

Peridynamic Modeling of the Failure of Heterogeneous Solids

Stewart Silling

Computational Physics Department, 9232
Sandia National Laboratories
Albuquerque, New Mexico 87185-0820
sasilli@sandia.gov

ARO Workshop on
Analysis and Design of New Engineered Materials and Systems with Applications

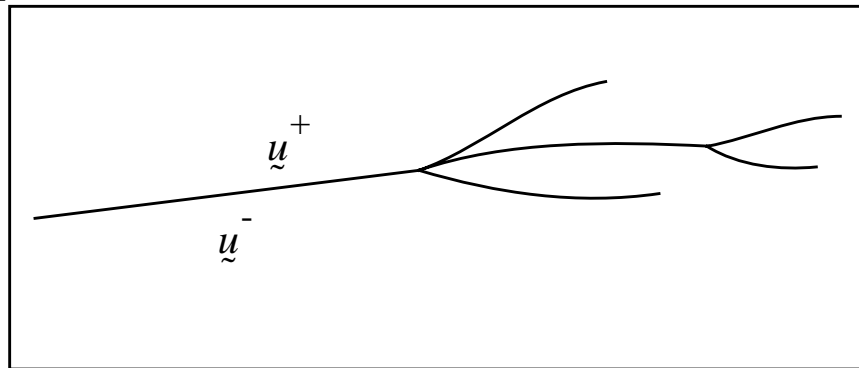
February 5, 2002

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.

Need for a new theory of solid mechanics

Computational Physics & Mechanics

- Classical formulation uses partial differential equations.
- The necessary spatial derivatives may not exist everywhere in the body.
- Example: Fracture (\underline{u} is discontinuous)



- Special techniques (of which there are many) are needed to model cracks in the classical theory.

Goal

Develop a model in which exactly the same equations hold everywhere, regardless of any discontinuities.

- ◆ To do this, get rid of spatial derivatives.

Basic idea of the peridynamic theory

- Equation of motion:

$$\rho \ddot{\underline{u}} = \underline{L}_u + \underline{b}$$

where \underline{L}_u is a functional.

- A useful special case:

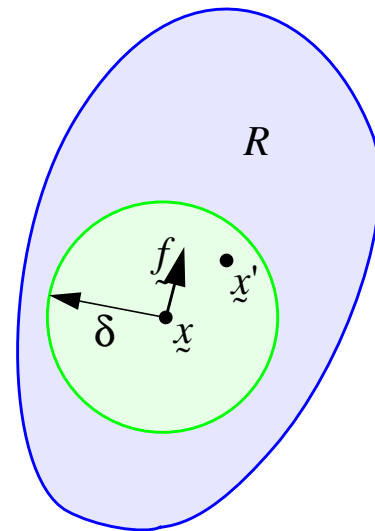
$$\underline{L}_u(\underline{x}, t) = \int_R \underline{f}(\underline{u}(\underline{x}', t) - \underline{u}(\underline{x}, t), \underline{x}' - \underline{x}) dV_{\underline{x}'}.$$

where \underline{x} is any point in the reference configuration, and \underline{f} is a vector-valued function.

More concisely:

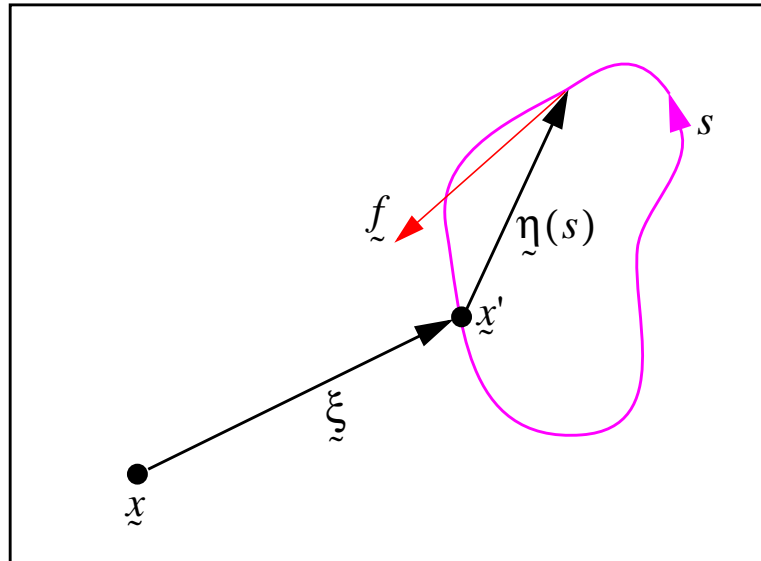
$$\underline{L} = \int_R \underline{f}(\underline{u}' - \underline{u}, \underline{x}' - \underline{x}) dV'.$$

- \underline{f} is the pairwise force function. It contains all constitutive information.
- It is convenient to assume that \underline{f} vanishes outside some horizon δ .



Microelastic materials

A material is microelastic if, holding any \underline{x} fixed, the work done by \underline{f} in moving any \underline{x}' around a closed path is 0.



In this case, Stokes' Theorem implies:

- ◆ There exists a scalar-valued function w , called the micropotential, such that

$$\underline{f}(\underline{\eta}, \underline{\xi}) = \frac{\partial w}{\partial \underline{\eta}}(\underline{\eta}, \underline{\xi})$$

where

$$\underline{\xi} = \underline{x}' - \underline{x}$$

$$\underline{\eta} = \underline{u}' - \underline{u}$$

Can further show:

- ◆ There exists a scalar function H such that

$$\underline{f}(\underline{\eta}, \underline{\xi}) = (\underline{\xi} + \underline{\eta}) H(|\underline{\xi} + \underline{\eta}|, \underline{\xi})$$

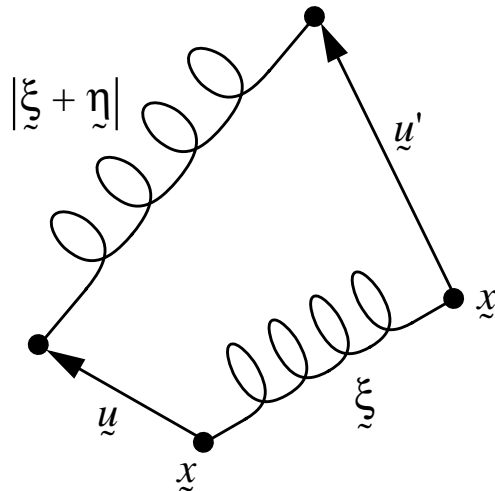
Interpretation of microelasticity

So the micropotential can depend only on:

- the current separation distance $|\xi + \eta|$
- the reference separation vector ξ .

Meaning: any two points \tilde{x} and \tilde{x}' are connected by a (possibly nonlinear) spring.

The spring properties can depend on the reference separation vector.



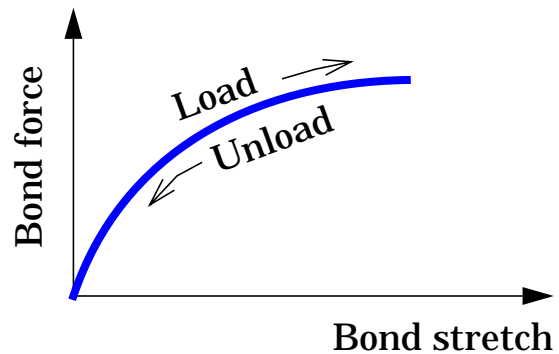
- Can prove: “microelastic implies macroelastic”:
 - Work done by external forces is stored in a recoverable form

Some material models

Computational Physics & Mechanics

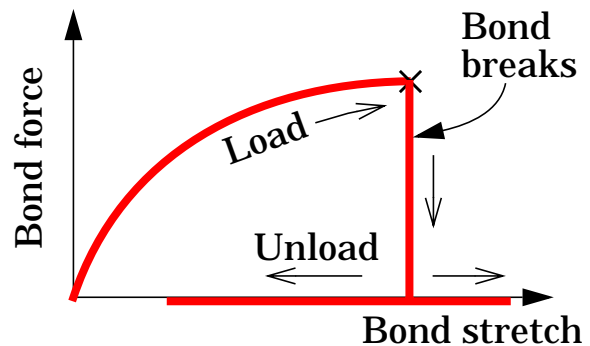
- Microelastic

- ◆ Each pair of particles is connected by a spring.
- ◆ Linear
- ◆ Bilinear
- ◆ etc.



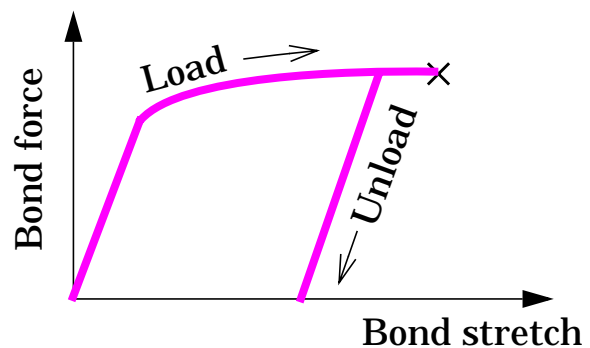
- Brittle microelastic

- ◆ Springs break irreversibly



- Microplastic

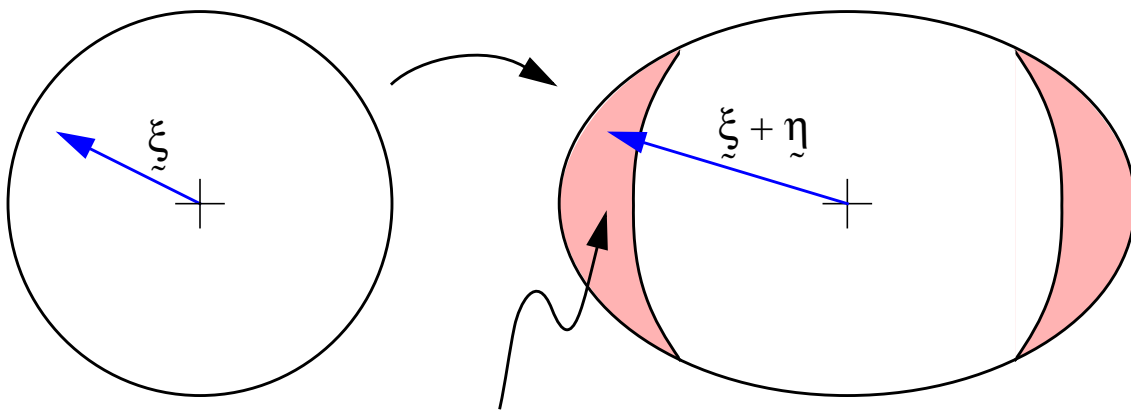
- ◆ Permanent bond deformation upon unloading.



- All of the above can have explicit rate dependence.

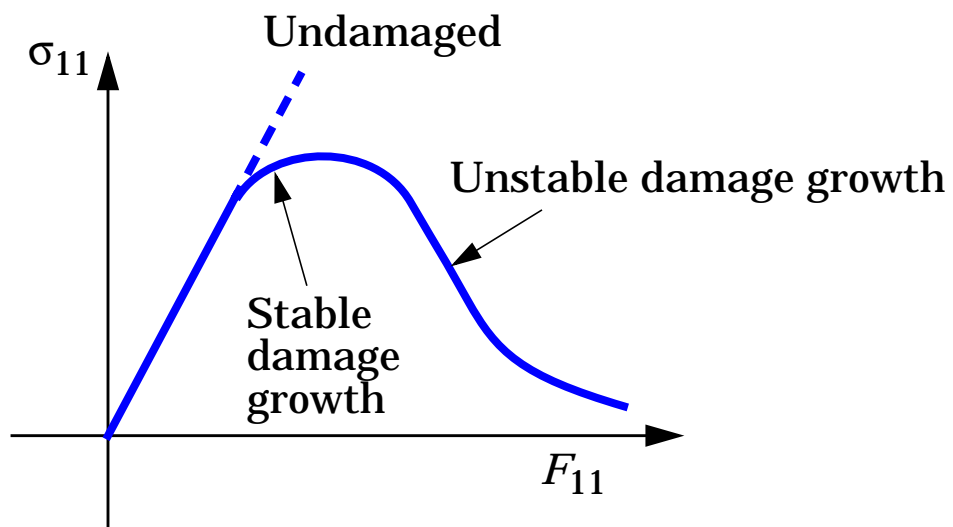
How bond breakage leads to material fracture

- Continuum damage is caused by deformation:



Broken springs: $|\xi + \eta| - |\xi| \geq \epsilon$

- This causes a change in the “stress-strain” curve:



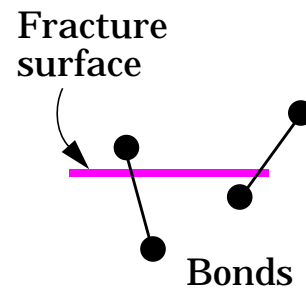
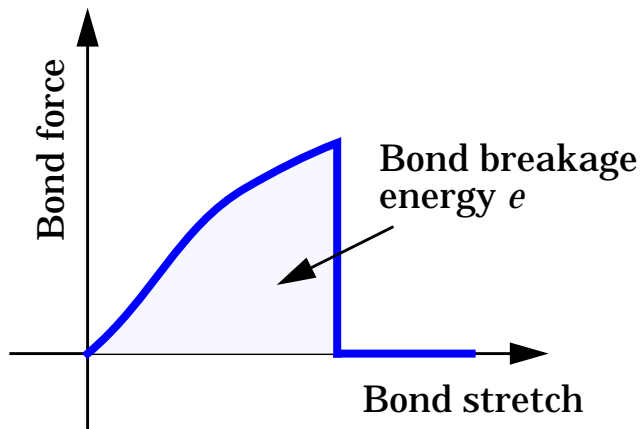
- Need to understand the mathematical conditions under which discontinuities can emerge.

Determination of constitutive parameters



Computational Physics & Mechanics

- Linear microelastic:
 - Basic:
 - ◆ Spring constant is fit to wave speed data.
 - Advanced:
 - ◆ Can fit wave dispersion data if available.
 - ◆ Bond properties can depend on initial bond length.
- Microplastic:
 - Fit to uniaxial stress-strain curve.
- Bond breakage properties:
 - Fit breakage stretch to fracture toughness data.



Sum over bonds that are broken by the fracture:

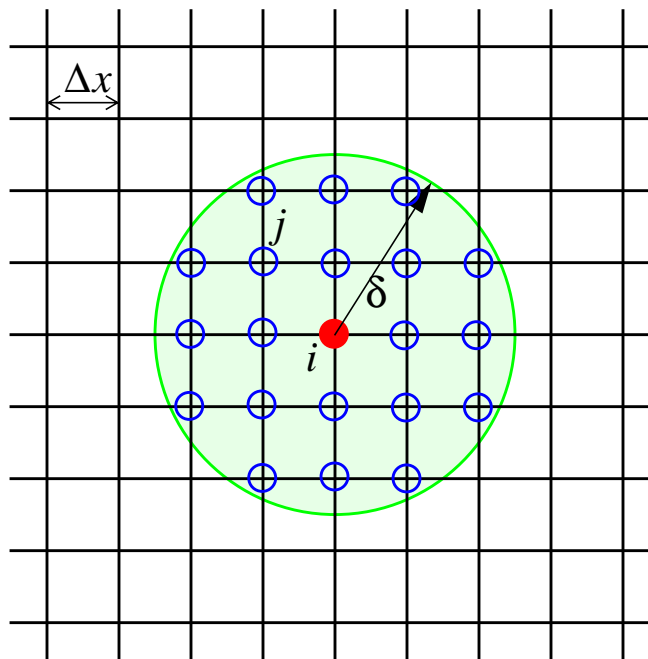
$$\text{Fracture energy} = \sum \text{bond breakage energy}$$

Numerical solution method for dynamic problems



Computational Physics & Mechanics

- Theory lends itself to mesh-free numerical methods.
 - No elements.
 - Changing connectivity.
- Brute-force integration in space.



$$\rho \ddot{u}^i = \sum_{|x^j - x^i| < \delta} f(\ddot{u}^j - \ddot{u}^i, x^j - x^i)(\Delta x)^3$$

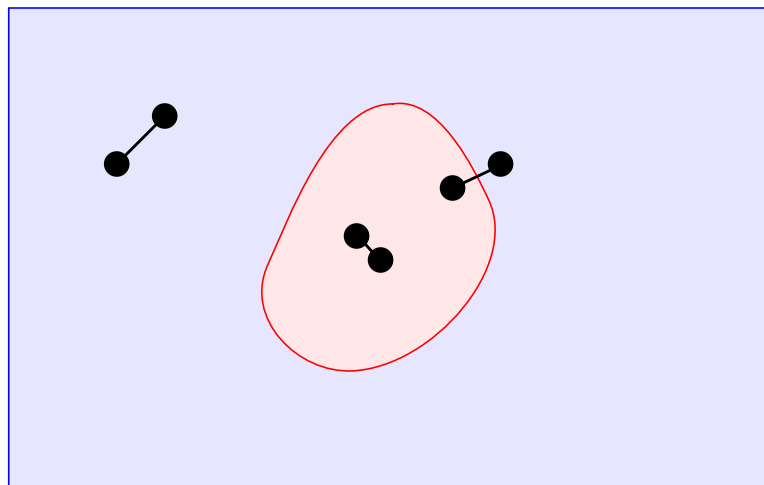
- Solution method has been found to scale well (almost linear speedup) when run on the Intel Teraflops computer at Sandia.
- Stable time step does not depend on mesh spacing (!)

Peridynamic fracture model is “autonomous”



Computational Physics & Mechanics

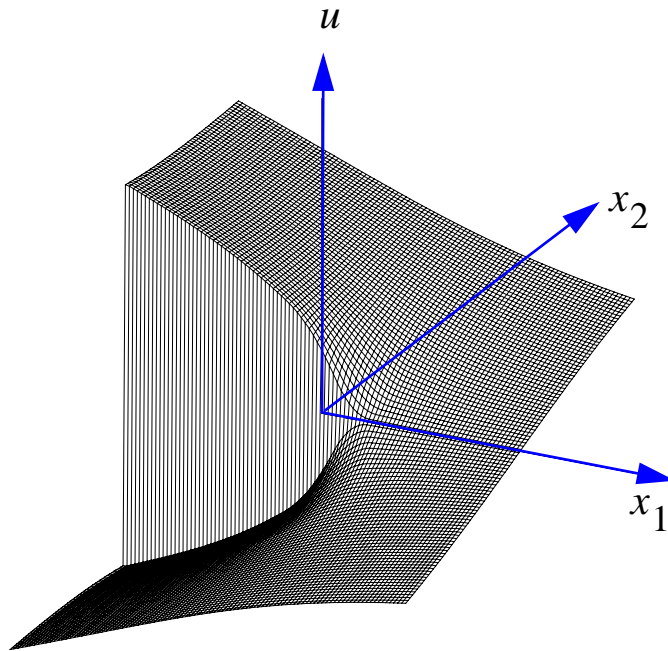
- Cracks grow when and where it is energetically favorable for them to do so.
- Path, growth rate, arrest, branching, mutual interaction are predicted by the constitutive model and equation of motion (alone).
 - No need for any externally supplied relation controlling these things.
- Any number of cracks can occur and interact.
- Interfaces between materials have their own bond properties.



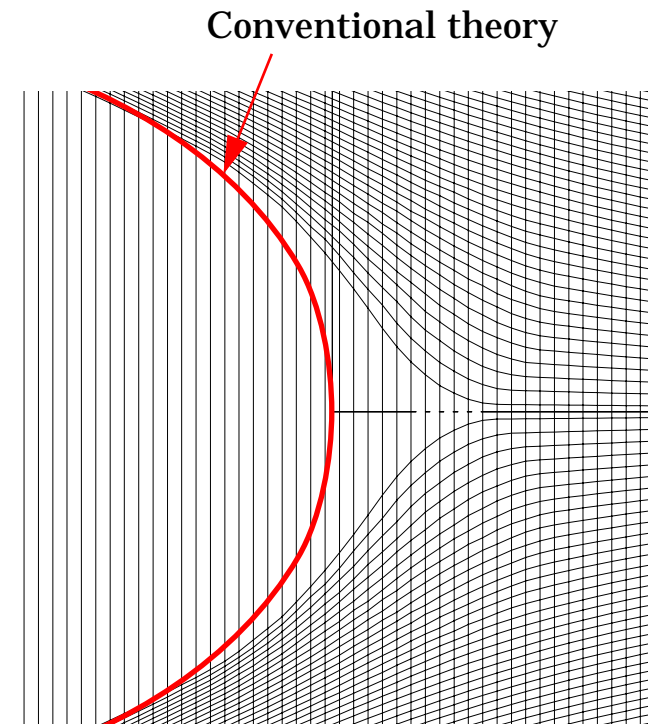
Mode-III crack tip field

Computational Physics & Mechanics

- Same equations are applied everywhere.
- Crack faces have cusp shape near tip.
 - No need for additional hypotheses (e.g. Barenblatt).



Surface into which a plane deforms

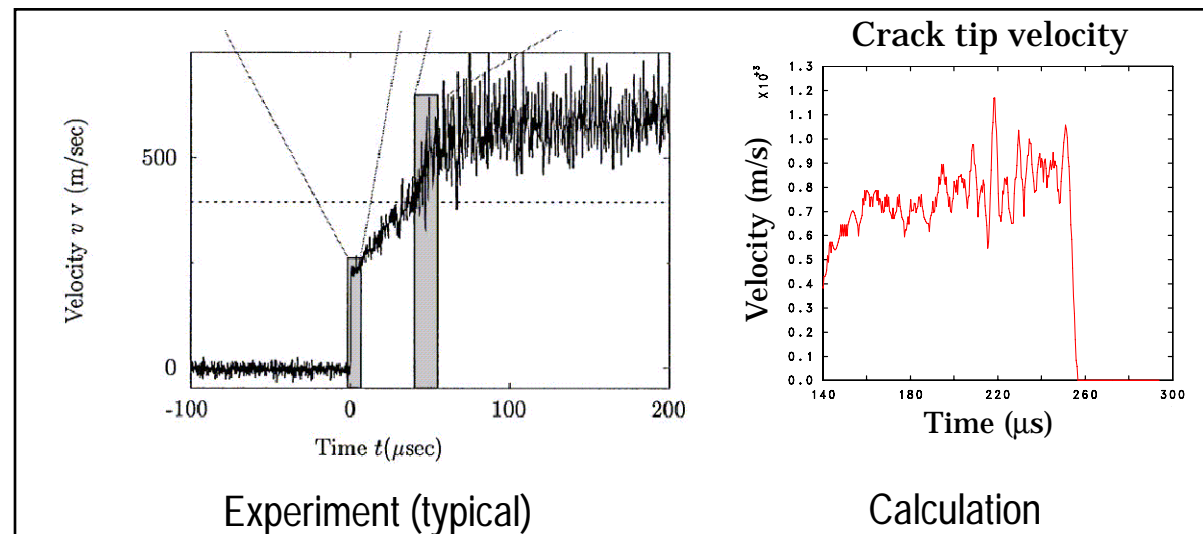
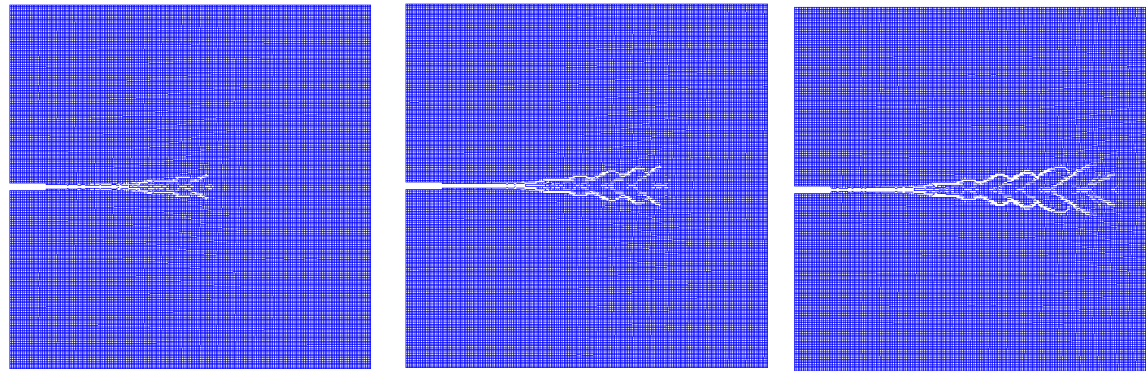
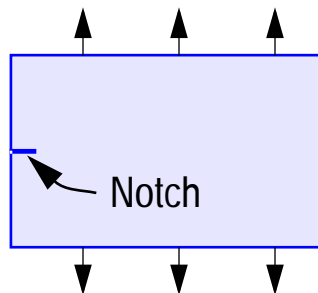


Enlarged view of crack tip

Dynamic brittle fracture

Computational Physics & Mechanics

- Stretching of a PMMA plate¹

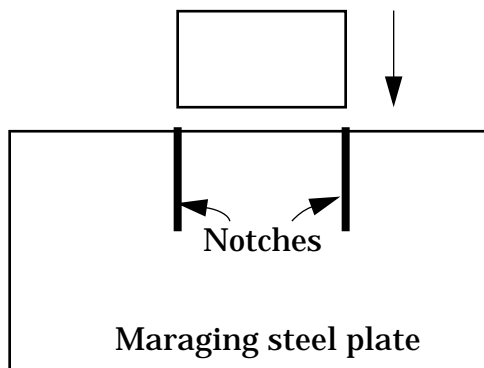


1. J. Fineberg and M. Marder, *Physics Reports* 313 (1999) 1-108

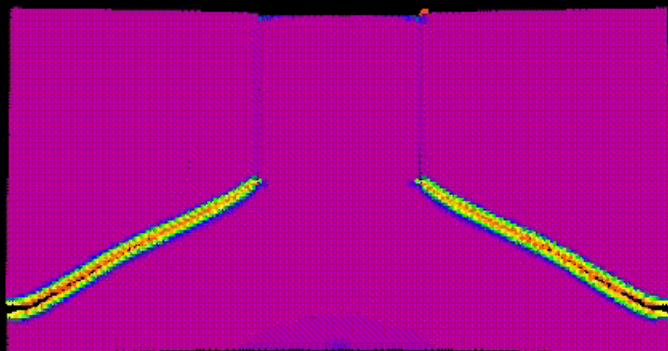
Dynamic fracture in a tough steel: Kalthoff-Winkler experiment



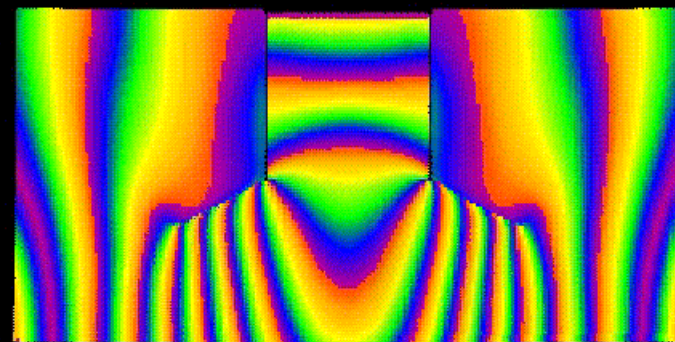
Computational Physics & Mechanics



- Code predicts correct crack angles.



Crack paths

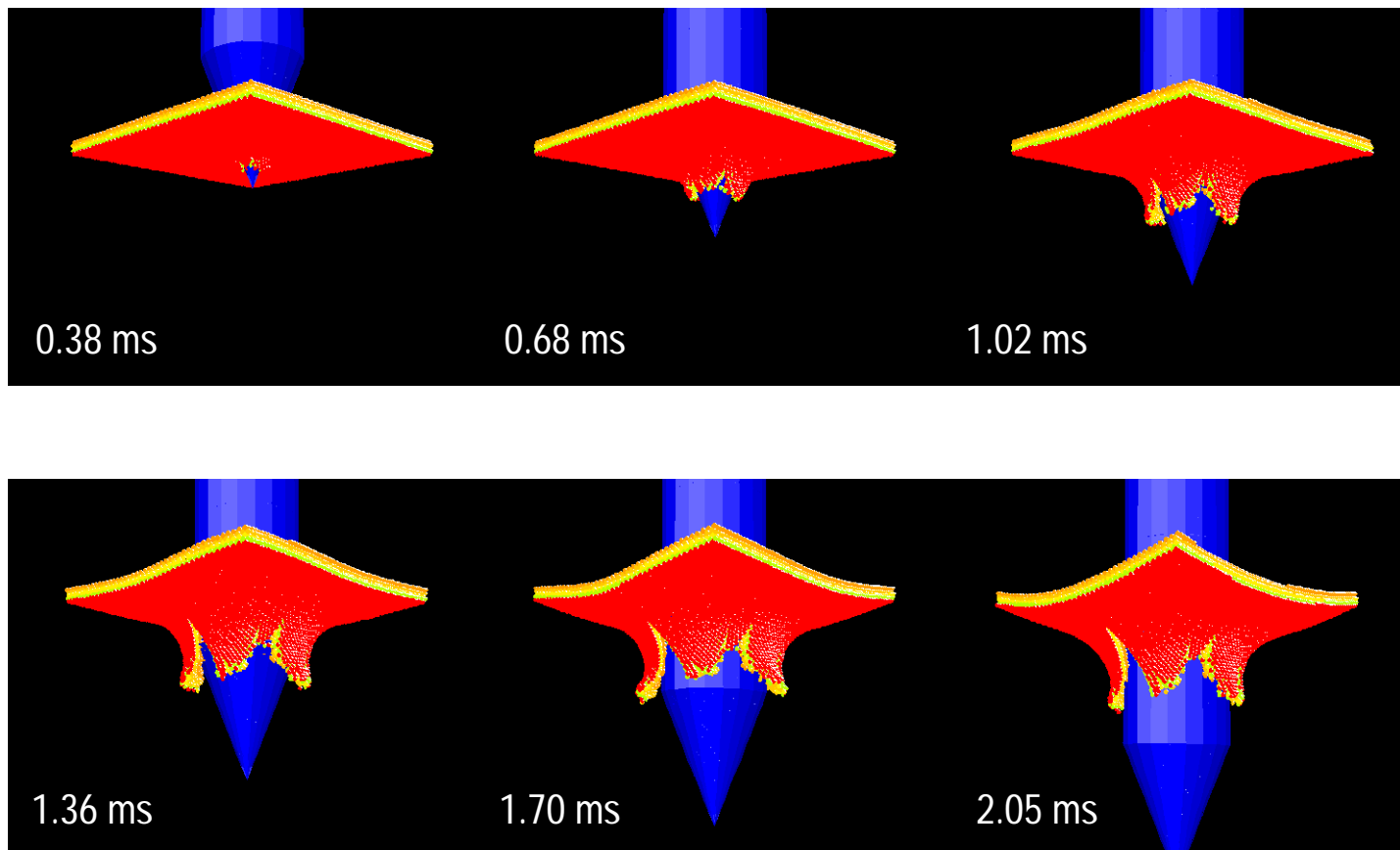


Simulated Moire fringes

Perforation of thin ductile targets

Computational Physics & Mechanics

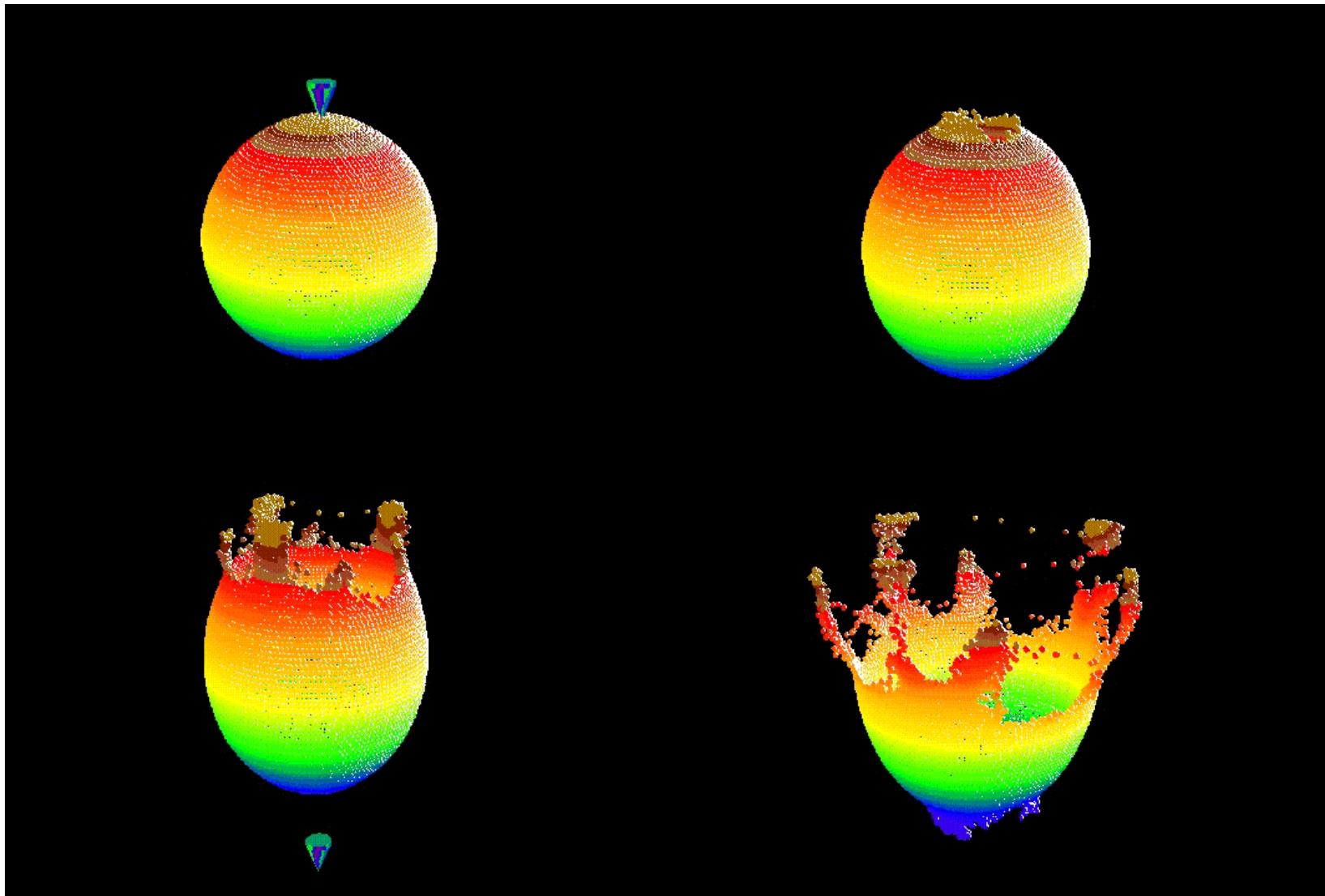
- Peak force occurs at about 0.4ms (end of drilling phase):¹



1. Not all of the target is shown.

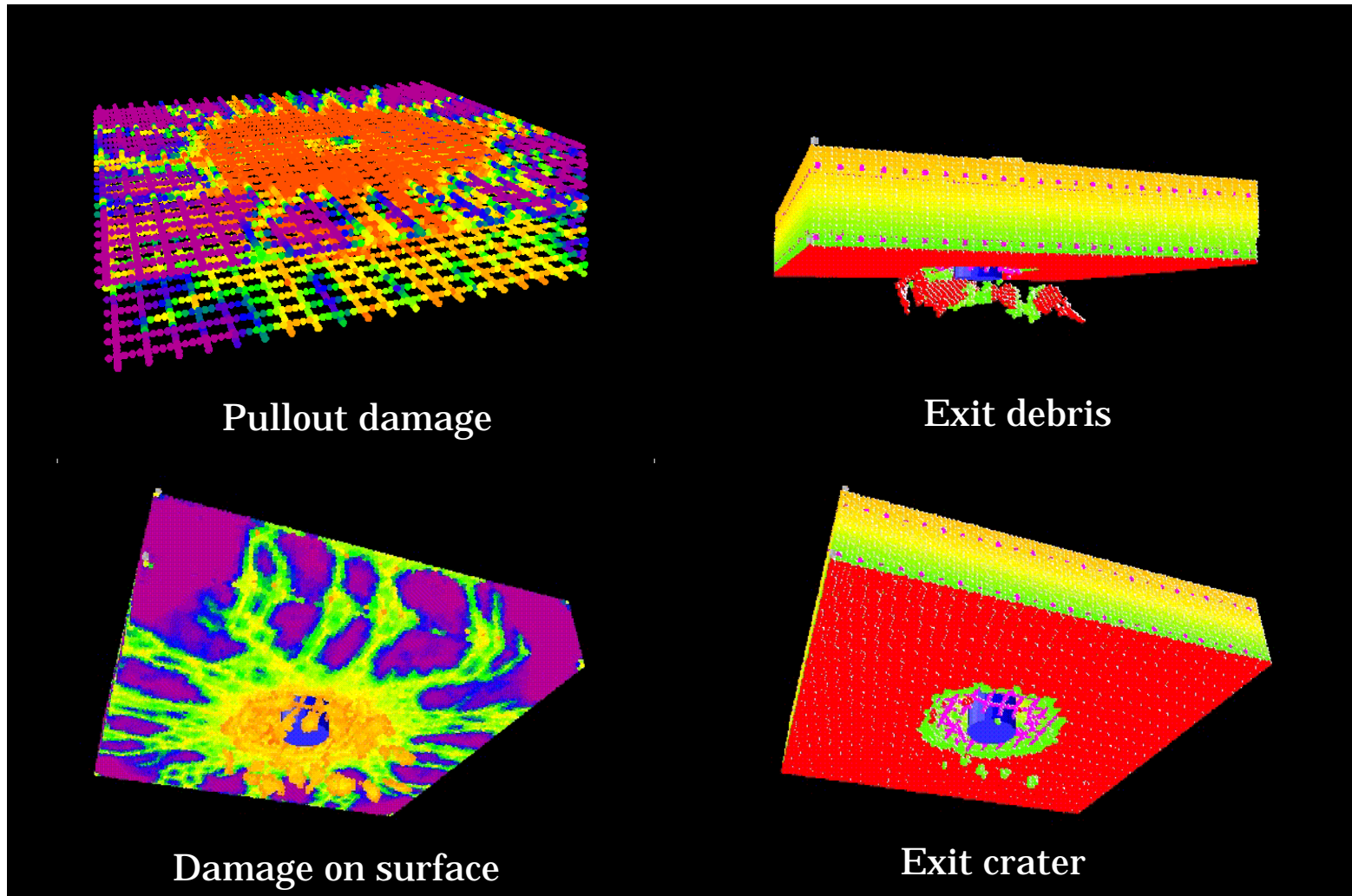
Dynamic fracture in a balloon

Computational Physics & Mechanics



Nonhomogeneous materials: Perforation of reinforced concrete

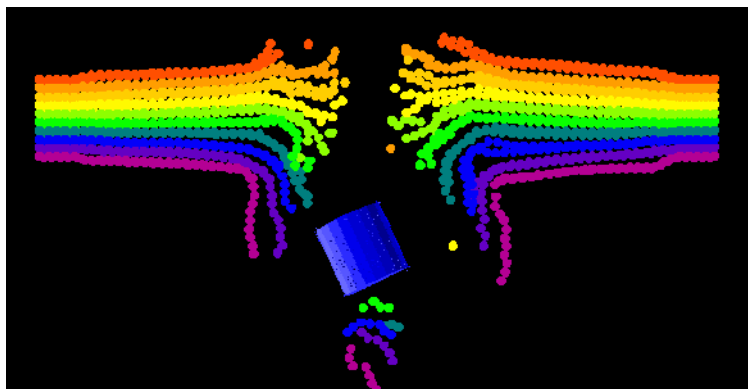
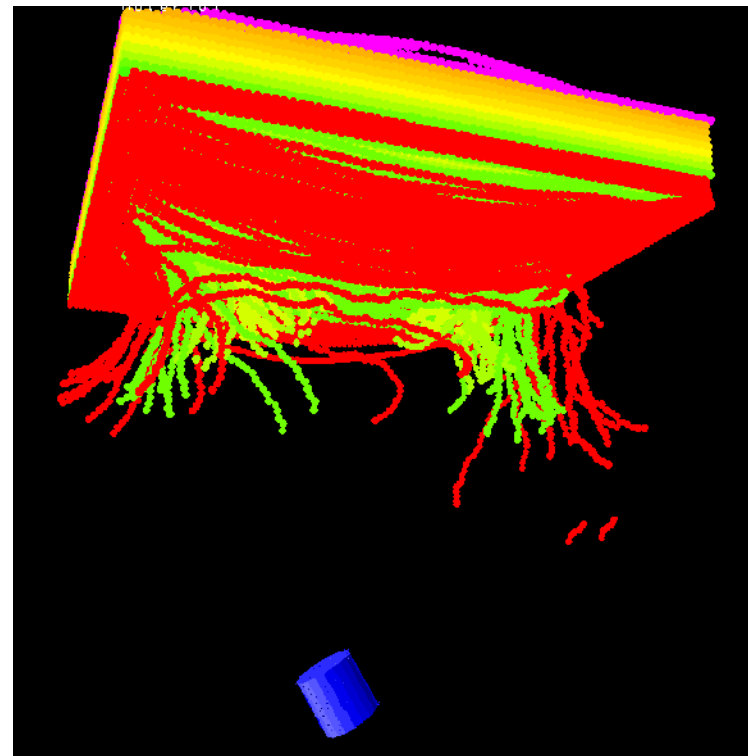
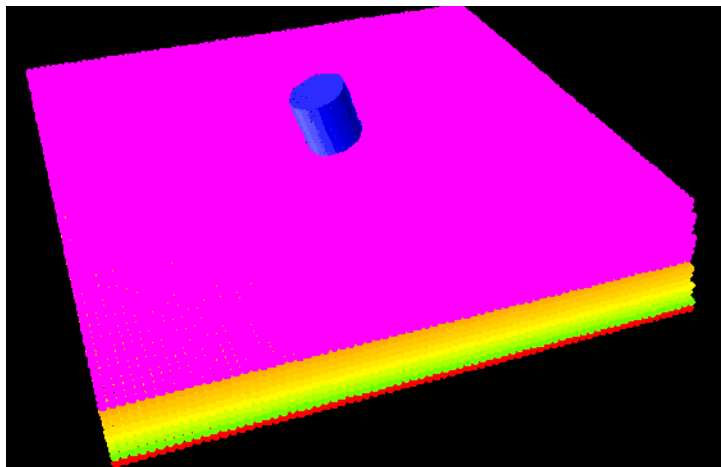
Computational Physics & Mechanics



Nonhomogeneous materials: Perforation of a fabric

Computational Physics & Mechanics

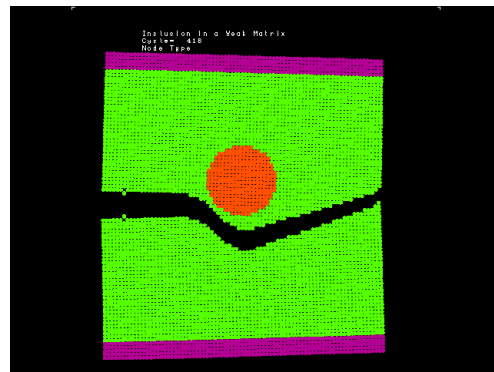
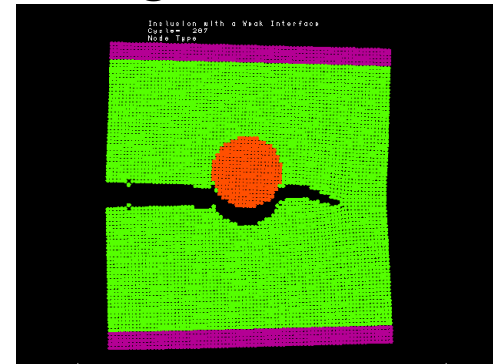
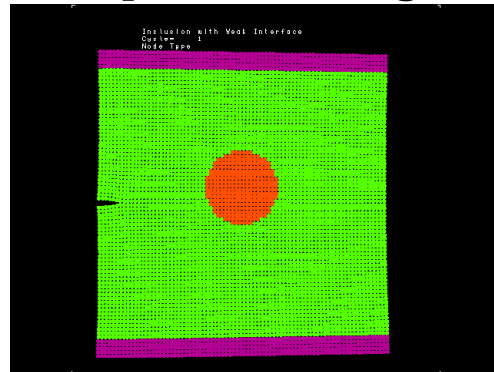
- Model includes fiber breakage, contact, and adhesion:



Nonhomogeneous materials: Fracture in a composite unit cell

Computational Physics & Mechanics

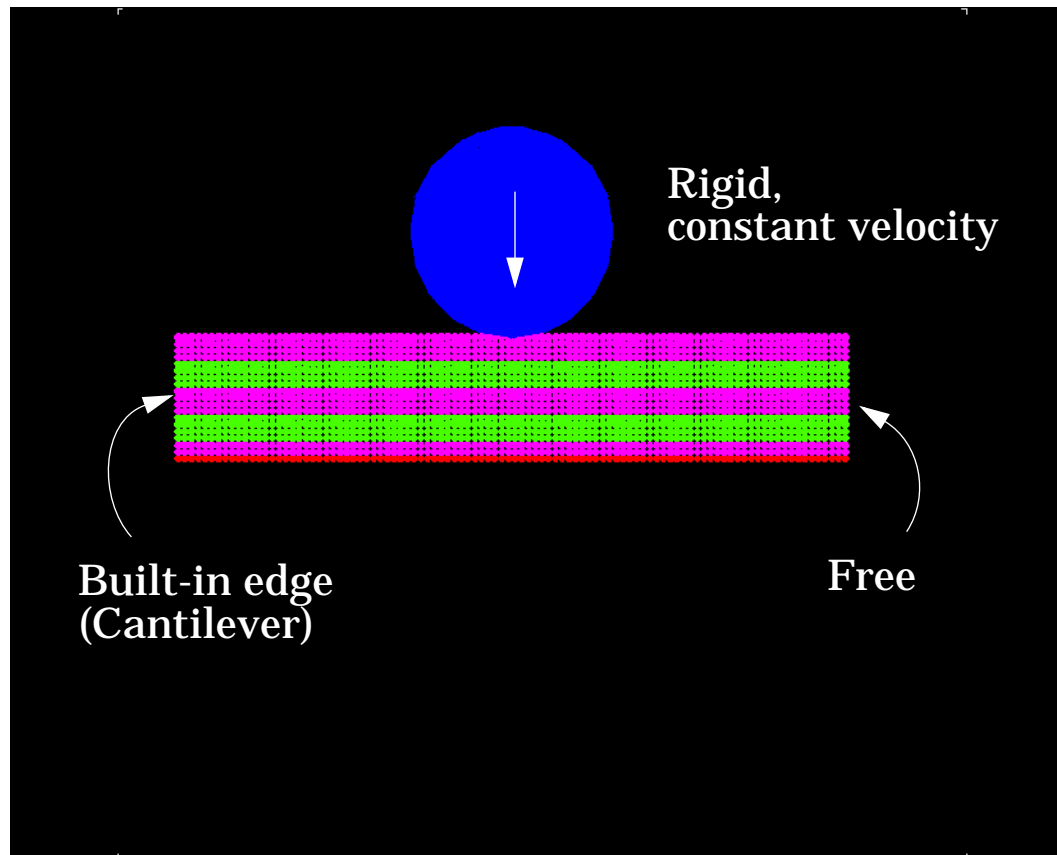
- Crack path, growth, and stability depend only on material properties.
- No need for separate laws governing crack growth.



Layered material example: Where does failure first occur?

Computational Physics & Mechanics

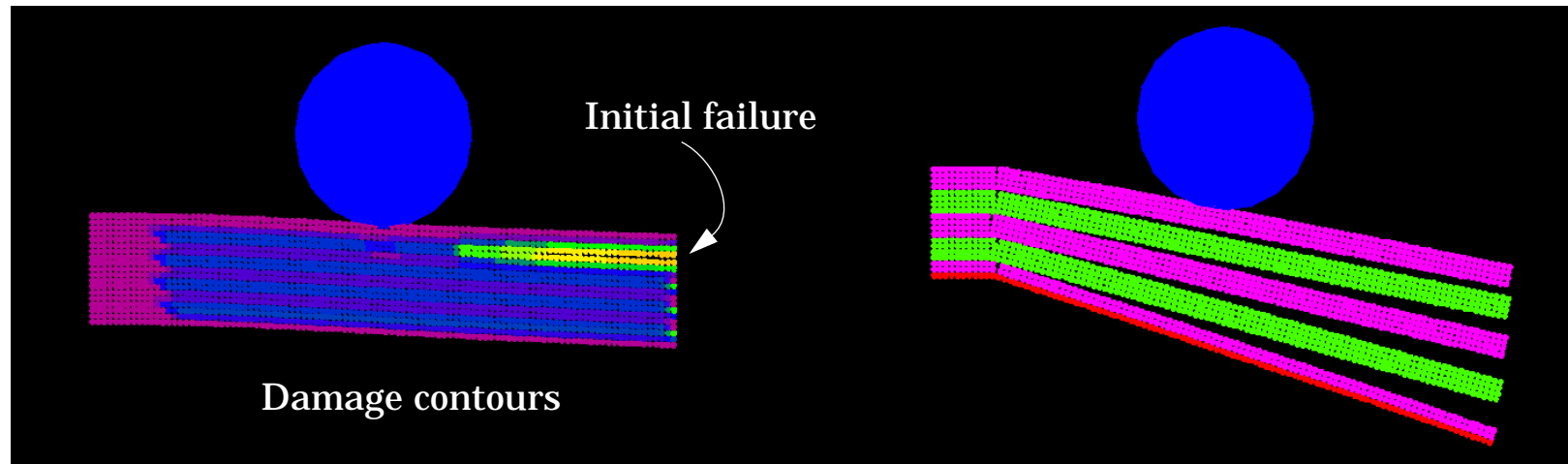
- Layers have identical properties.
- Interfaces have half the strength of the layers.



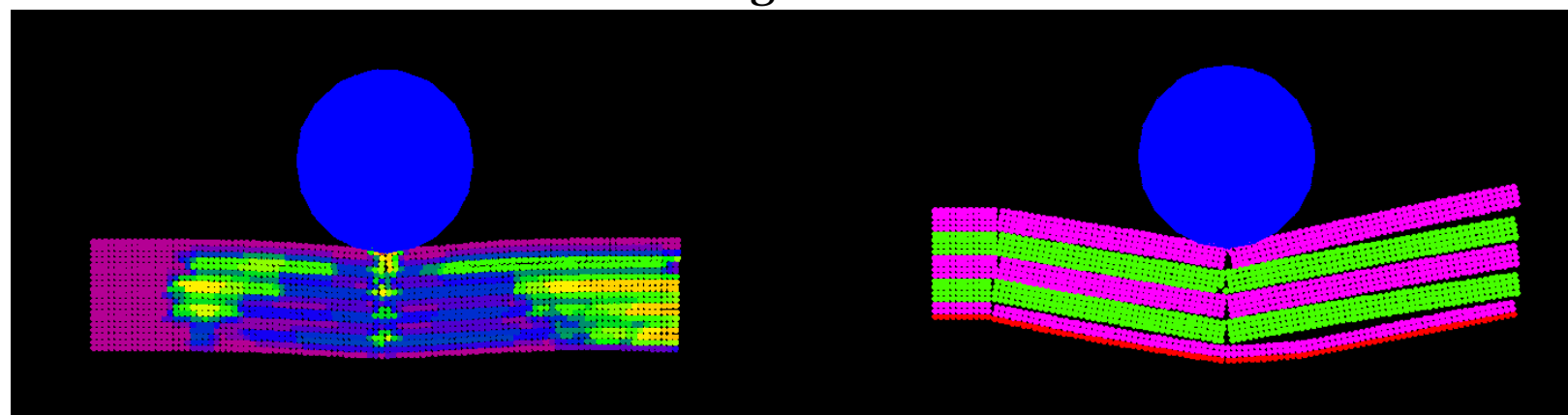
Initial failure site and mode depends on loading rate

Computational Physics & Mechanics

Low rate



High rate

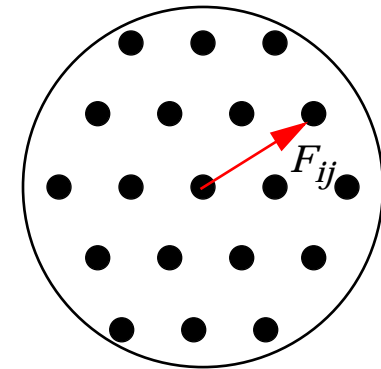


Correspondence with atomic-scale physics



Computational Physics & Mechanics

- Can a constitutive model be derived rigorously from an atomic-scale physical description?
 - Classical theory: people have been trying for a long time.
 - Peridynamic theory may be a more natural way to do this because of its similarity to molecular dynamics.
 - ◆ This is currently being attempted by Bhattacharya (Caltech) and Abeyaratne (MIT).
 - May lead to a good way to do multiscale modeling.





Conclusions



Computational Physics & Mechanics

- Method appears to have the potential to model:
 - Heterogeneous materials of great complexity.
 - Complex fracture systems without the need to keep track of each crack.

Possible research directions

- Mechanics of heterogeneous materials
 - Understand how failure progresses from one material to another.
 - Improved material models.
 - Validation against interface crack data.
 - Fatigue cracks.
 - Multiscale modeling.
 - Learn how to do complex material systems.
- Theory and numerical solutions
 - Improved solvers.
 - ◆ Multigrid, iterative, implicit, etc.