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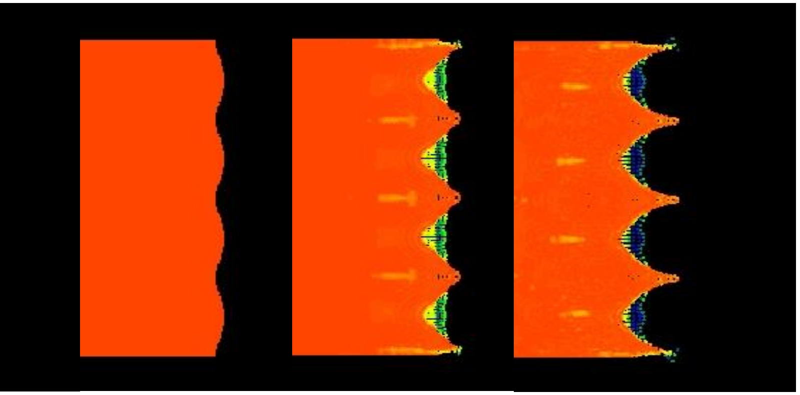

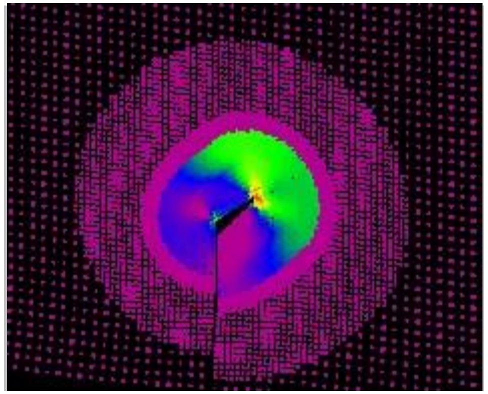

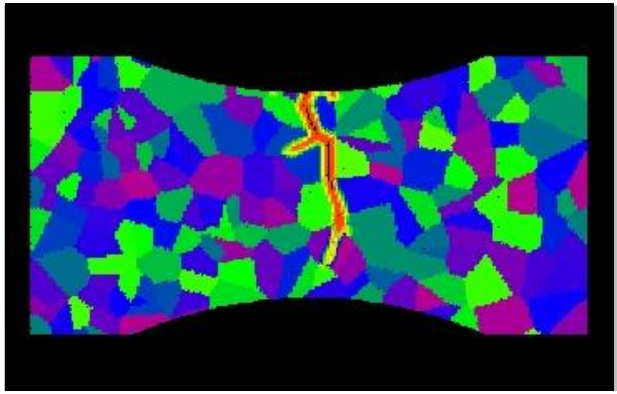

Unifying the mechanics of continua, cracks, and particles

Stewart Silling   John Mitchell
Sandia National Laboratories
Albuquerque, New Mexico

3M Company, St. Paul, Minn., July 31, 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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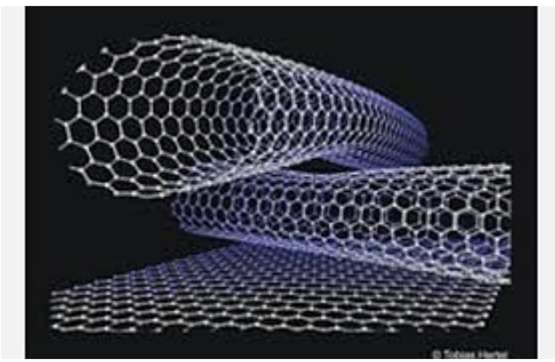
Outline

- Purpose of peridynamics
- Basic equations
- Examples
  - Mesoscale damage modeling
  - Mechanics of membranes and adhesion
  - Impact and penetration
- Software (JM)
- Material models (JM)

What should be modeled as a classical continuum?

- Commercial finite element codes approximate the equations of classical continuum mechanics.
  - Assumes a <u>continuous body</u> under <u>smooth deformation</u>.
  - When is this the right approximation?

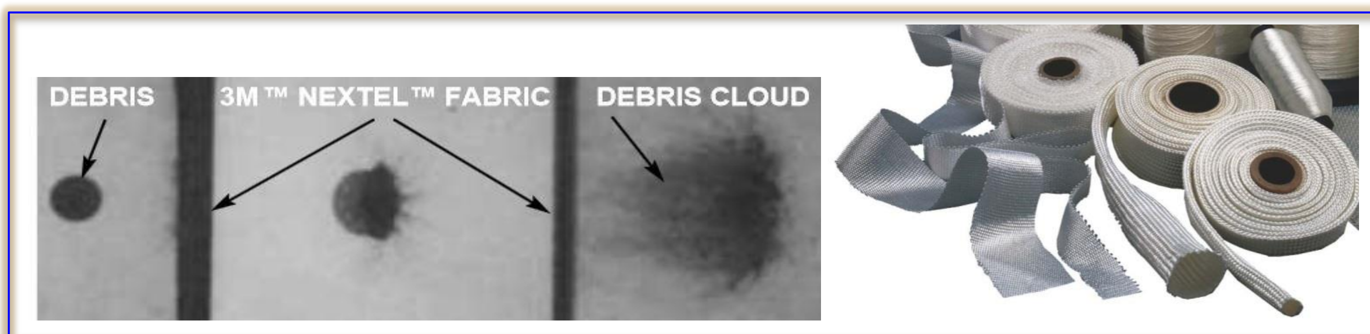
$$\boxed{\nabla \cdot \sigma + b = 0}$$



Carbon nanotubes (image: nsf.gov)

Fragmented glass (image: Washington Glass School)

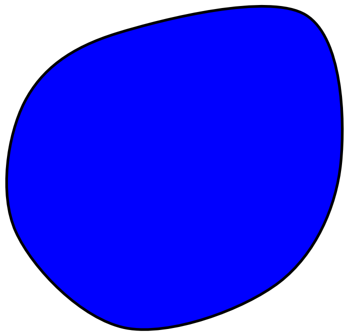
Augustin-Louis Cauchy, 1840
(image: Library of Congress)



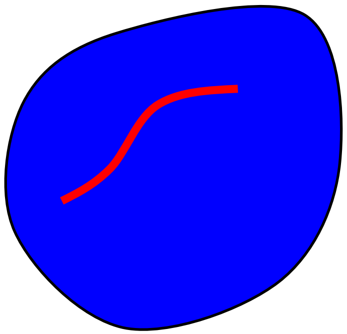
Hypervelocity impact onto ceramic fabric (image: 3m.com)

Purpose of peridynamics

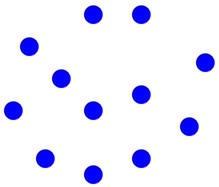
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body
with a defect

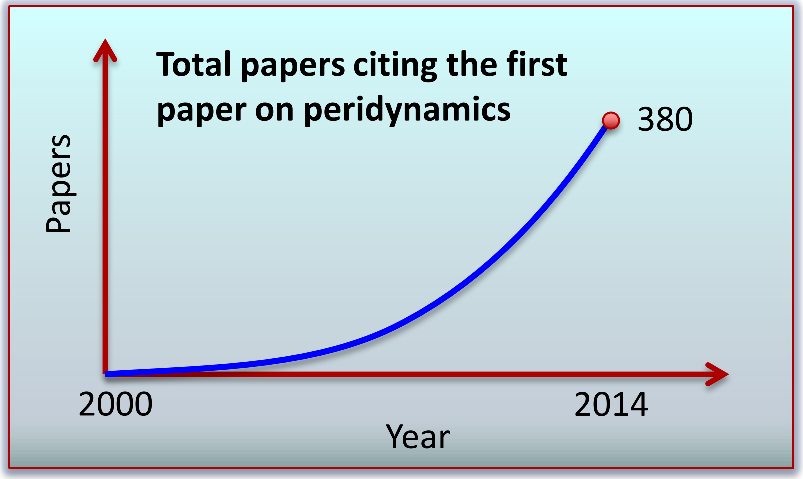


Discrete particles

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

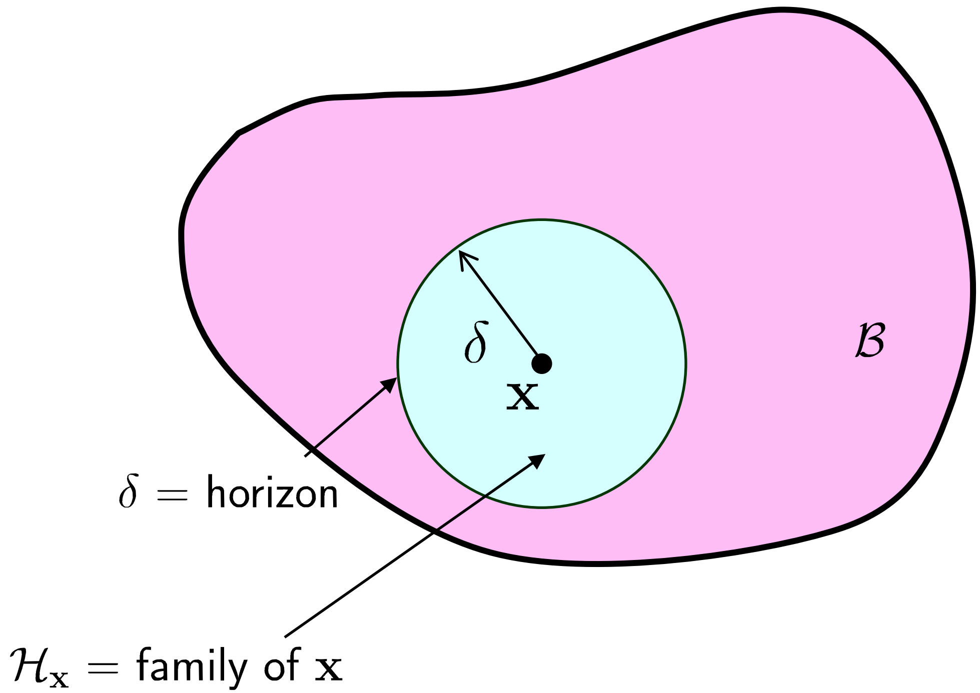
Peridynamics: Who's interested?

- Research has been conducted at:
  - MIT
  - Caltech
  - Harvard University
  - University of Illinois, Urbana-Champaign
  - University of New Mexico
  - University of Arizona
  - University of California, Berkeley
  - University of Texas, San Antonio
  - University of Texas, Austin
  - Penn State University
  - Columbia University
  - University of Alabama
  - Louisiana State University
  - Carnegie Mellon University
  - Michigan State University
  - Florida State University
  - University of Nebraska, Lincoln
  - … others worldwide
- Sponsors include:
  - Army
  - Air Force
  - Navy
  - Department of Energy
  - Boeing
  - Big oil companies
  - Intel
  - Raytheon
  - NSF
  - Orica USA Corp



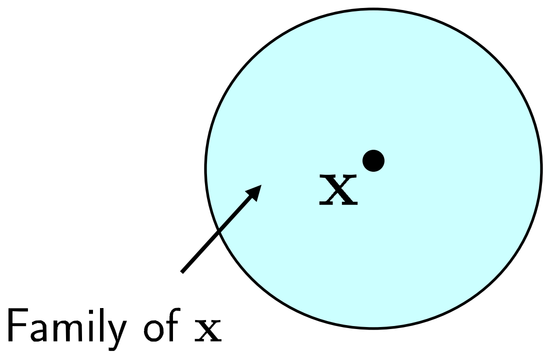
Peridynamics basics: Horizon and family

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

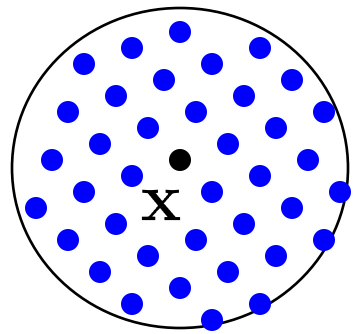


Strain energy at a point

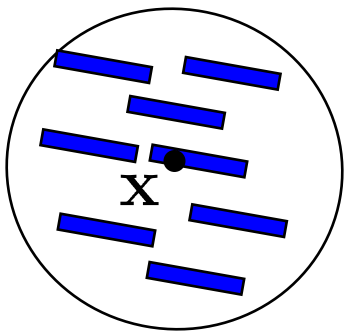
Continuum



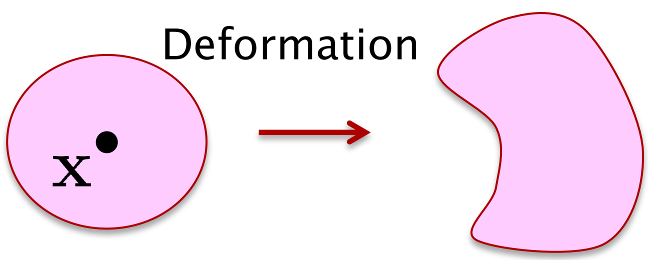
Discrete particles



Discrete structures



Deformation



- 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:

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

where W is the strain energy density, $\mathbf{y}$ is the deformation map, $\mathbf{b}$ is the applied external force density, and $\mathcal{B}$ is the body.

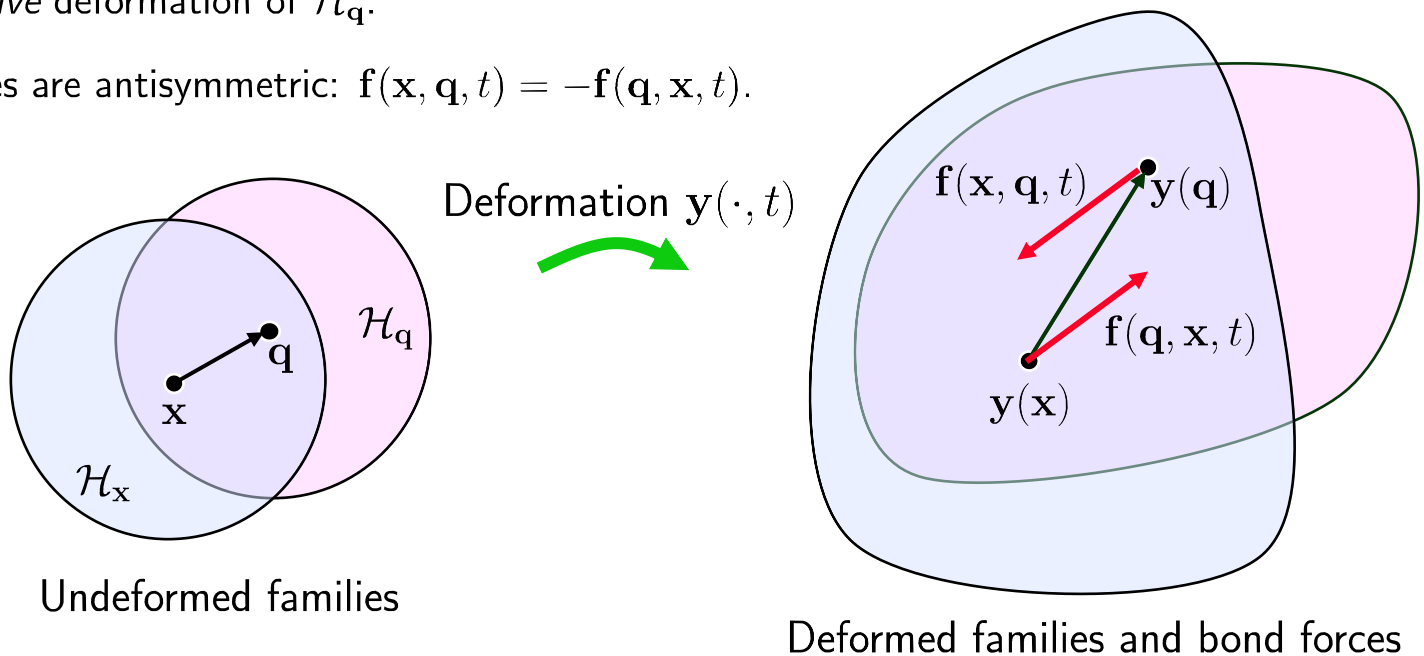
- Euler-Lagrange equation is the equilibrium equation:

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

for all $\mathbf{x}$.

Material modeling: What determines bond forces?

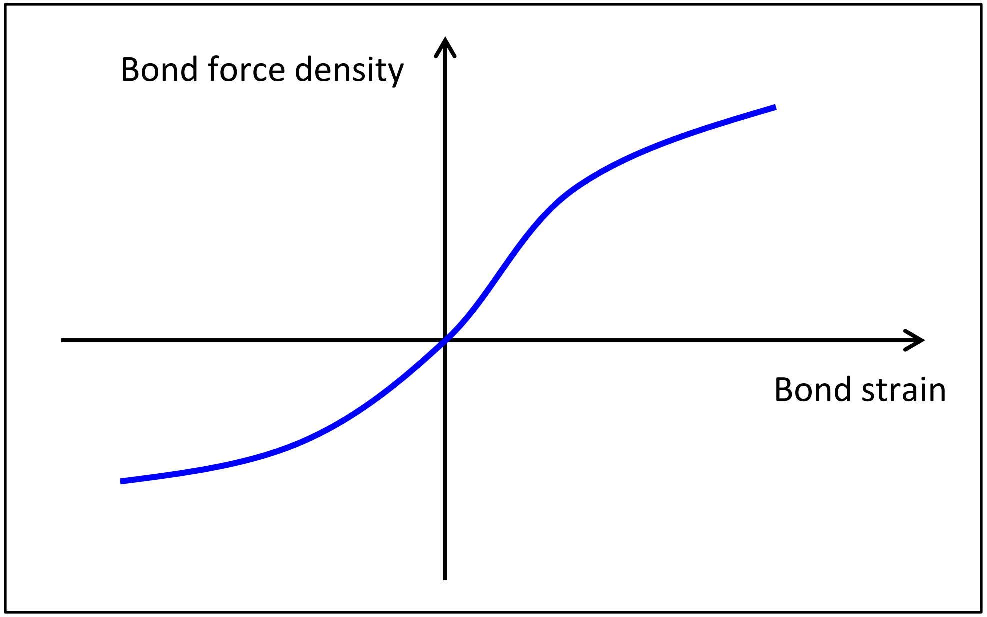
- Each pairwise bond force vector $\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$ is determined jointly by:
- the *collective* deformation of $\mathcal{H}_{\mathbf{x}}$, and
- the *collective* deformation of $\mathcal{H}_{\mathbf{q}}$.
- Bond forces are antisymmetric: $\mathbf{f}(\mathbf{x}, \mathbf{q}, t) = -\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$.



In state notation: $\mathbf{f}(\mathbf{q}.\mathbf{x}) = \mathbf{T}[\mathbf{x}]\langle\mathbf{q} - \mathbf{x}\rangle - \mathbf{T}[\mathbf{q}]\langle\mathbf{x} - \mathbf{q}\rangle$

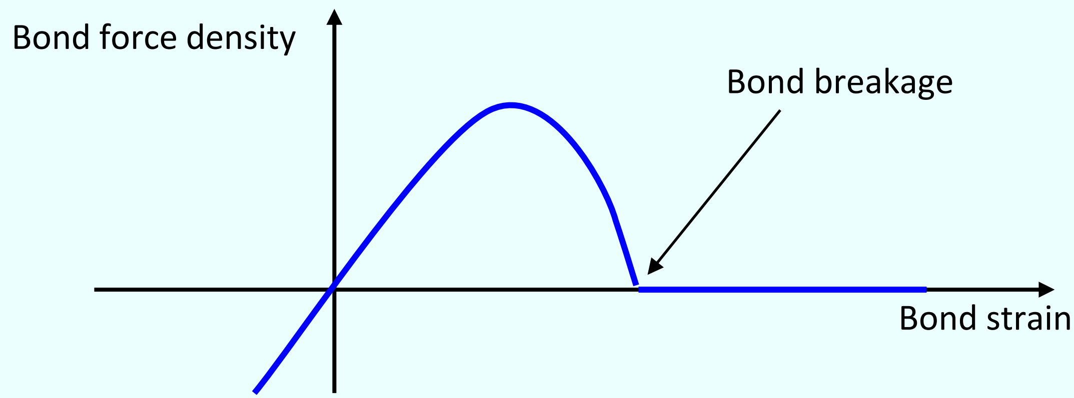
Bond based materials

- If each bond response is independent of the others, the resulting material model is called bond-based.
- The material model is then simply a graph of bond force density vs. bond strain.
- Main advantage: simplicity.
- Main disadvantage: restricts the material response.
    - Poisson ratio always = 1/4.



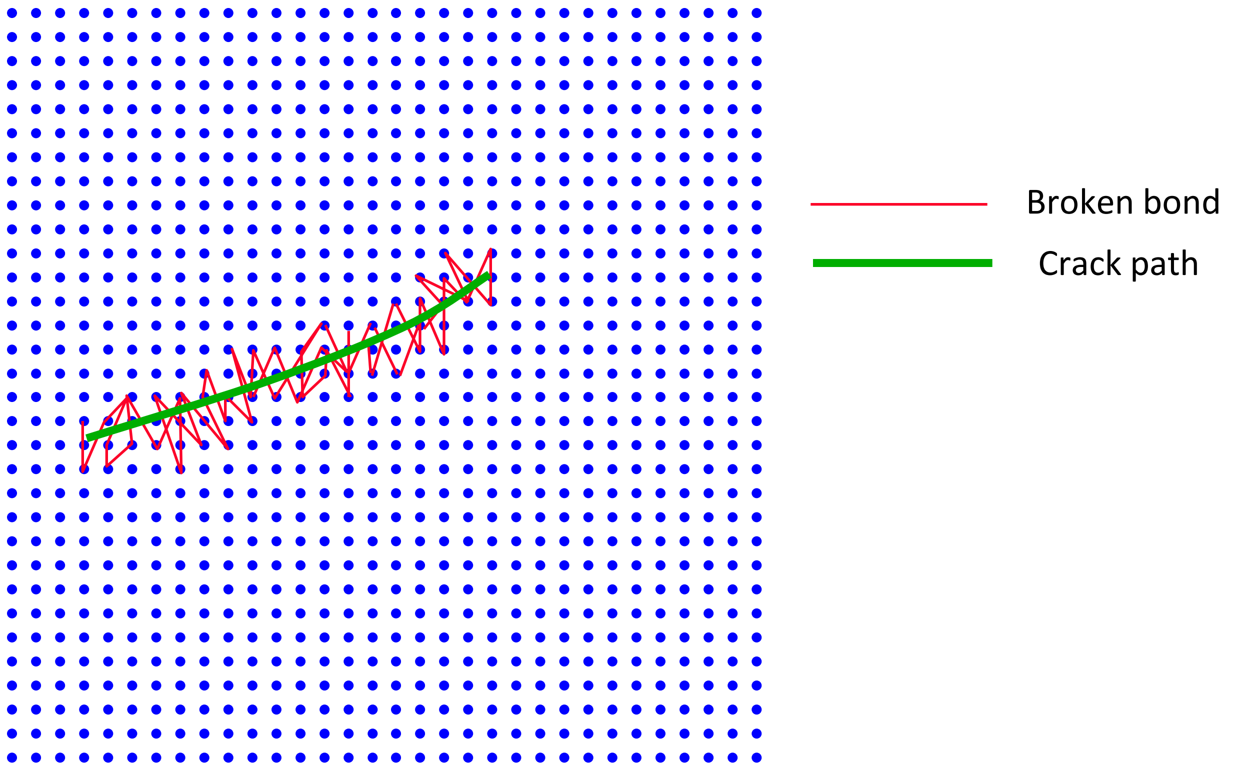
Damage due to bond breakage

- 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

Bond breakage leads to autonomous crack growth



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

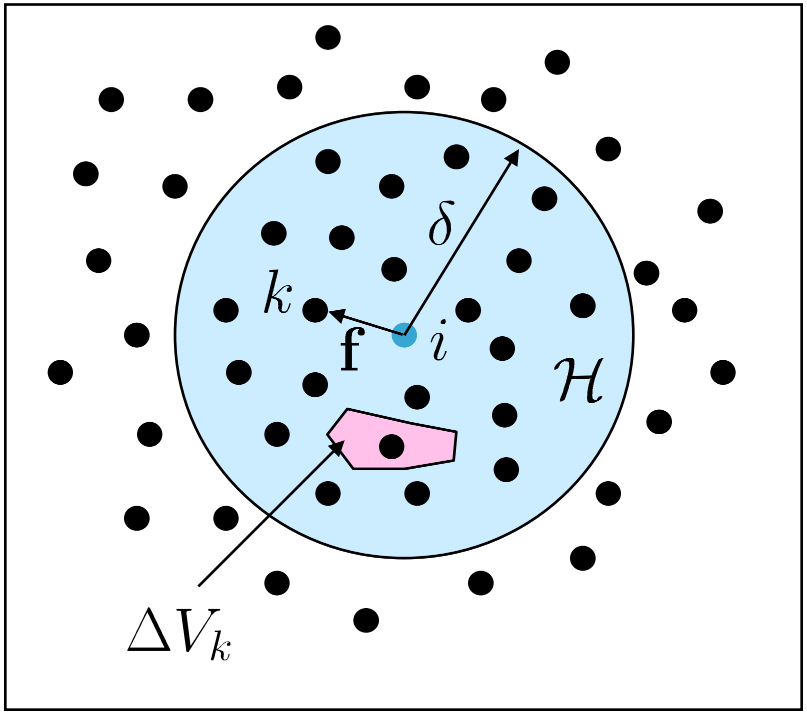
EMU numerical method

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

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

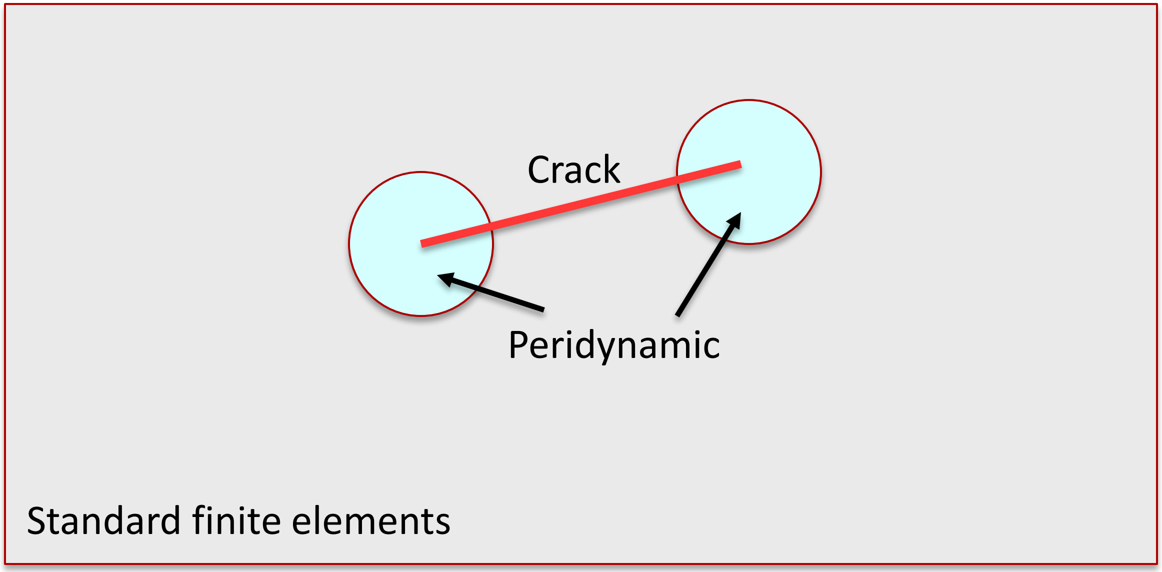
$$\downarrow$$

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



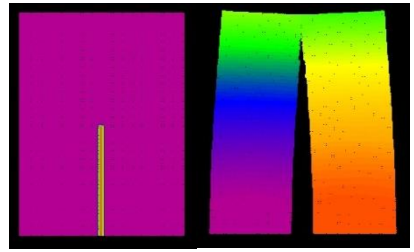
Practical issues caused by nonlocality

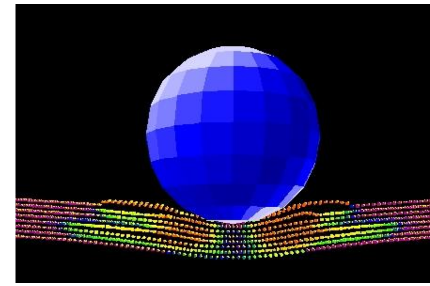
- Material properties change near free surfaces.
  - Solutions: correction factor, position-dependent material models.
- Zero energy modes in certain material models.
  - Solution: apply correction forces.
- Large number of interactions result in slow computations.
  - Solutions: better quadrature, local-nonlocal coupling.

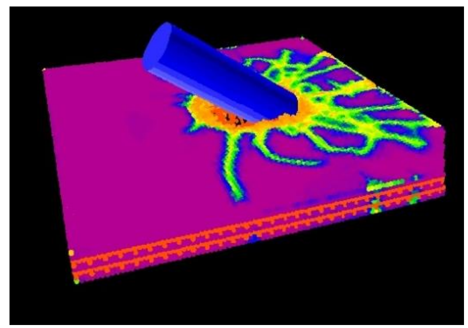


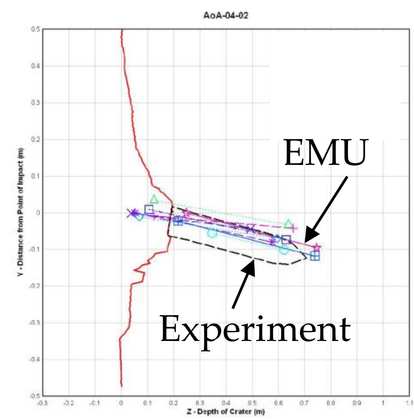
Examples of validation for peridynamics

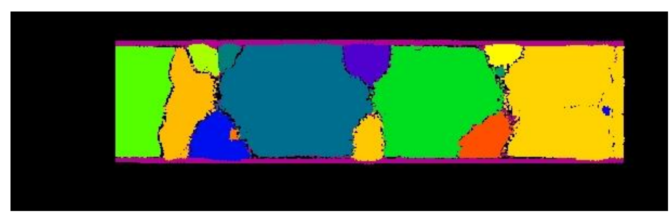
- Single crack brittle energy balance
- 3-point bend test
- Dynamic fracture
  - Crack growth velocity
  - Trajectory
  - Branching
- Impact into concrete and aluminum
  - Residual velocity
  - Penetration depth
  - Crater size
- Fatigue
  - S-N curves for aluminum and epoxy
  - Paris law curves for 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





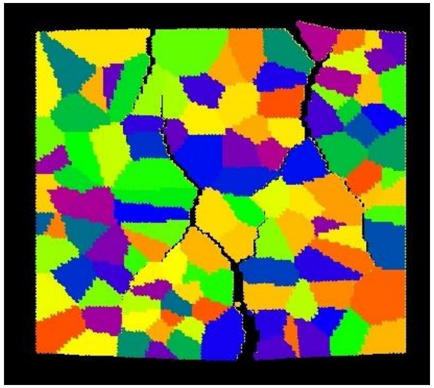




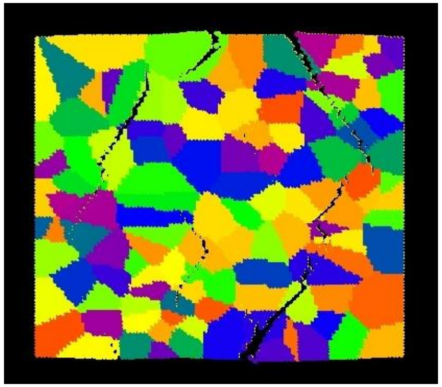


Polycrystals: Mesoscale model*

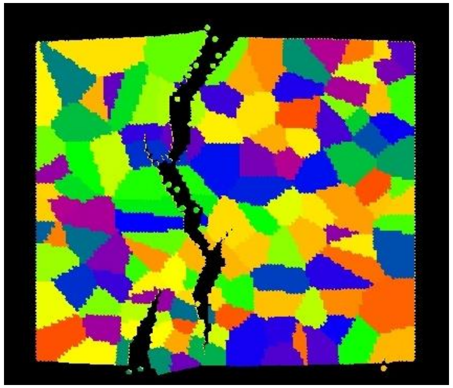
- Bonds between grains have properties that characterize the interface.



$\beta = 0.25$



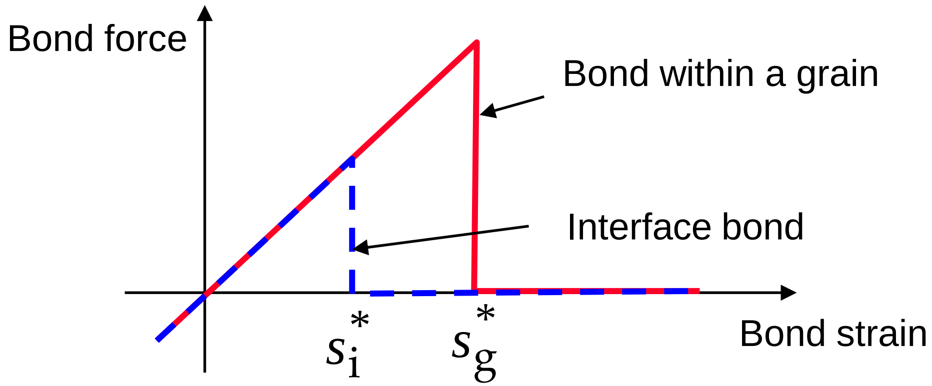
$\beta = 1$



$\beta = 4$

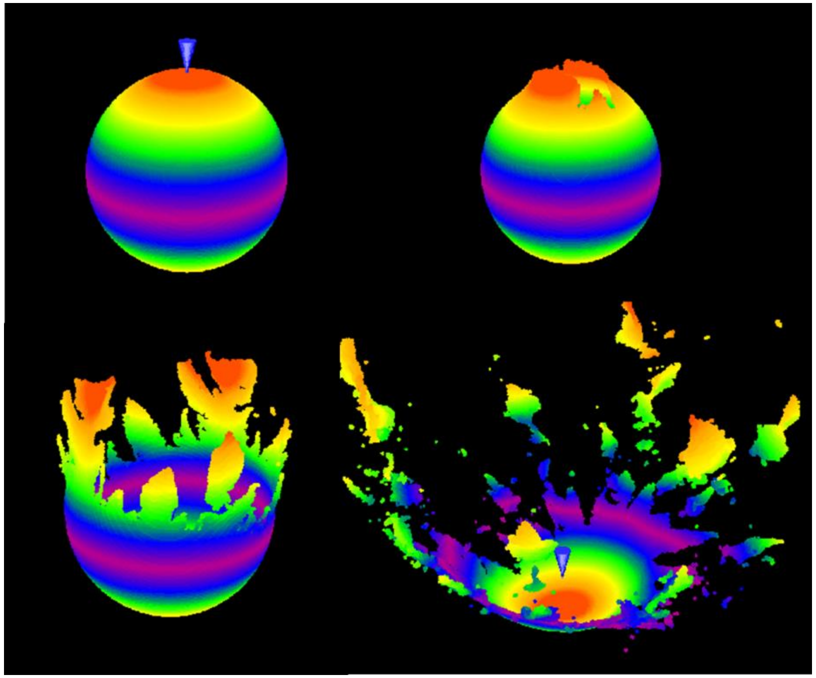
$$\boxed{\beta = \frac{s_i^*}{s_g^*}}$$

Large β favors trans-granular fracture.

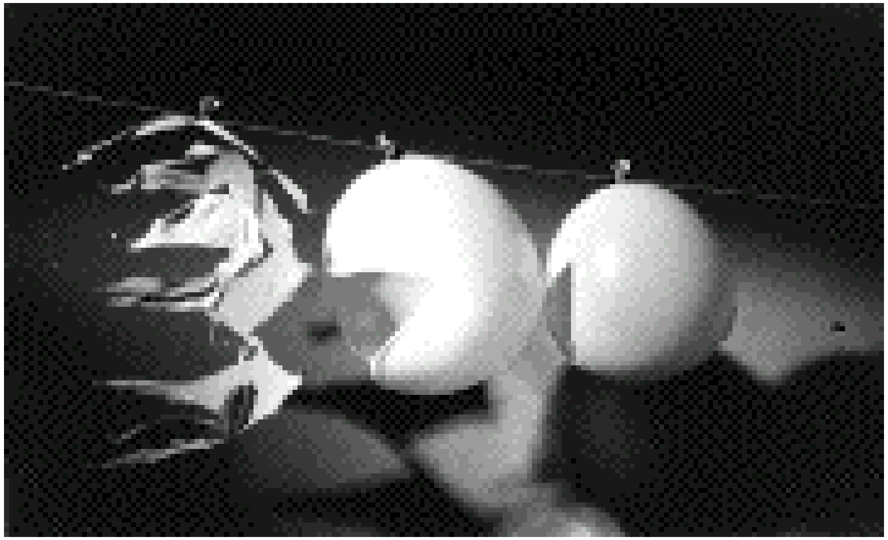


* Work by F. Bobaru & students (University of Nebraska – Lincoln)

Dynamic fracture in membranes

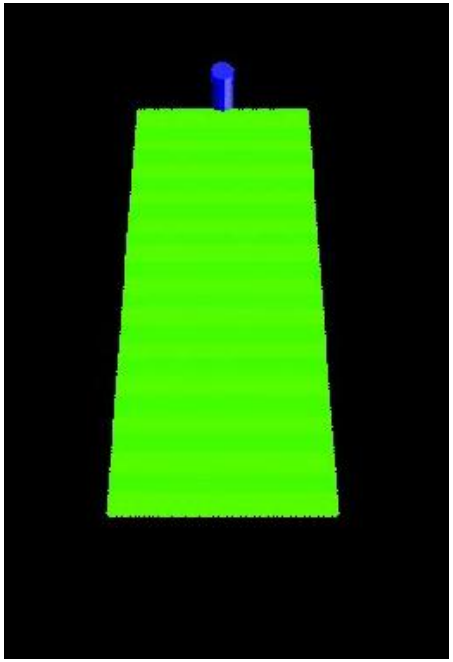


EMU model of a balloon penetrated by a fragment



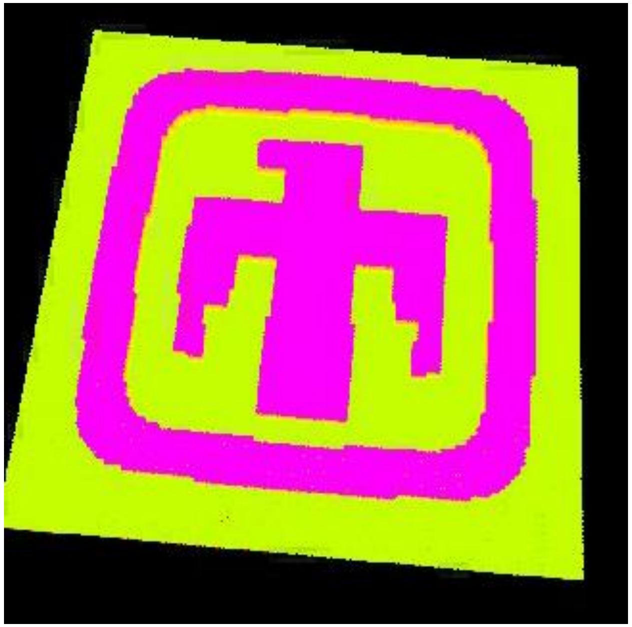
Early high speed photograph by Harold Edgerton (MIT collection)
http://mit.edu/6.933/www/Fall2000/edgerton/edgerton.ppt

Examples: Membranes and thin films



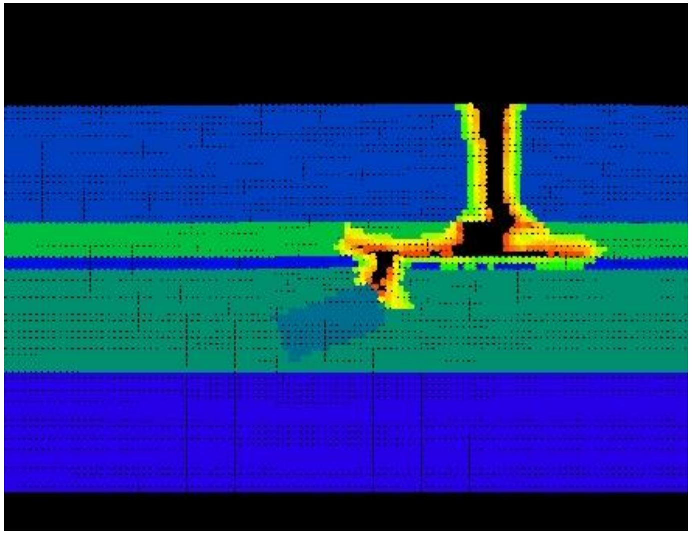
Oscillatory crack path

Video



Aging of a film

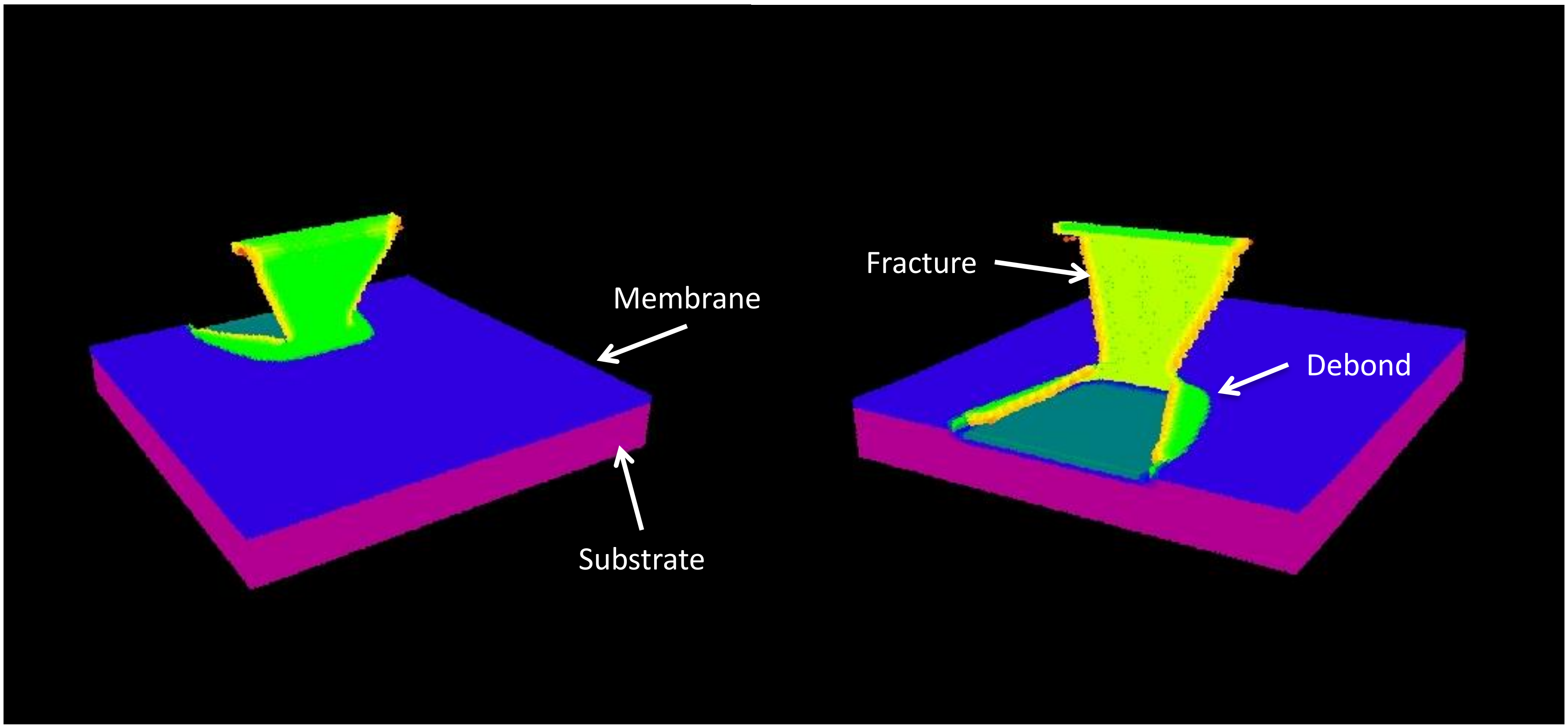
Video



Environmental fatigue in coatings

Fracture and debonding of membranes

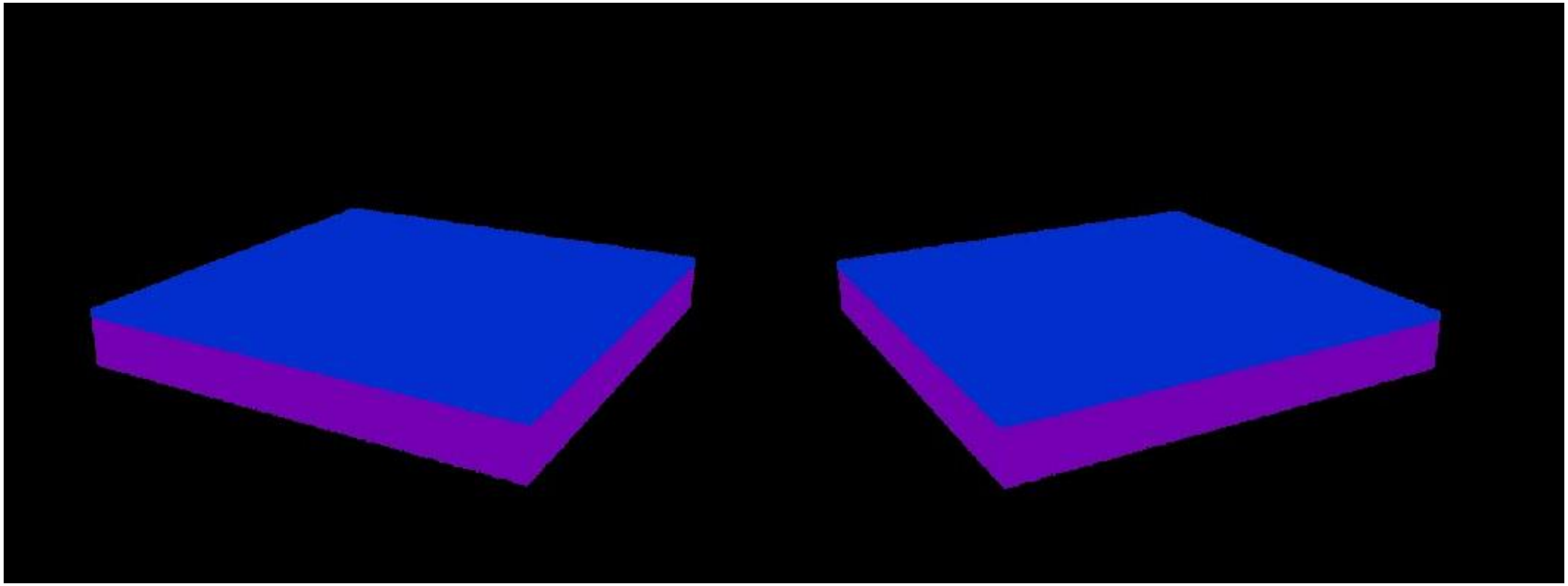
- Simulation of peeling illustrates interplay between fracture (tearing) and debonding (peeling).



Fracture and debonding of membranes

- Debond precedes fracture front.

Two views of the same simulation

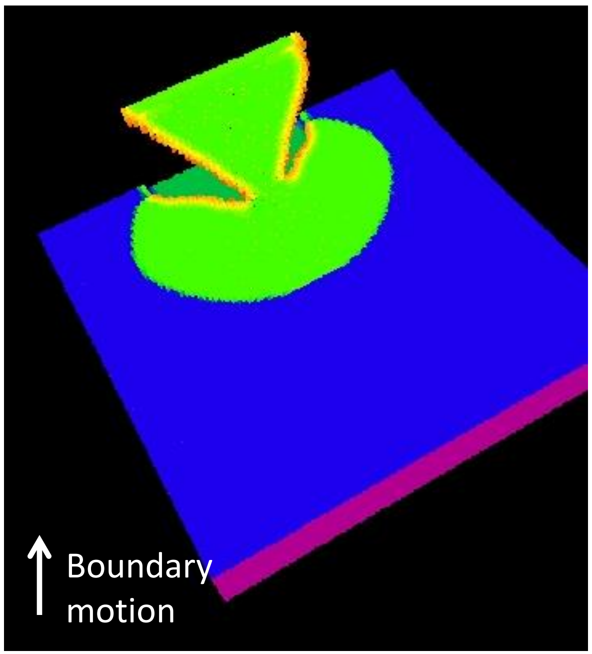


VIDEOS

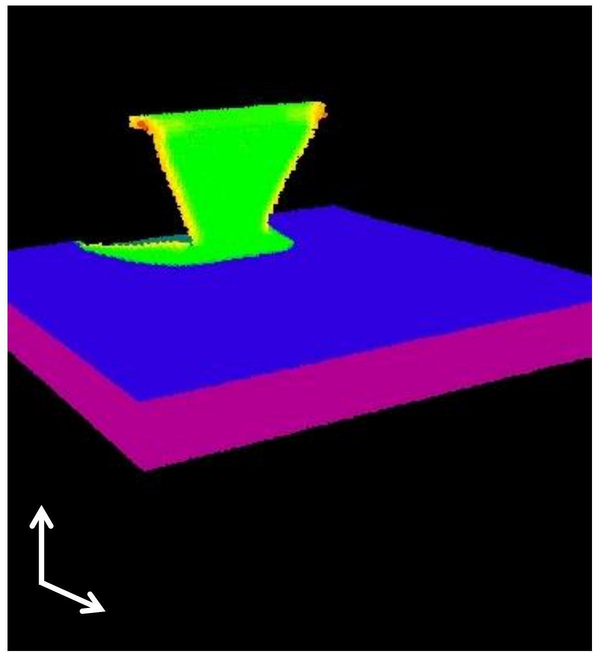
Fracture and debonding of membranes

- Direction of pull strongly affects the amount of debonding ahead of the fracture.

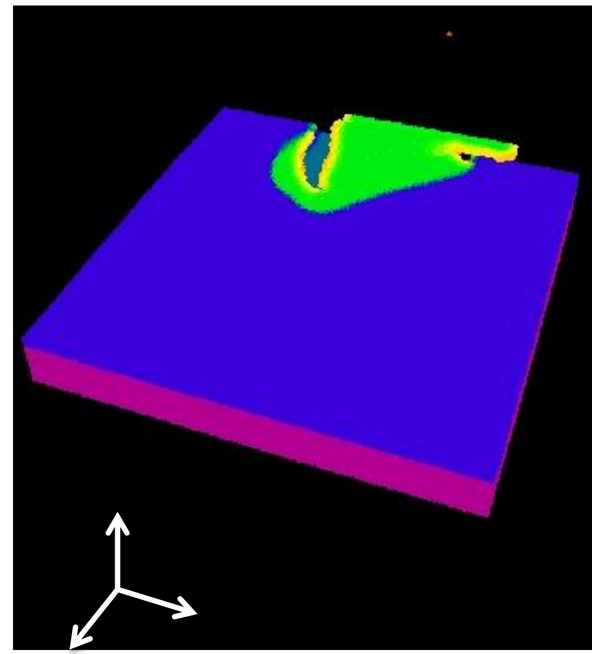
Pull straight up



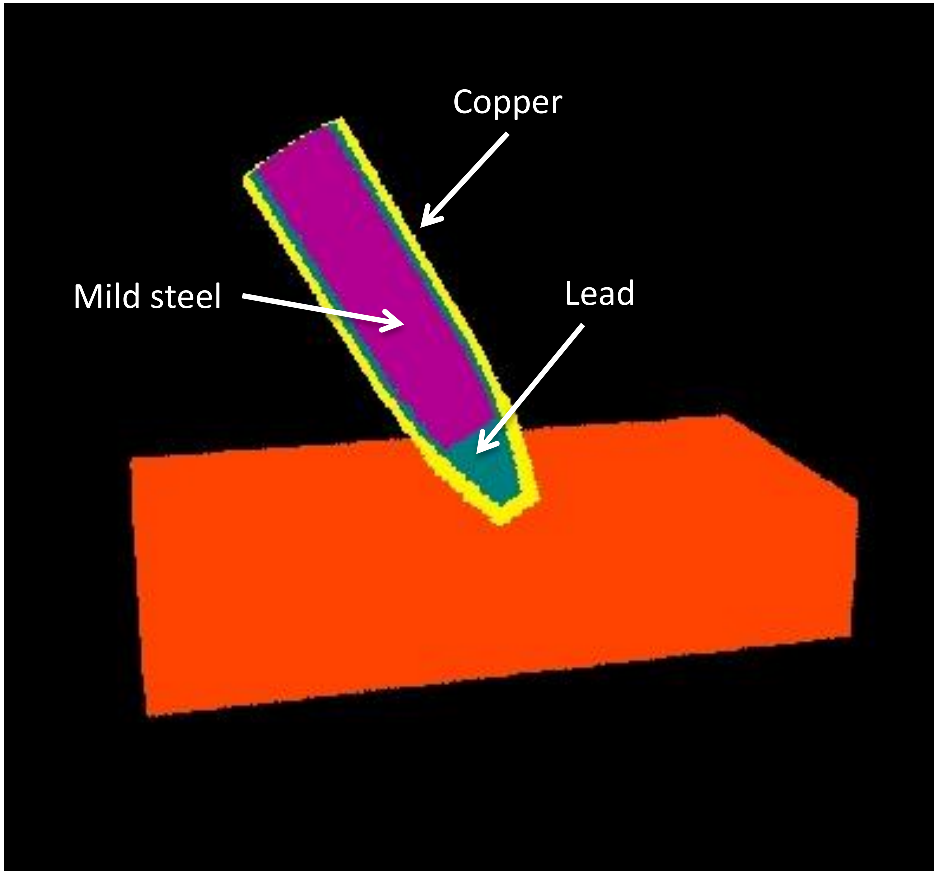
Pull up and forward



Pull up, forward, and sideways

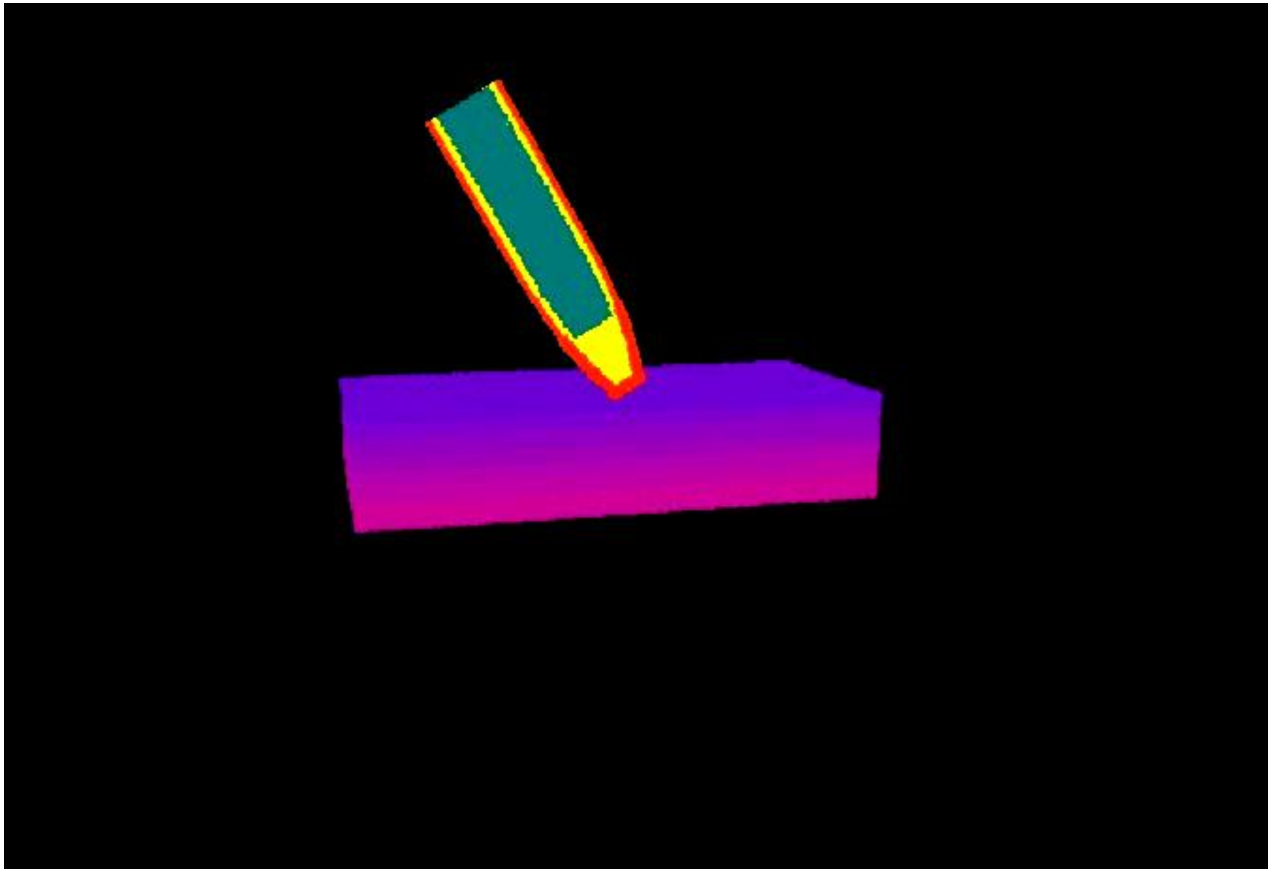


Modeling impact and penetration: Small arms round into a brittle plate



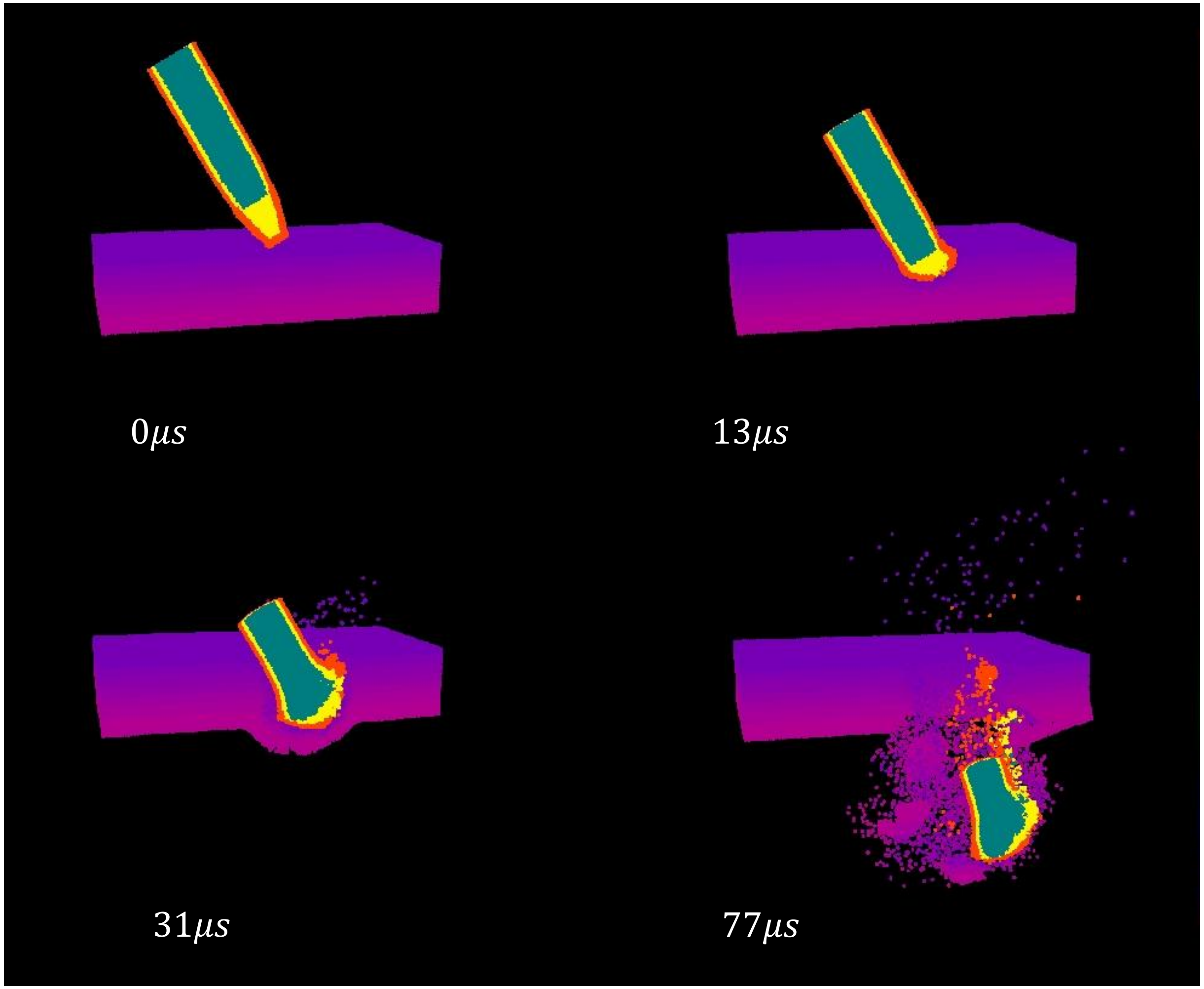
Small arms round into a brittle plate

- Peridynamic model reproduces large deformation and fragmentation of target.



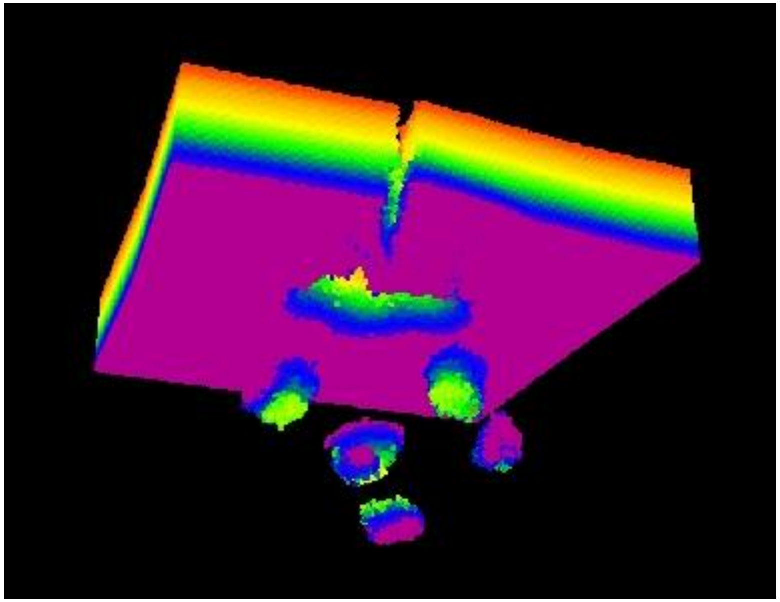
VIDEO

Small arms round into a brittle plate

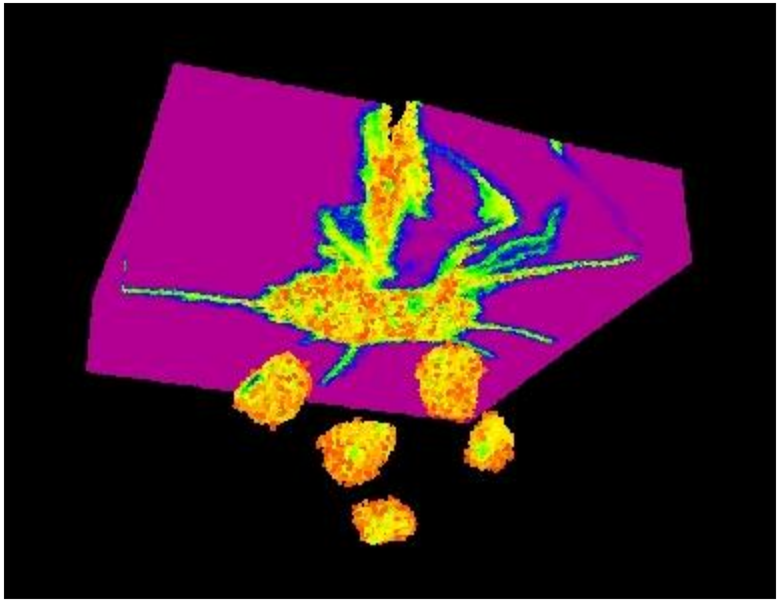


Small arms round into a brittle plate

- Method predicts a reasonable crater shape and crack distribution.



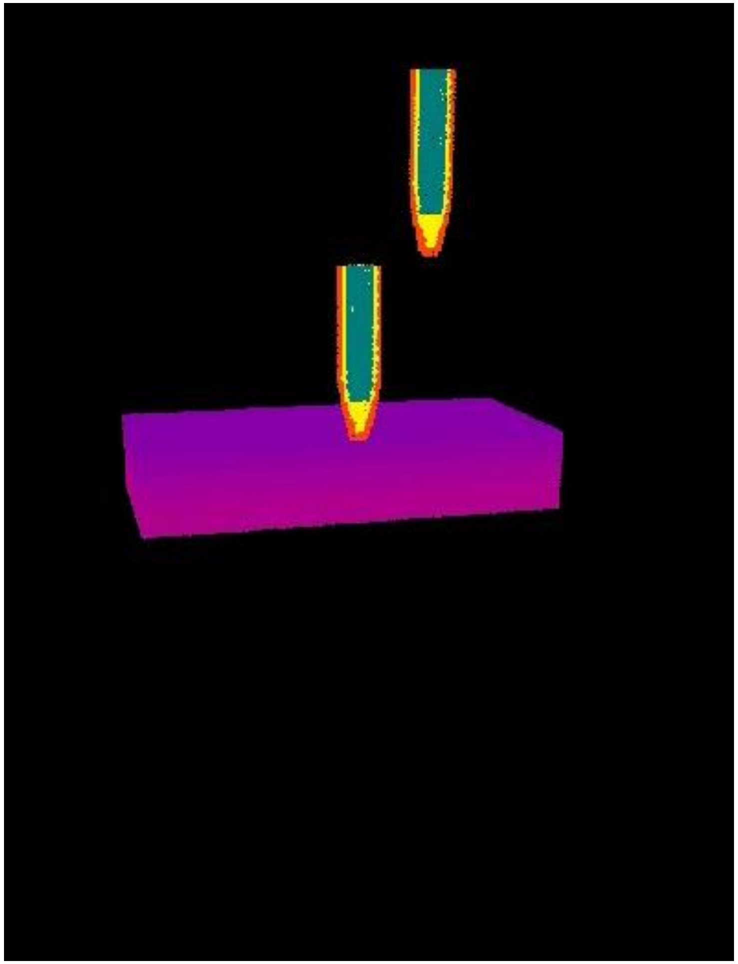
Crater shape and debris



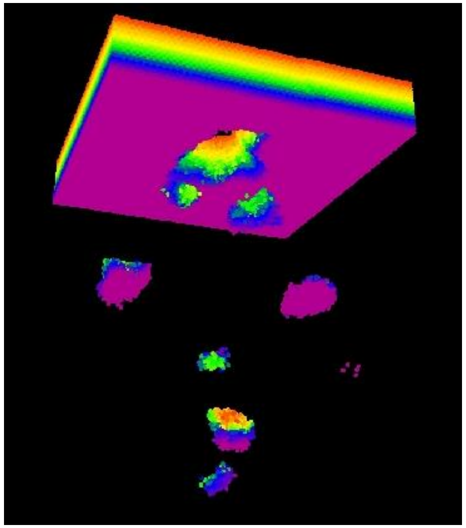
Peridynamic damage
(broken bonds)

Multiple hits on a target

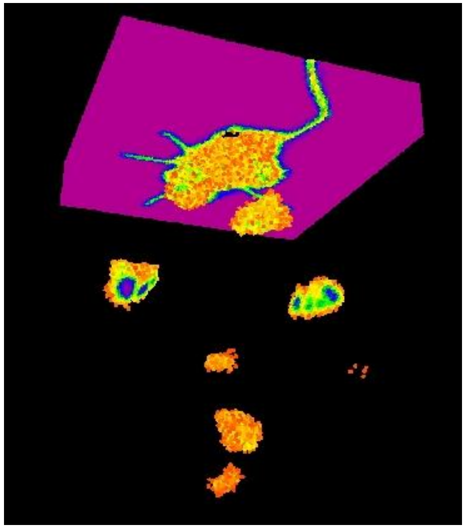
- Damage from first hit affects the second.



VIDEO



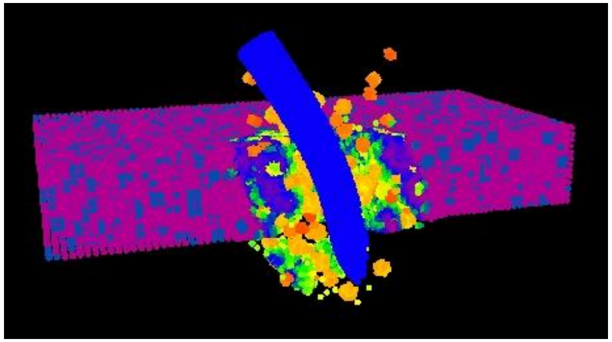
Crater shape

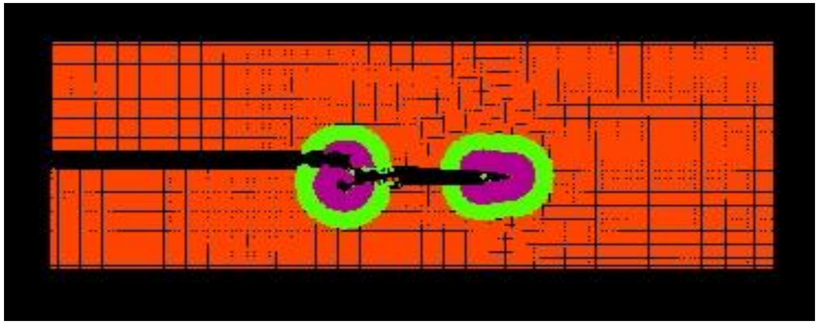


Damage

Some current research areas

- Penetration mechanics
- Heirarchical multiscale method and coarse graining





- Local-nonlocal coupling
- Material modeling
- Progressive failure in composites
- Ductile failure
- Transition to a production software method
- Calibration of a peridynamic damage model using molecular dynamics
- Eulerian version of peridynamics for fluids and fluid-structure interaction
- Better numerical discretization method

Summary

- Peridynamics a generalization of traditional continuum mechanics.
  - Equations are compatible with the physical nature of cracks and long-range forces.
  - Cracks nucleate and grow spontaneously.
  - The standard theory (PDEs) is a special case of peridynamics.
- Applications include:
  - Fracture and fragmentation.
  - Mechanics of membranes and adhesion.
  - Mesoscale & nanoscale.
  - Impact and penetration.
- Not yet a production tool – users need to understand how it behaves.