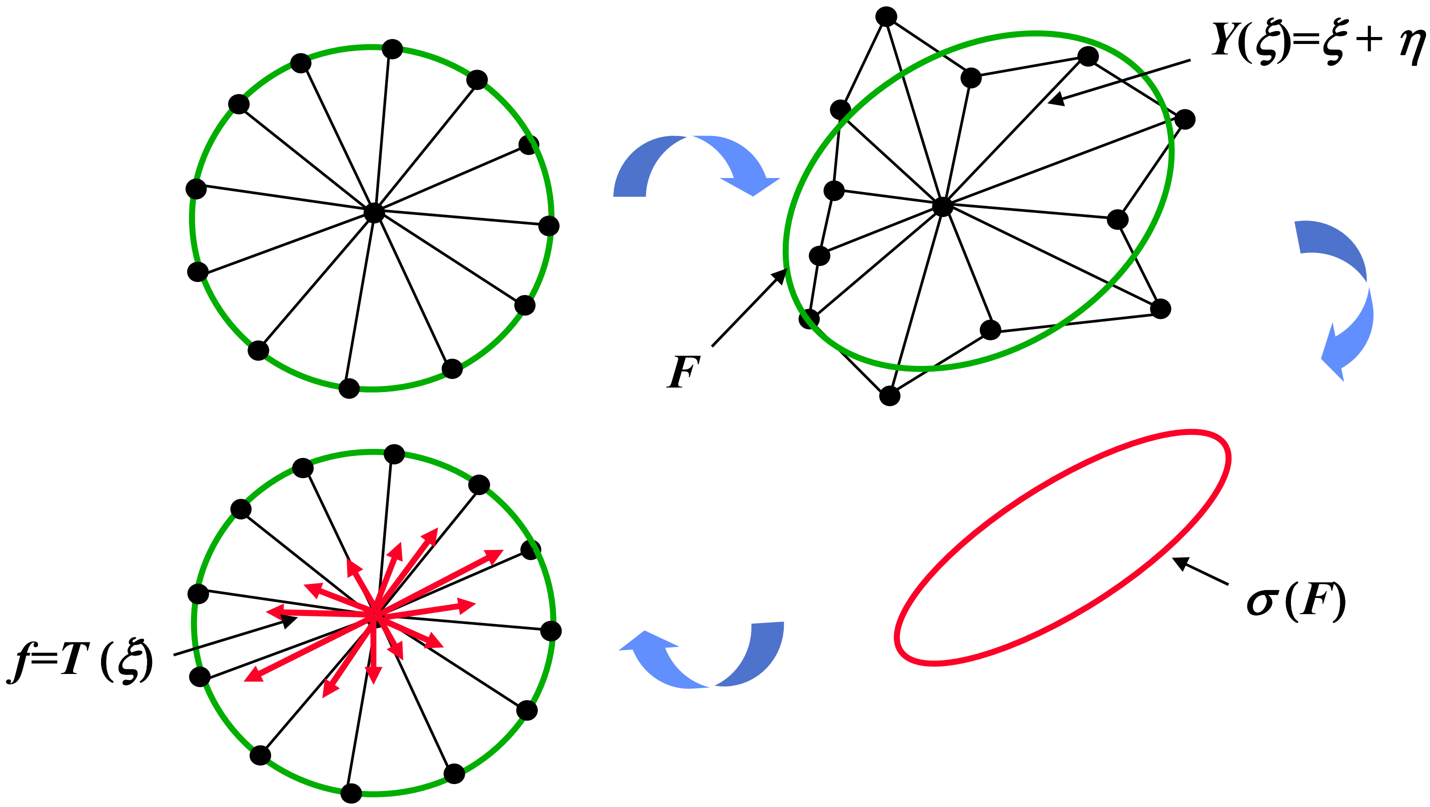
Peridynamic states:
Using material models from classical theory

- Map a deformed state to a deformation gradient tensor.
- Use a conventional stress-strain material model.
- Map the stress tensor onto the bond forces within the state.



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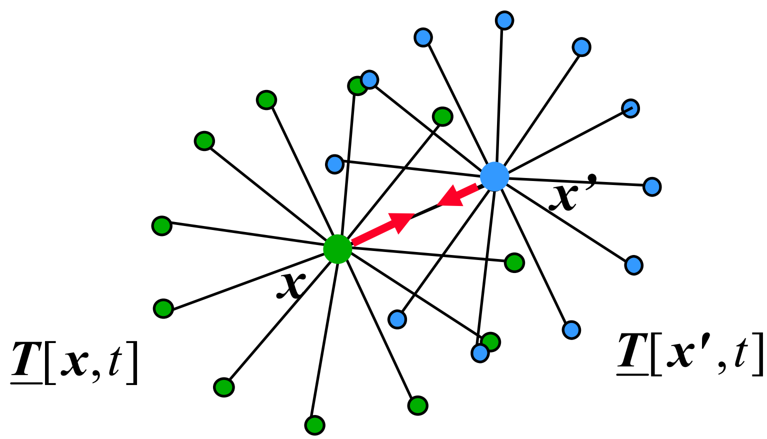
State-based equation of motion

- A force state at $\boldsymbol{x}$ gives the force in each bond connected to $\boldsymbol{x}$: $\quad \boldsymbol{f} = \underline{\boldsymbol{T}}(\xi)$
- Bond-based:

$$\rho\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_R \boldsymbol{f}(\boldsymbol{u}'-\boldsymbol{u}, \boldsymbol{x}'-\boldsymbol{x})dV' + \boldsymbol{b}(\boldsymbol{x},t)$$

- State-based:

$$\rho\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \frac{1}{2}\int_R \{\underline{\boldsymbol{T}}[\boldsymbol{x},t](\boldsymbol{x}'-\boldsymbol{x}) - \underline{\boldsymbol{T}}[\boldsymbol{x}',t](\boldsymbol{x}-\boldsymbol{x}')\}dV' + \boldsymbol{b}(\boldsymbol{x},t)$$



Force states at $\boldsymbol{x}$ and $\boldsymbol{x}'$ combine

Elastic state-based materials

- Suppose W is a scalar valued function of a state such that

$$\underline{\hat{T}}(\underline{Y}) = W_{Y}(\underline{Y}) \qquad \text{for all } \underline{Y}$$

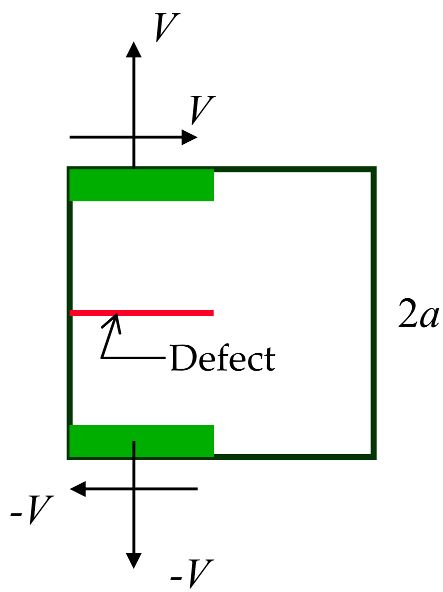
Frechet derivative (like a gradient)

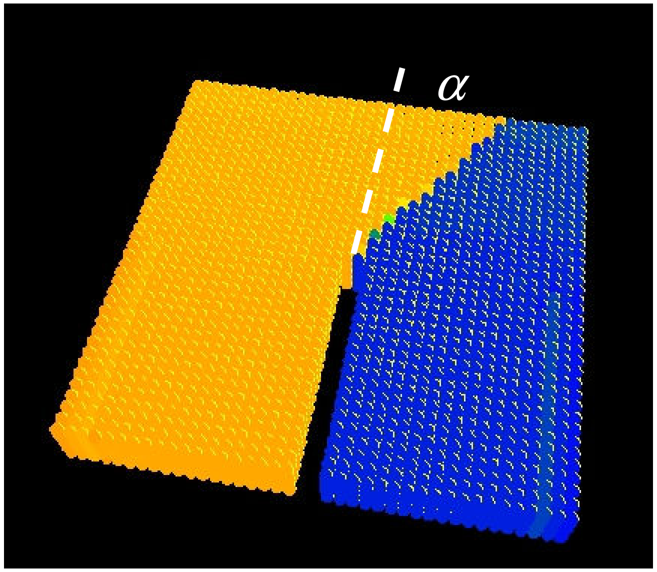
- Bodies composed of this elastic state-based material conserved energy in the usual sense of elasticity.

$$\frac{\partial}{\partial t}\int W dV = \int b \cdot \dot{u} dV$$

Peridynamic state model: Effect of Poisson ratio on crack angle

Thick, notched brittle linear elastic plate is subjected to combined tension and shear





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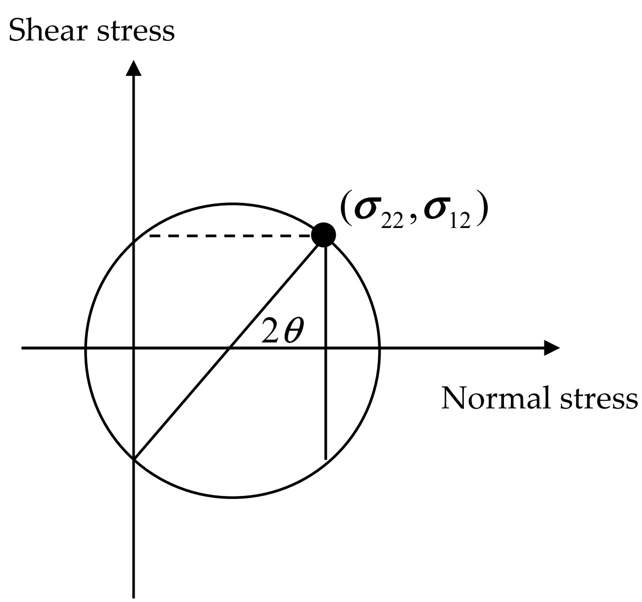
Peridynamic state model: Effect of Poisson ratio on crack angle, ctd.

- Hold E constant and vary ν.
  - Larger ν means smaller μ.
- Does this change the crack angle?
- Approximate analysis near initial crack tip based on Mohr's stress circle:
  - Find orientation θ of plane of max principal stress.



$$\sigma_{11} = 0 \qquad \sigma_{22} = EVt/a \qquad \sigma_{12} = \mu Vt/a$$

$$\mu = E/2(1+\nu)$$

$$2\theta = \tan^{-1}(2\sigma_{12}/\sigma_{22}) = \tan^{-1}(1/(1+\nu))$$

$$\nu = 0.1 \Rightarrow \theta = 21.1^o$$

$$\nu = 0.4 \Rightarrow \theta = 16.8^o$$

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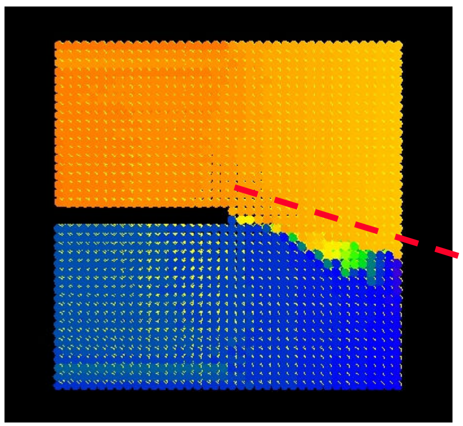
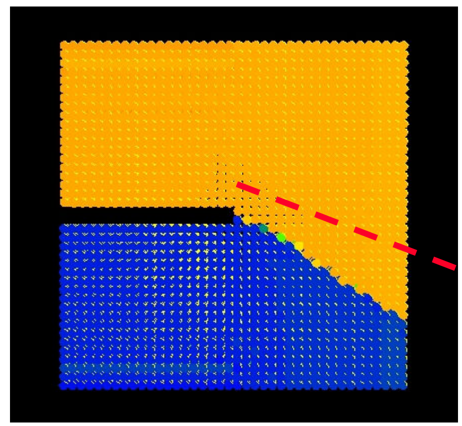
Peridynamic state model:
Effect of Poisson ratio on crack angle, ctd.

- Predicted crack angles near initial crack tip are close to orientation of max principal **stress**



$\boldsymbol{\theta} = 16.8^o$

ν= 0.4
Model result



$\boldsymbol{\theta} = 21.1^o$

ν= 0.1
Model result

Peridynamic states vs. FE: Elastic-plastic solid

- Direct comparison between a finite-element code and Emu with a conventional material model.

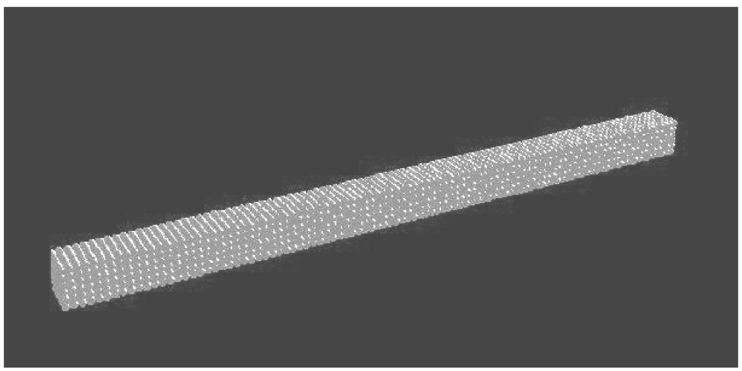


Figure 3. 3600 node discrete peridynamic lattice

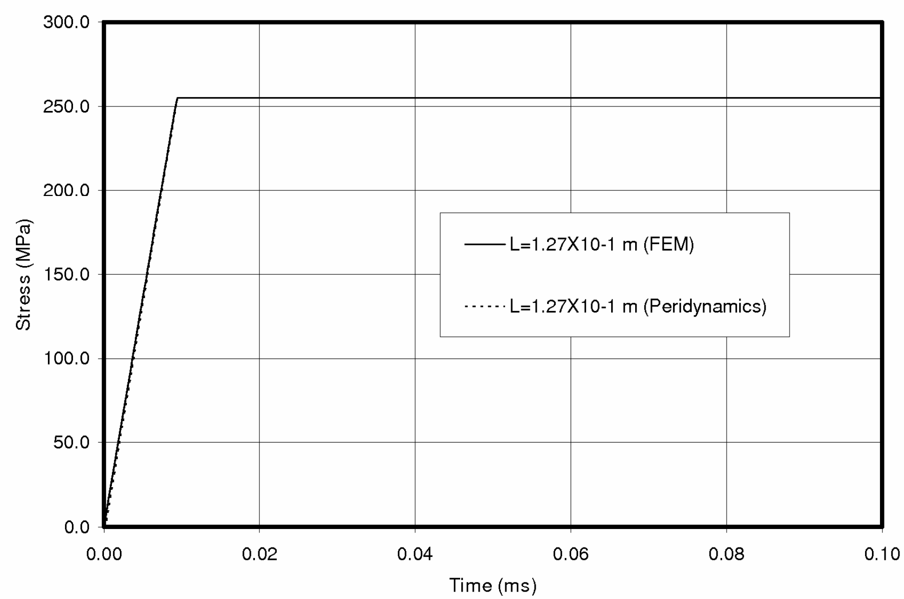


Figure 7. Stress in the bar at L=127 mm using both Peridynamics and FEM

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Summary:
Peridynamic vs. conventional model

- Peridynamic
  - Uses integral equations.
  - Same equations hold on or off discontinuities.
  - Nonlocal.
  - Force state (or deformation state) has "infinite degrees of freedom."
- Classical
  - Uses differential equations.
  - Discontinuities require special treatment (methods of LEFM, for example).
  - Local.
  - Stress tensor (or strain tensor) has 6 degrees of freedom.