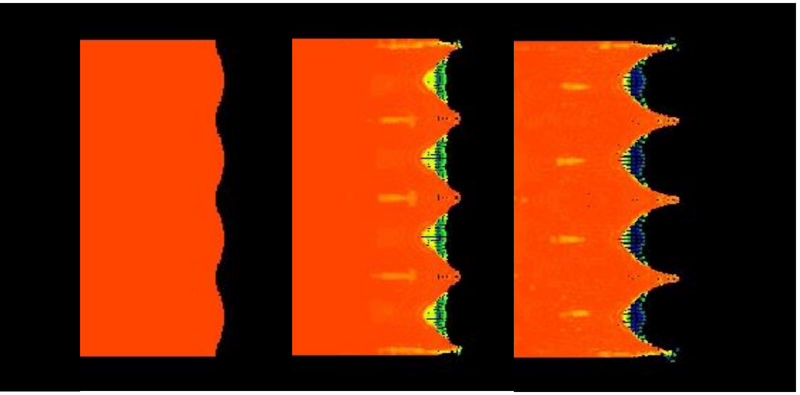
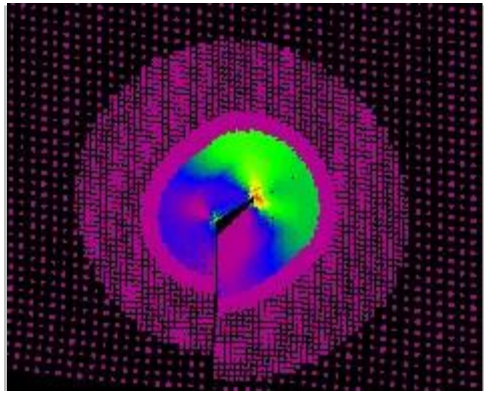
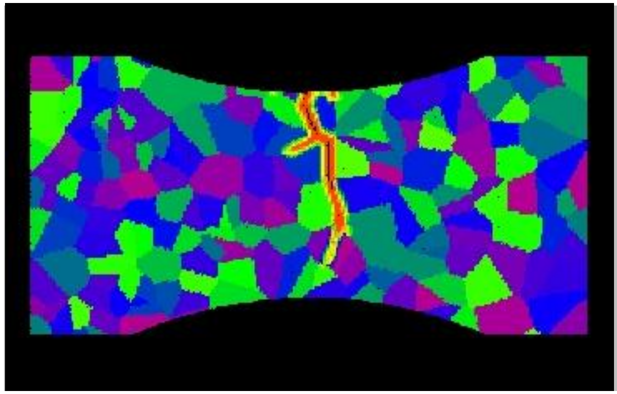
Exceptional service in the national interest

SAND2015-0148PE

Sandia National Laboratories







Peridynamics: Historical and future perspectives

Stewart Silling

Peridynamics MURI Meeting, December 13, 2015

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

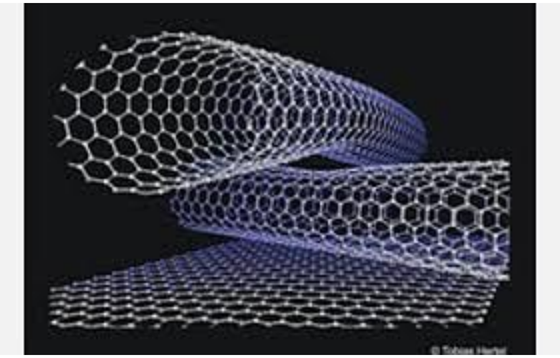
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Outline

- Purpose of peridynamics
- Basic equations
- Examples of capabilities
  - Success stories
- Strengths and weaknesses
  - Research priorities

What should be modeled as a classical continuum?

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



Carbon nanotubes (image: nsf.gov)

$$\nabla \cdot \sigma + b = 0$$

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

Fragmented glass (image: Washington Glass School)

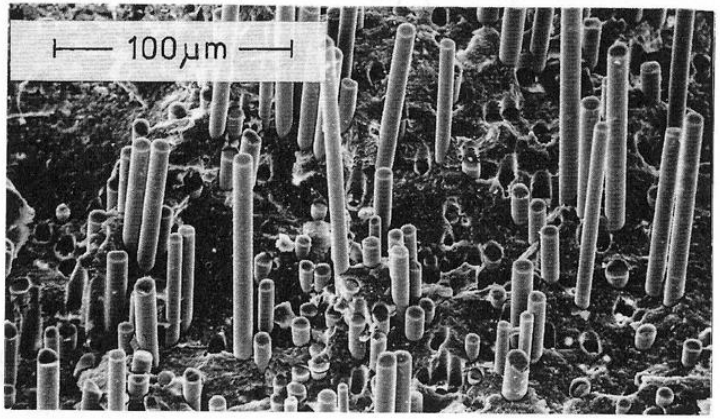
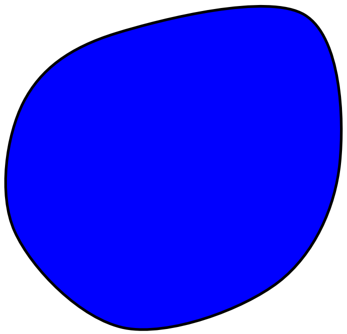


Figure 11.20 Pull-out: (a) schematic diagram; (b) fracture surface of 'Silceram' glass-ceramic reinforced with SiC fibres. (Courtesy H. S. Kim, P. S. Rogers and R. D. Rawlings.)

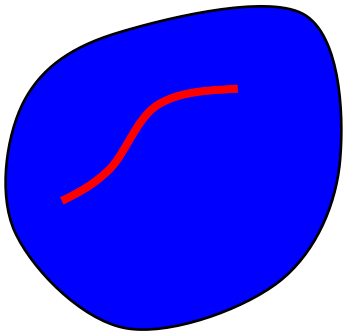
Complex failure progression in a composite

Purpose of peridynamics

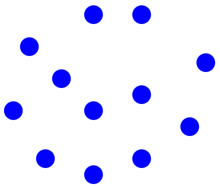
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body with a defect

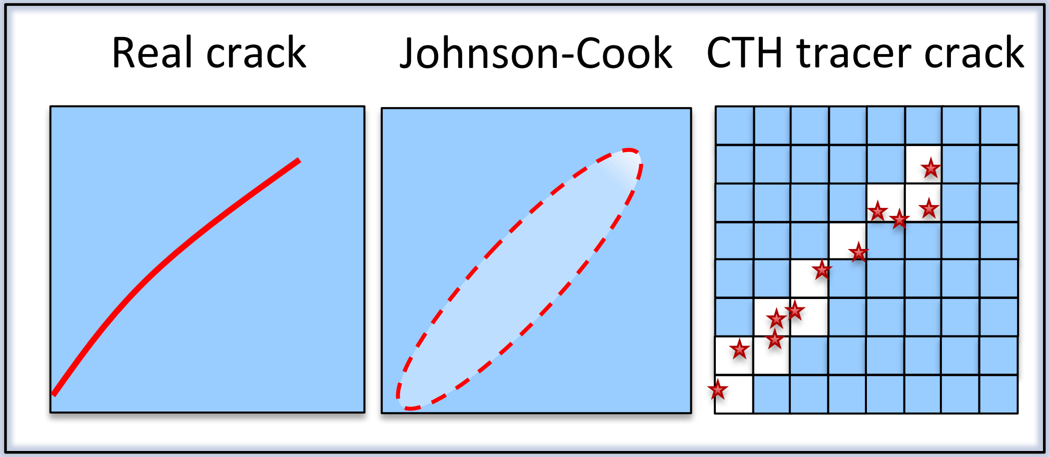


Discrete particles

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

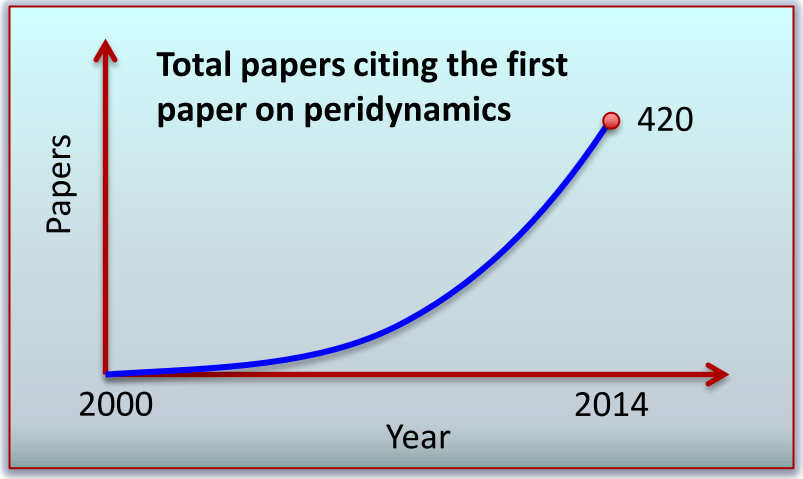
Personal view of PD history

- 1980's
  - Mathematical theory of singularities in elastic solids
- 1990's:
  - Johnson-Cook, similar models in CTH
  - Tracer crack & shear band model in CTH
  - 1998: "The realization"
- 2000's:
  - Bond-based peridynamics
    - Rush to applications
  - State-based peridynamics
  - Math, physics foundations
- 2010's:
  - Increasing interest worldwide
  - Sierra, Peridigm
  - Plasticity
  - Address practical issues
    - Wake-up calls
  - Thermodynamics
  - Shock waves
  - Multiscale
  - Multiphysics
  - LS-DYNA

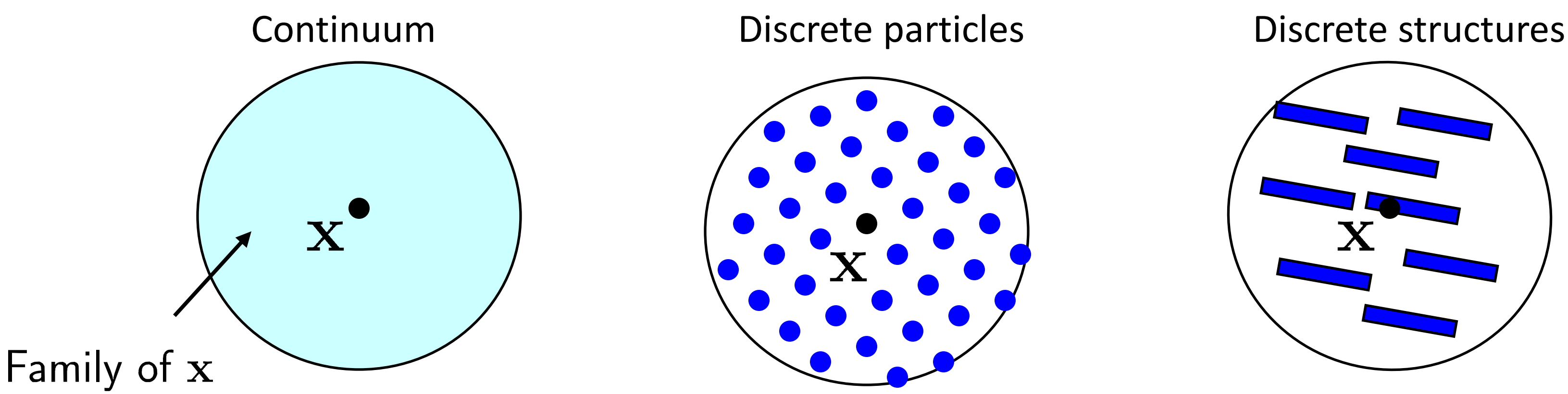


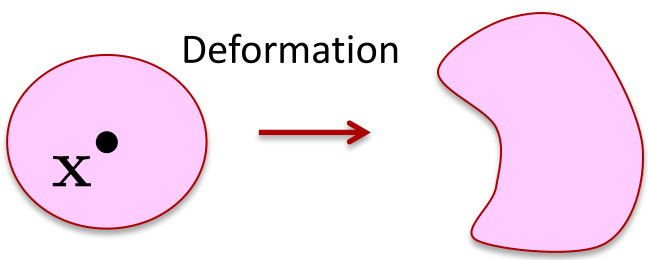
Peridynamics: Who’s interested?

- Research has been conducted at:
  - MIT
  - Caltech
  - Harvard University
  - Northwestern 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
  - KAUST
  - … others worldwide



Point of departure: Strain energy at a point



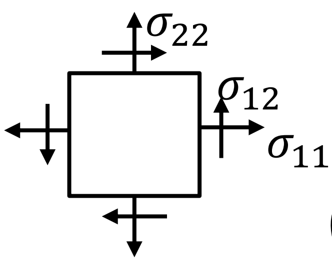


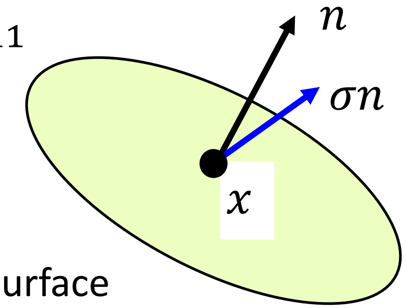
- Key assumption: the strain energy density at $\mathbf{x}$ is determined by the deformation of its family.

The nature of internal forces

Standard theory

Stress tensor field
(assumes continuity of forces)





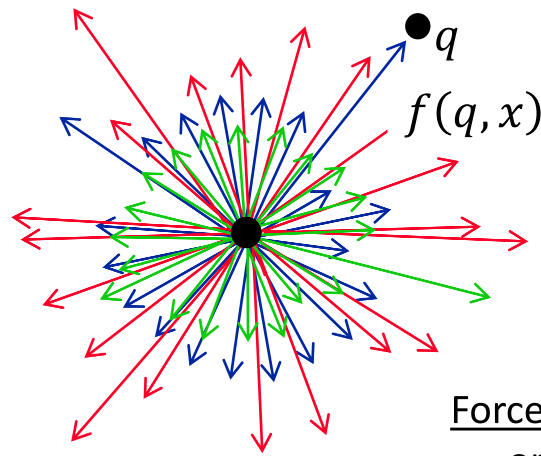
Stress tensor maps surface normal vectors onto surface forces

$$\rho\ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t)$$

Differentiation of surface forces

Peridynamics

Bond forces between neighboring points
(allowing discontinuity)



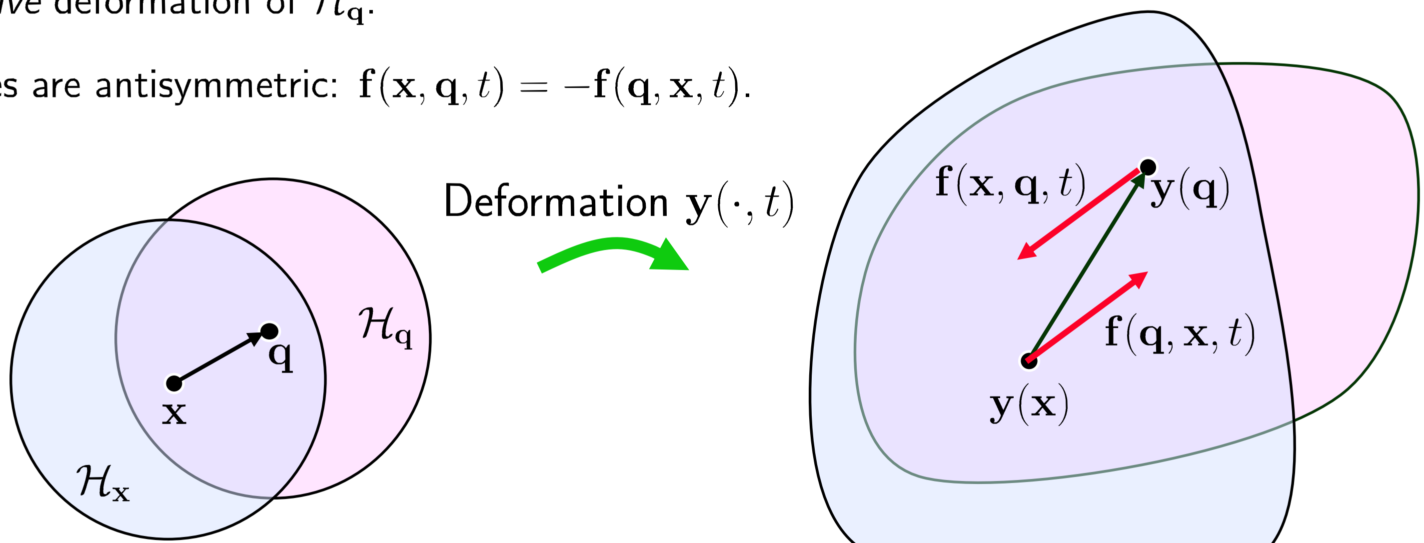
Force state maps bonds onto bond forces

$$\rho\ddot{u}(x,t) = \int_{H_x} f(q,x)dV_q + b(x,t)$$

Summation over bond forces

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: $\mathbf{f}(\mathbf{x}, \mathbf{q}, t) = -\mathbf{f}(\mathbf{q}, \mathbf{x}, t)$.



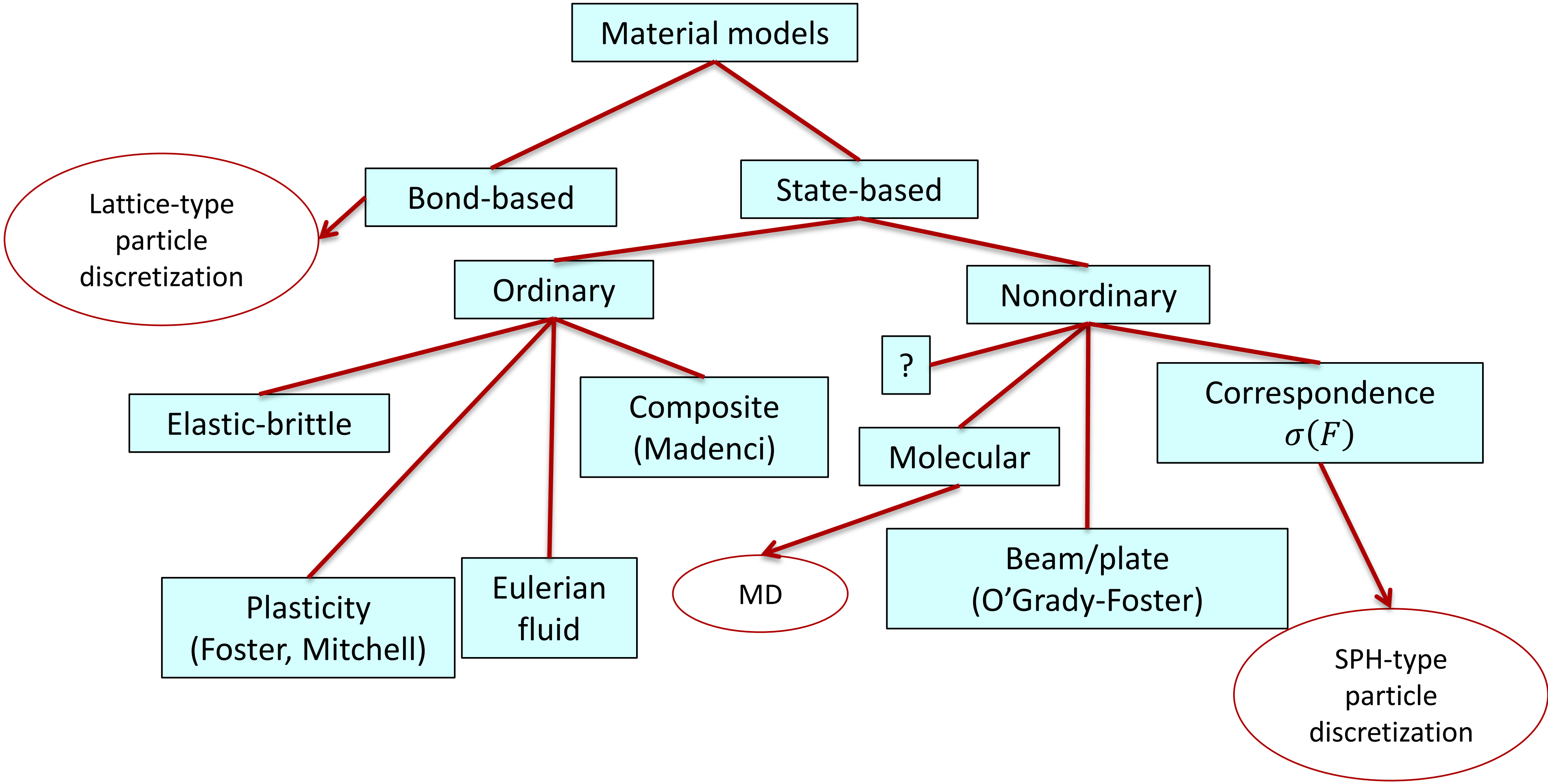
Undeformed families

Deformed families and bond forces

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

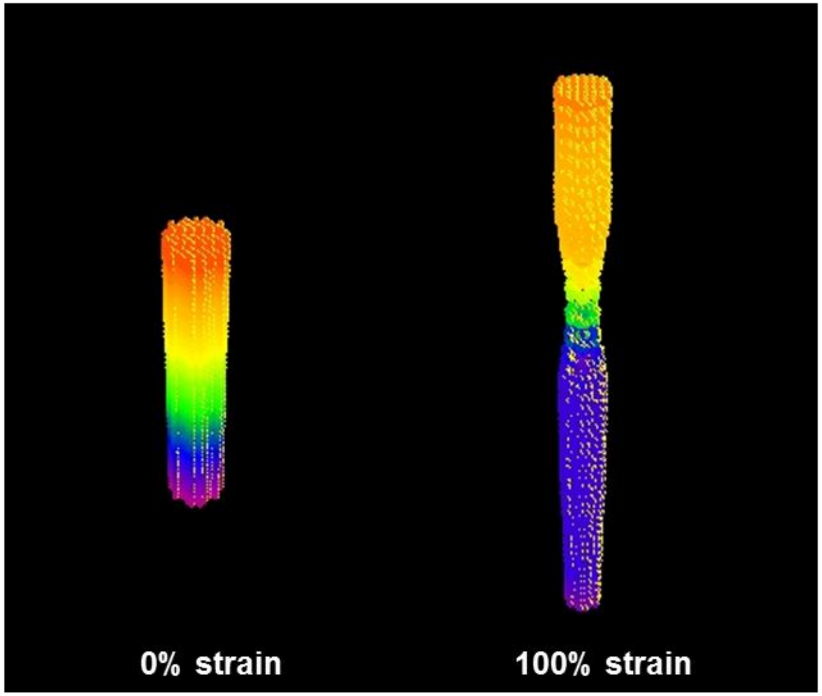
Types of material models

- A material model determines the bond forces in the family according to the deformation of the family.

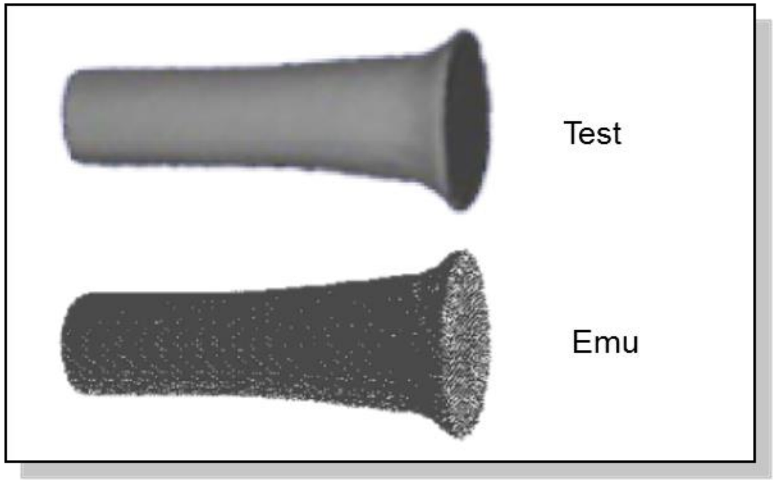


Any standard material model can be used in peridynamics

- Example: Large-deformation, strain-hardening, rate-dependent material model.
  - Material model implementation by John Foster.



Necking of a bar under tension



Taylor impact test

Peridynamic vs. local equations

- Peridynamic theory is similar in structure to the local theory but uses nonlocal operators.

State notation: $\underline{\text{State}}\langle\text{bond}\rangle = \text{vector}$

Relation	*Peridynamic theory*	*Standard theory*
Kinematics	$\underline{\mathbf{Y}}\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q}) - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \int_{\mathcal{H}} \big(\mathbf{t}(\mathbf{q},\mathbf{x}) - \mathbf{t}(\mathbf{x},\mathbf{q})\big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\mathbf{t}(\mathbf{q},\mathbf{x}) = \underline{\mathbf{T}}\langle\mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular momentum balance	$\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle\mathbf{q}-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle\mathbf{q}-\mathbf{x}\rangle\, dV_{\mathbf{q}} = \mathbf{0}$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{\mathbf{Y}}}$ (Fréchet derivative)	$\boldsymbol{\sigma} = W_{\mathbf{F}}$ (tensor gradient)
First law	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + q + r$	$\dot{\varepsilon} = \boldsymbol{\sigma}\cdot\dot{\mathbf{F}} + q + r$

$$\underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} := \int_{\mathcal{H}} \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \cdot \dot{\underline{\mathbf{Y}}}\langle\boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}$$

Peridynamic form of thermodynamics

- SS & Lehoucq, Adv Appl Mech (2010)
- Oterkus, Madenci & Agwai, JMPS (2014)

- First law expression:

$$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + r + h$$

where ε is the internal energy density, r is the source rate, h is the rate of heat transport.

- Second law expression:

$$\theta \dot{\eta} \geq r + h$$

where θ is the temperature and η is the entropy.

- Free energy:

$$\psi = \varepsilon - \theta \eta.$$

- Assume a material model of the form

$$\psi(\underline{\mathbf{Y}}, \theta)$$

- First + second laws imply (through Coleman-Noll or similar method):

$$\underline{\mathbf{T}} = \psi_{\underline{\mathbf{Y}}}, \qquad \eta = -\psi_\theta.$$

Frechet derivative

Multiphysics: Nonlocal diffusion

- Agwai, thesis, U.Ariz. (2011)
- Burch & Lehoucq (2011)
- Bobaru & Duangpanya, J.Comp.Phys. (2012)
- Du et al (2012)

- We can extend the dependence of free energy:

$$\psi(\underline{\mathbf{Y}}, \theta, z, \underline{\phi})$$

where z is the concentration of a chemical species, and $\underline{\phi}$ is the *damage state*.

- Recall momentum balance:

$$\rho(\mathrm{x})\ddot{\mathrm{y}}(\mathrm{x}, t) = \int_{\mathcal{H}} \mathrm{f}(\mathrm{x}', \mathrm{x}, t)\; d\mathrm{x}' + \mathrm{b}(\mathrm{x}).$$

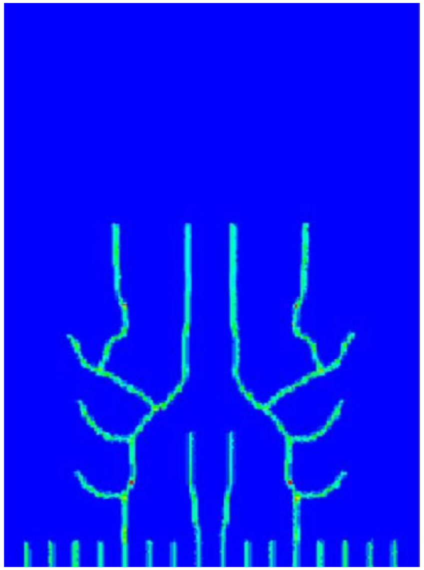
- Nonlocal forms of transport equations for heat, concentration:

$$C_v\dot{\theta}(\mathrm{x}, t) = \int_{\mathcal{H}} q(\mathrm{x}', \mathrm{x}, t)\; d\mathrm{x}' + r(\mathrm{x})$$

where C_v=specific heat, q=bond heat flux, r=energy source rate;

$$\dot{z}(\mathrm{x}, t) = \int_{\mathcal{H}} J(\mathrm{x}', \mathrm{x}, t)\; d\mathrm{x}' + s(\mathrm{x})$$

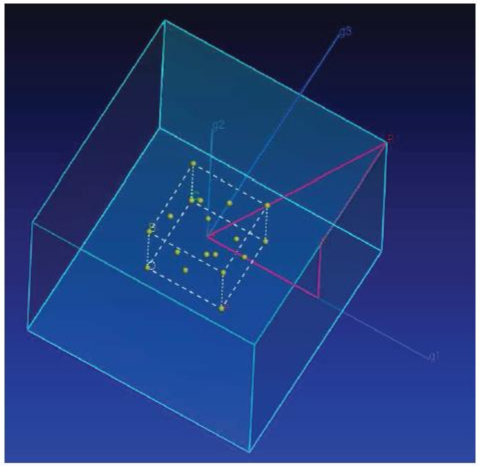
where J=concentration flux, s=source rate.



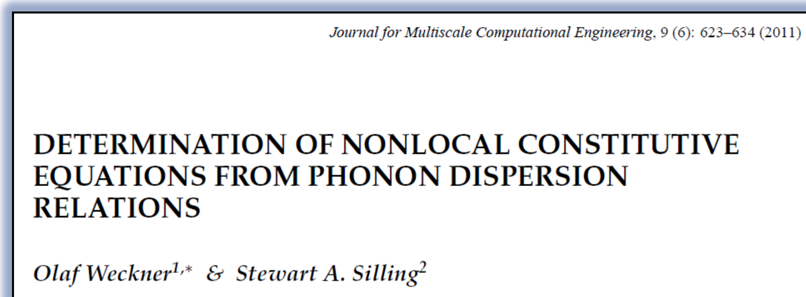
Simulated crack growth in a glass plate driven by thermal gradients (Kilic & Madenci, 2009)

Bond response can be found from phonon dispersion curves

Sandia National Laboratories

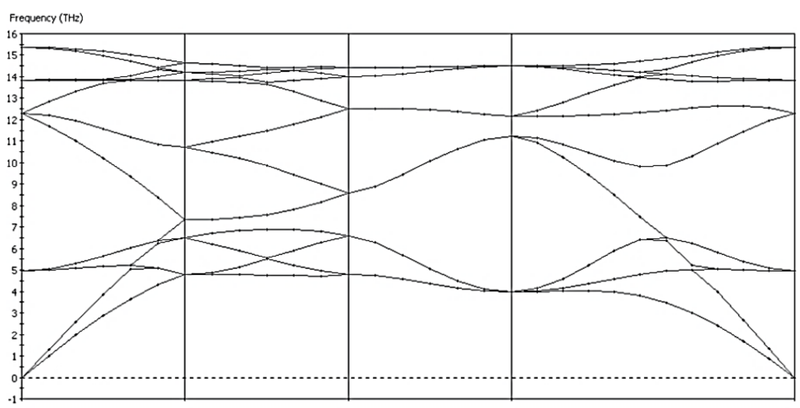


Si crystal structure

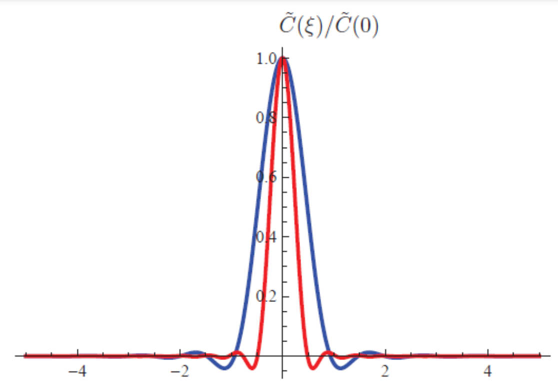

Journal for Multiscale Computational Engineering, 9 (6): 623–634 (2011)

DETERMINATION OF NONLOCAL CONSTITUTIVE EQUATIONS FROM PHONON DISPERSION RELATIONS

Olaf Weckner[1,*] & *Stewart A. Silling*[2]



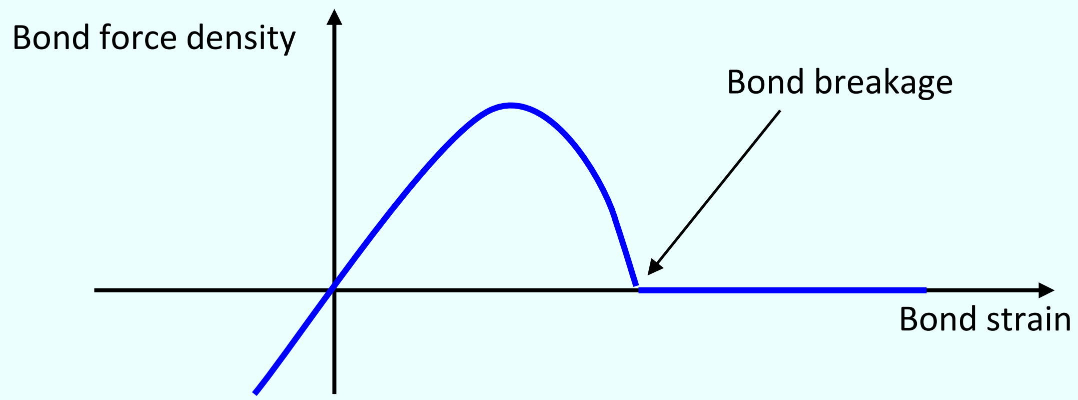
Si dispersion curves



Si peridynamic bond stiffness as a function of bond length

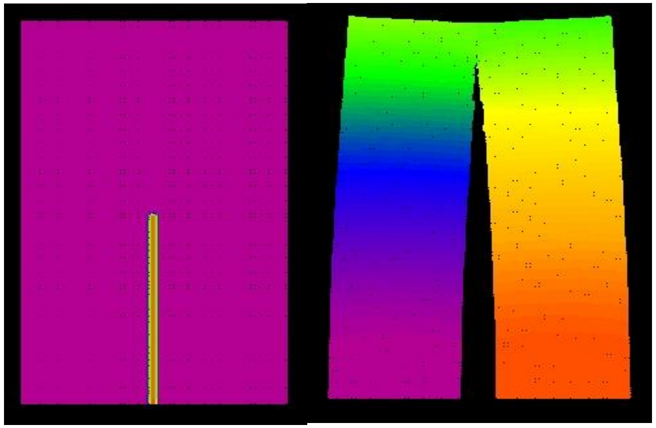
Damage due to bond breakage

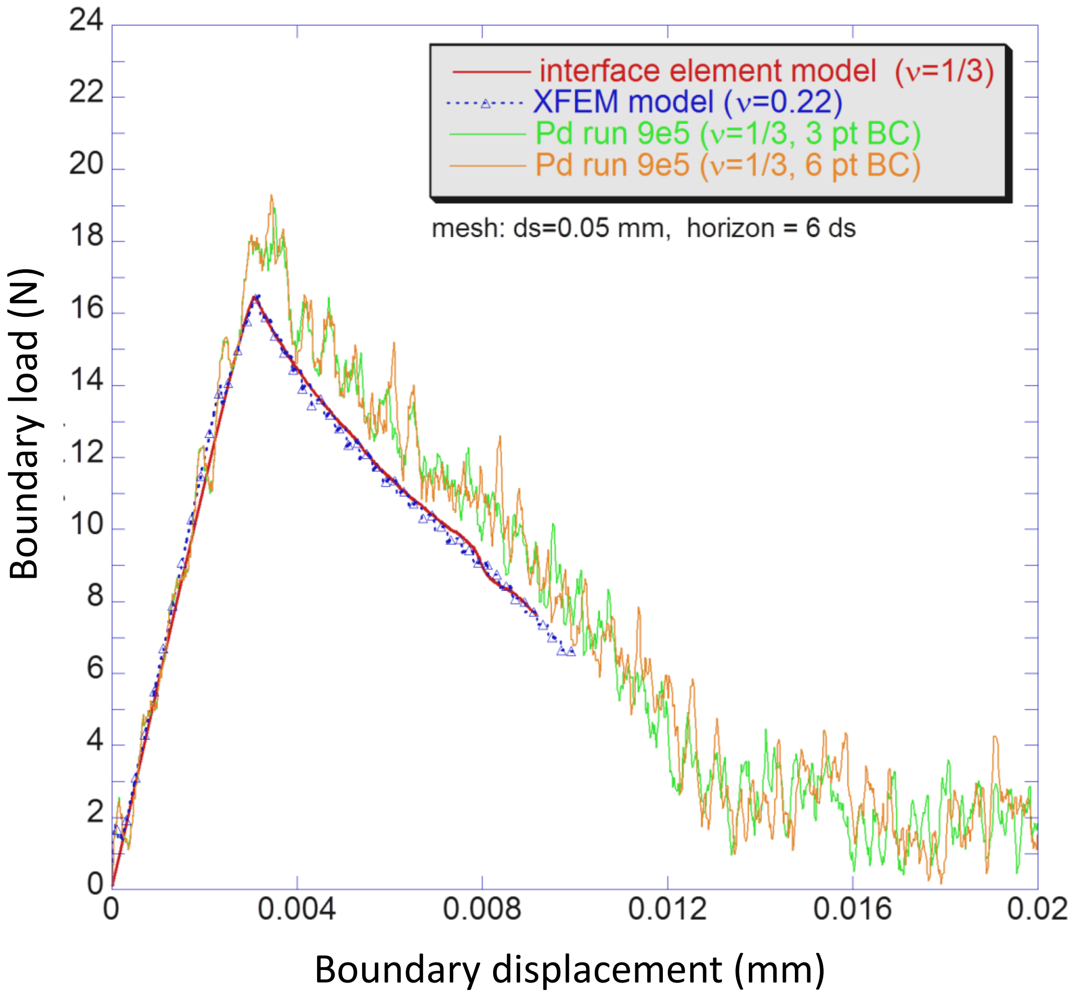
- Recall: each bond carries a force.
- Damage is implemented at the bond level.
  - Bonds break irreversibly according to some criterion.
  - Broken bonds carry no force.
- Examples of criteria:
  - Critical bond strain (brittle).
  - Hashin failure criterion (composites).
  - Gurson (ductile metals).



Critical bond strain damage model

Peridynamics gives similar answers to XFEM and cohesive elements*

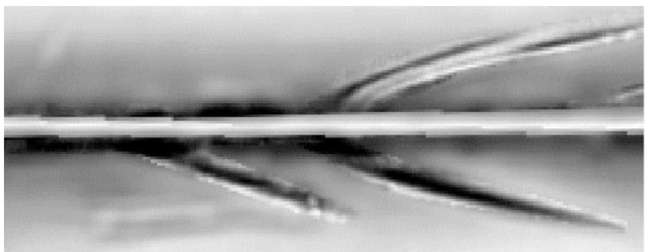




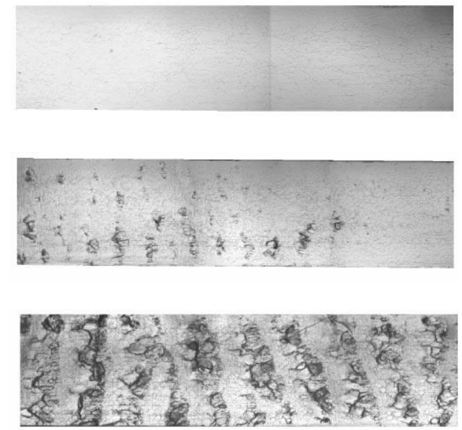
*SS and Jim Cox

Dynamic fracture in PMMA

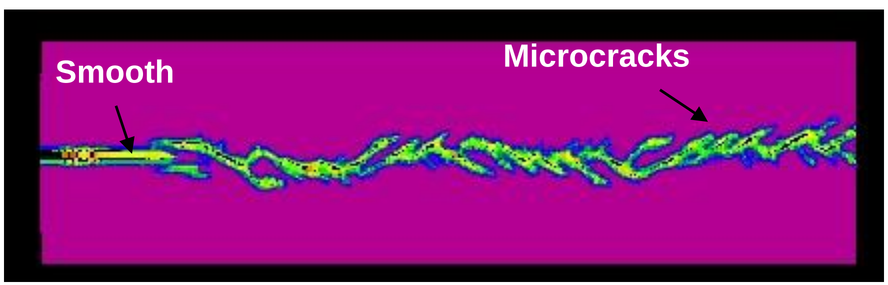
- Peridynamic simulation shows crack surface features related to fracture instability.
- These are difficult to reproduce with standard methods.



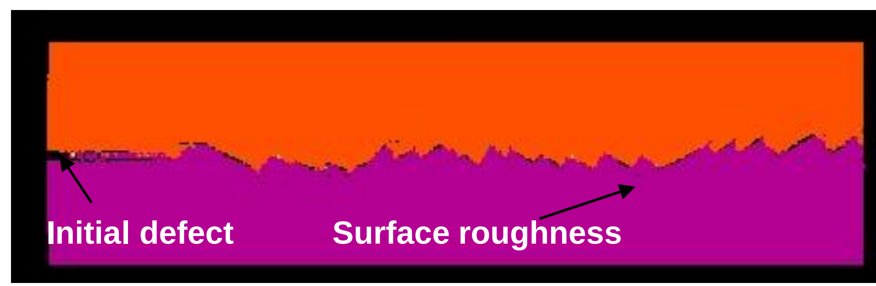
Microbranching



Mirror-mist-hackle transition*



EMU damage

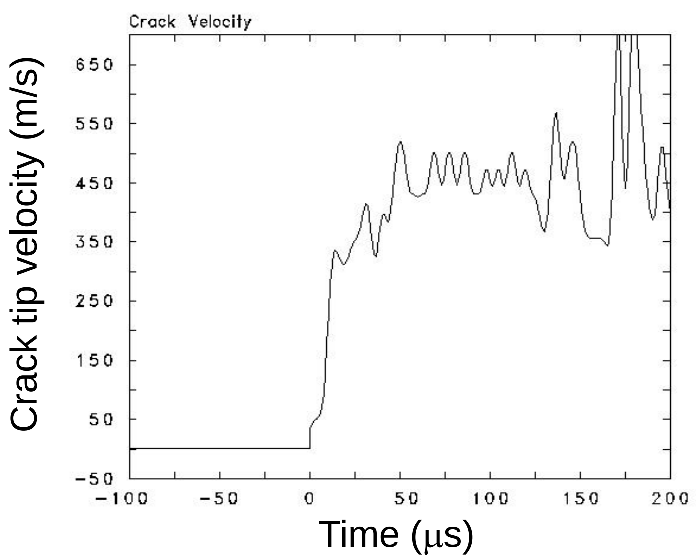


EMU crack surfaces

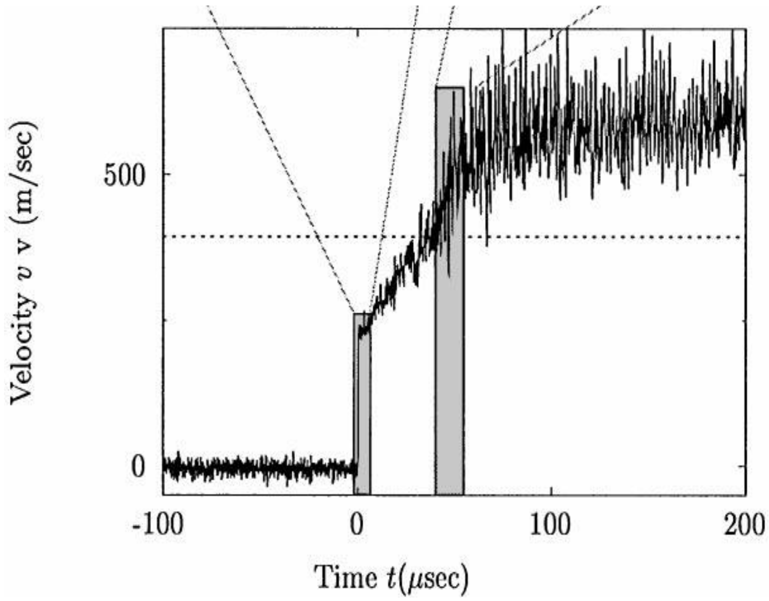
* J. Fineberg & M. Marder, *Physics Reports* 313 (1999) 1-108

Dynamic fracture in PMMA, ctd: Crack tip velocity

- Simulation reproduces the main features of dynamic crack velocity history.



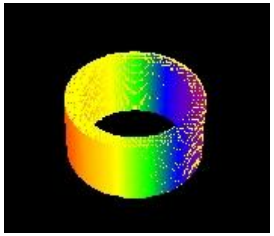
EMU



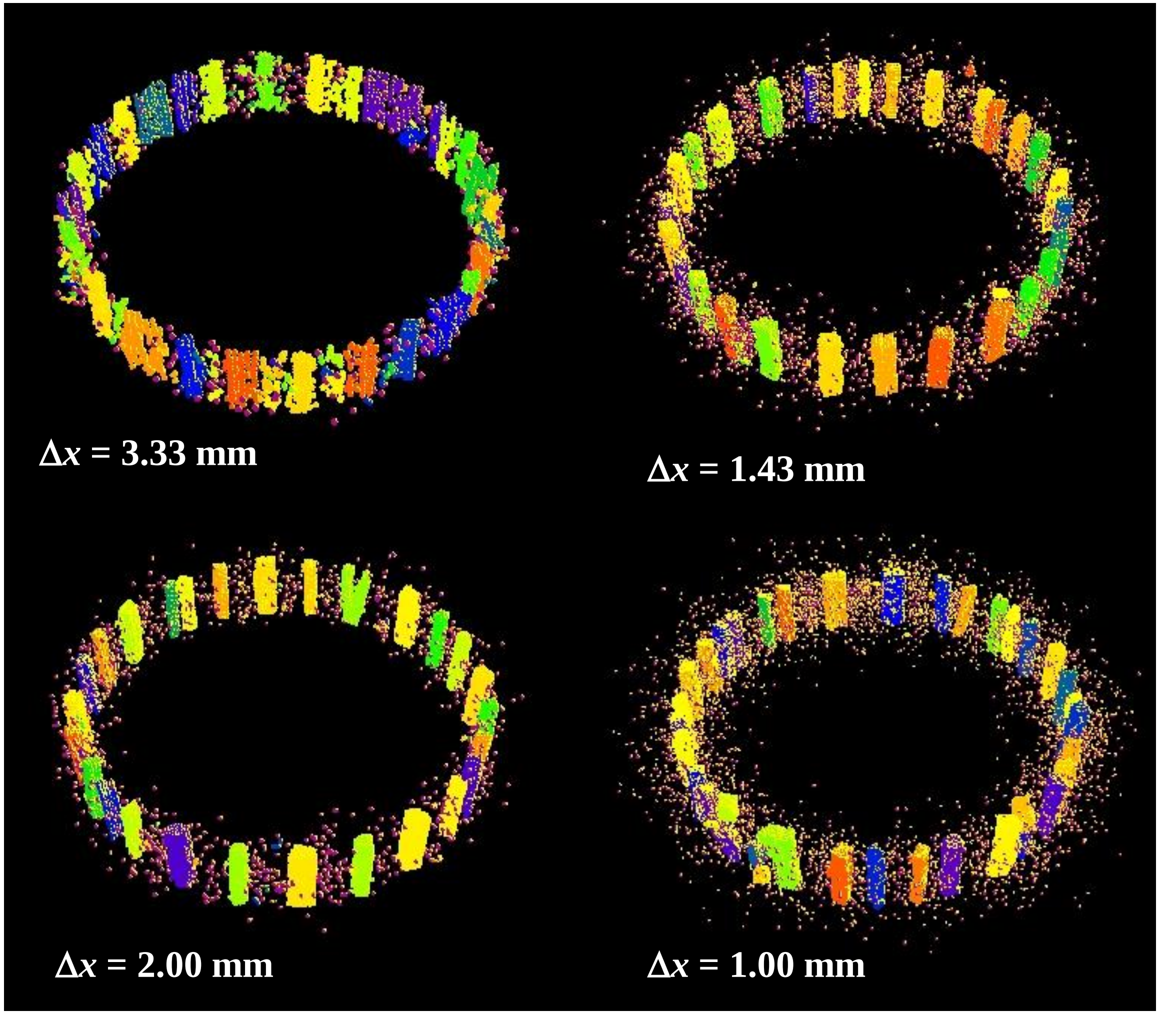
Experiment*

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

Fragmentation is not strongly dependent on mesh spacing



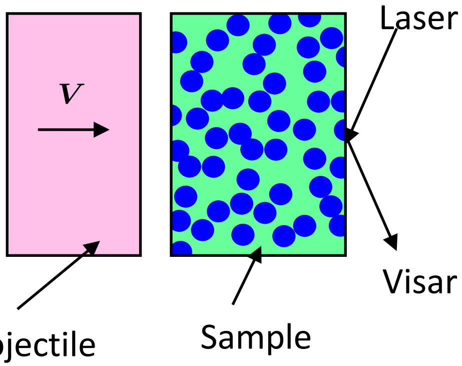
Brittle ring with initial radial velocity

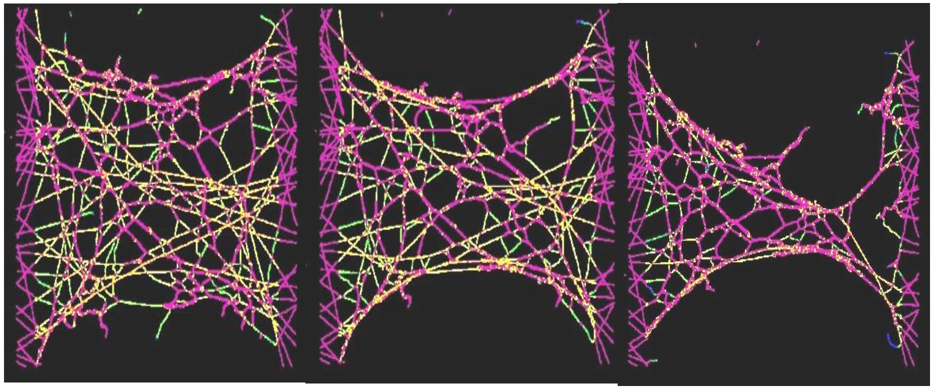


$$\delta = 3\Delta x$$

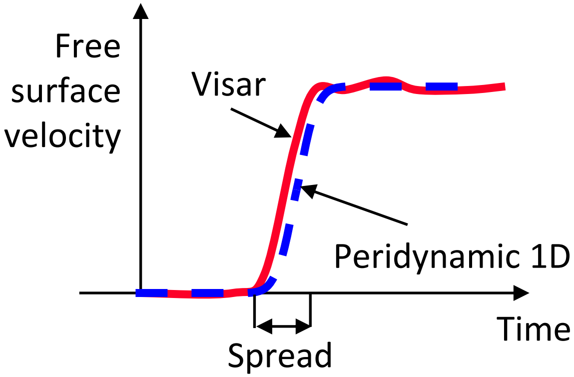
Importance of nonlocality

- Peridynamics is consistent with all laws of classical physics.
- It uses nonlocal interactions between material points.
  - The Cauchy theory is local.
  - Locality is often mistakenly assumed to be a law of physics.
- Molecular scale, nanoscale interactions are always nonlocal.
- Complex fluids are nonlocal.
- Any heterogeneous medium is nonlocal.
- Any discretized model of the local equations is nonlocal.





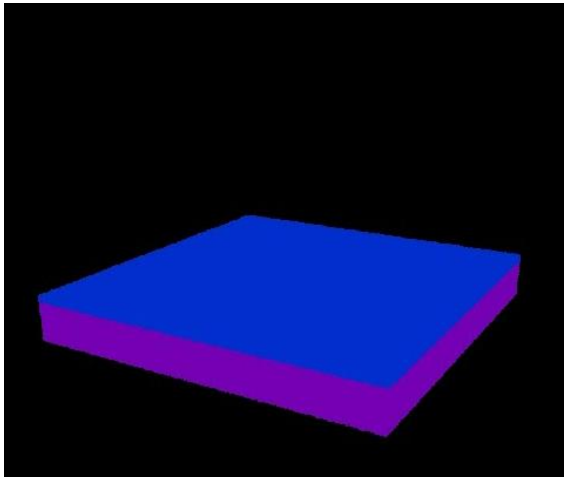
Peridynamic model of a nanofiber membrane
(F. Bobaru, Univ. of Nebraska)



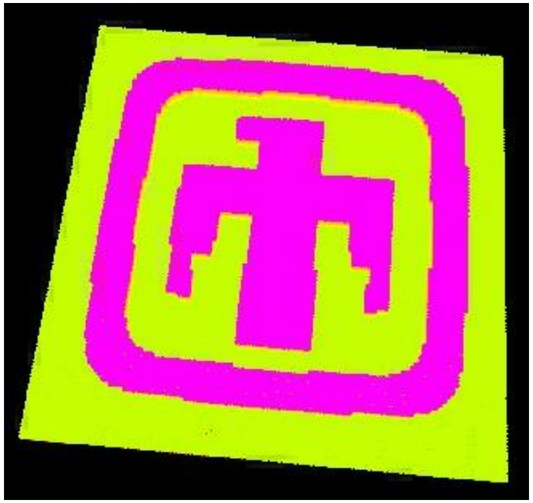
Local model would predict zero spread.

Method reveals subtleties in the mechanics of thin structures

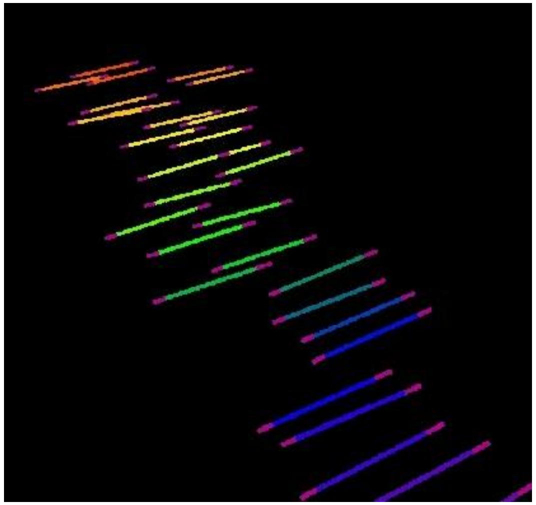
- Autonomous crack growth and long-range forces are crucial.



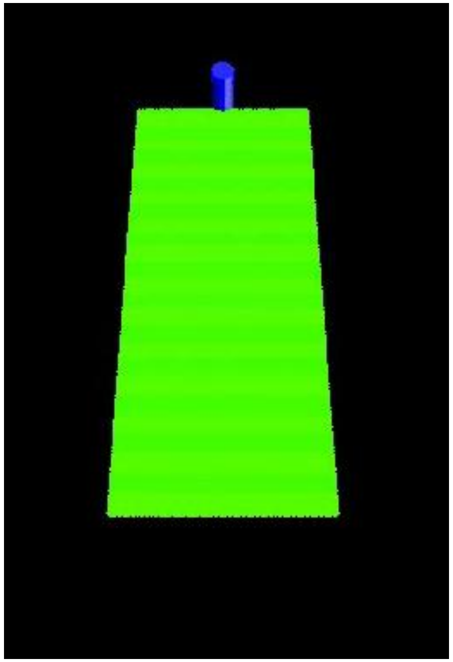
Membrane decohesion



Aging



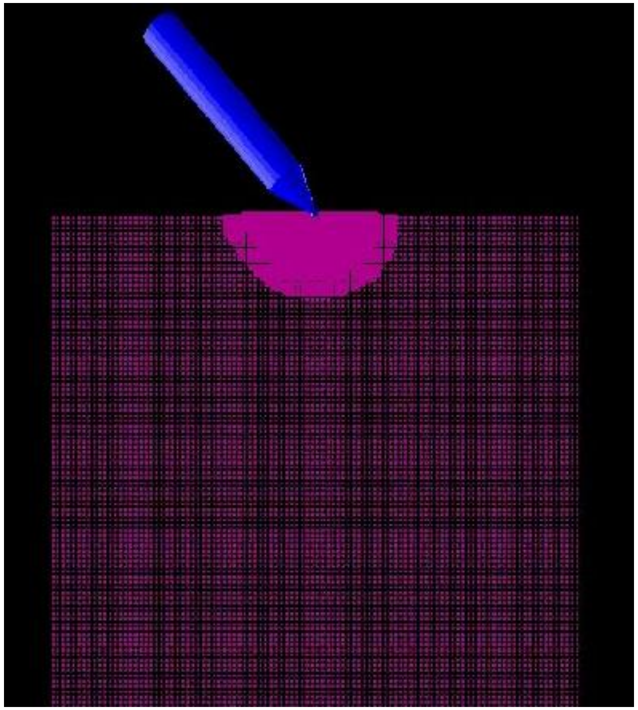
Self assembly



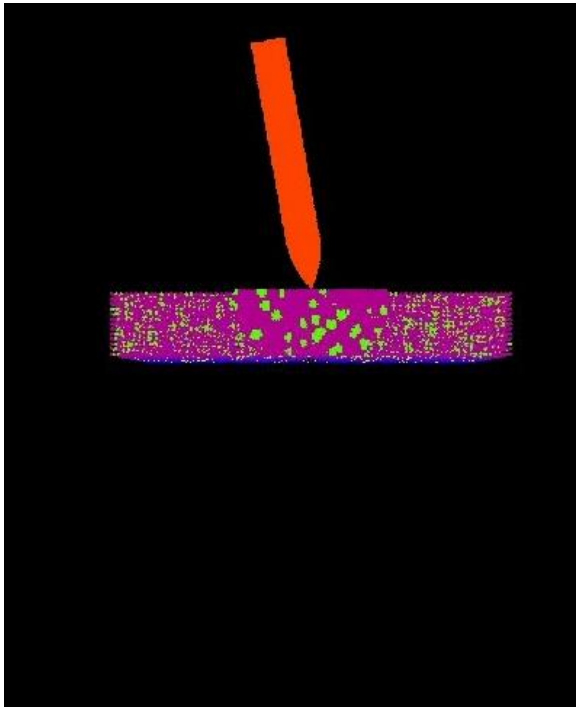
Oscillatory crack path

Examples: Impact and penetration (JMP)

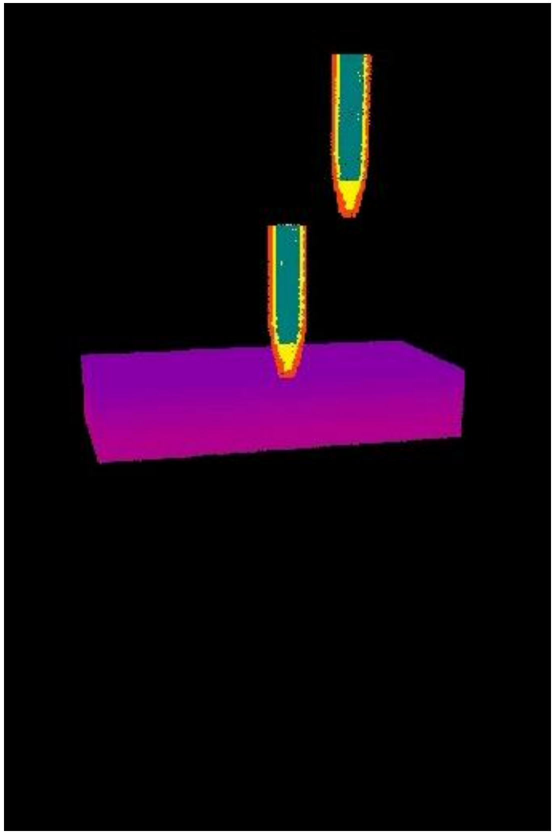
VIDEOS



Ricochet from heterogeneous target



Tail slap in a deformable penetrator

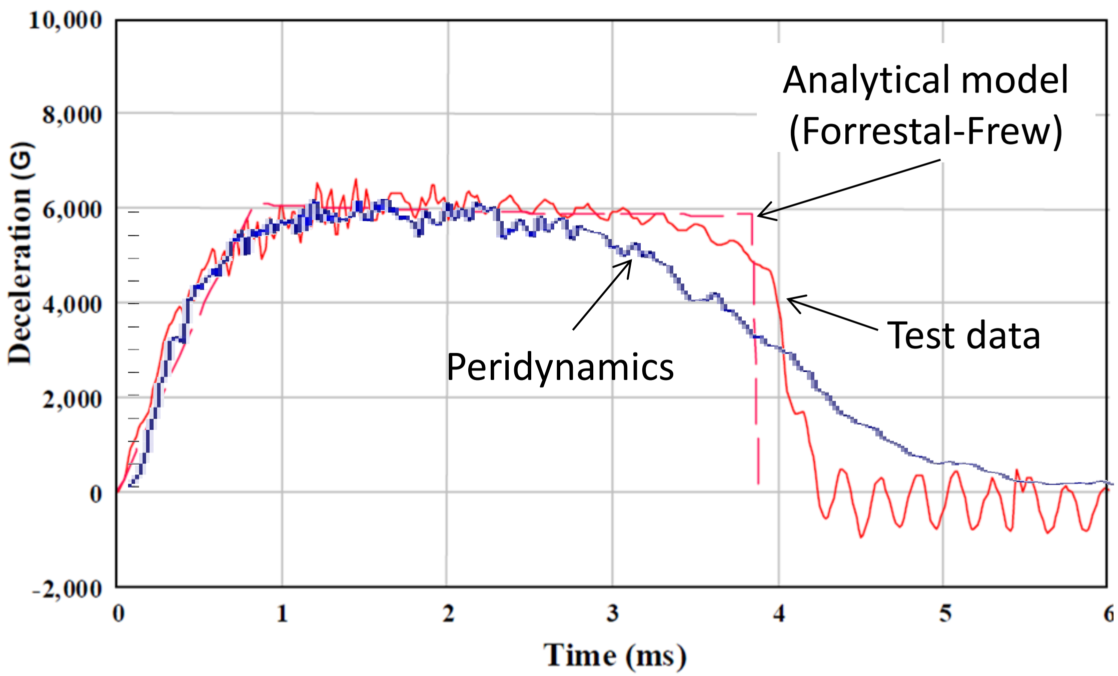


Small arms multihit

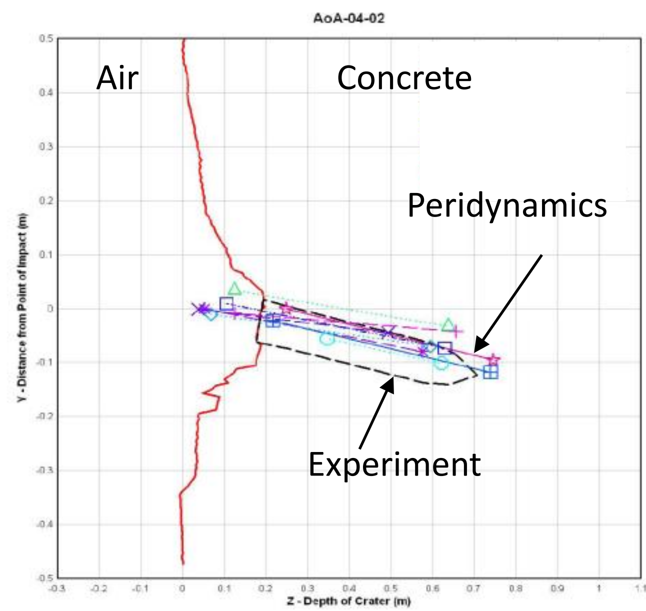
Earth penetrating munitions

- Peridynamic simulations have been validated extensively under the JMP.
- Examples:

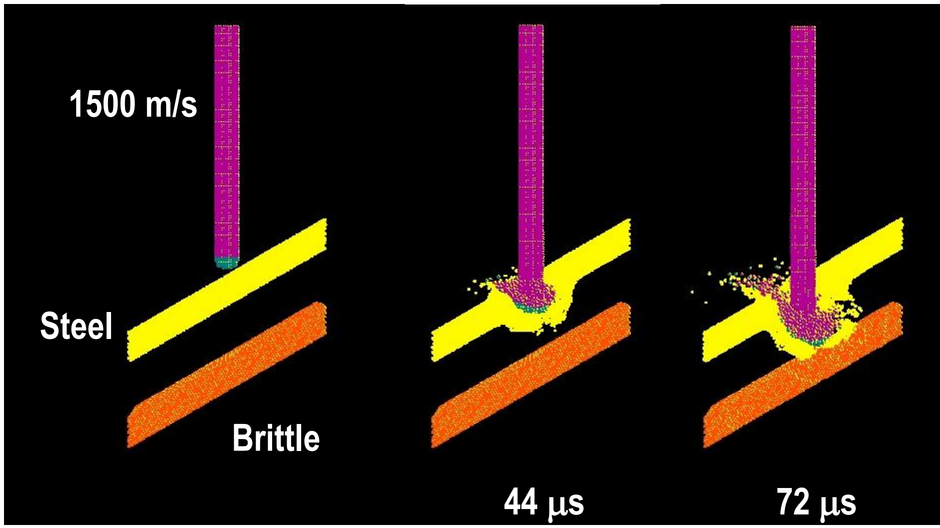
On-board accelerometer data vs. model

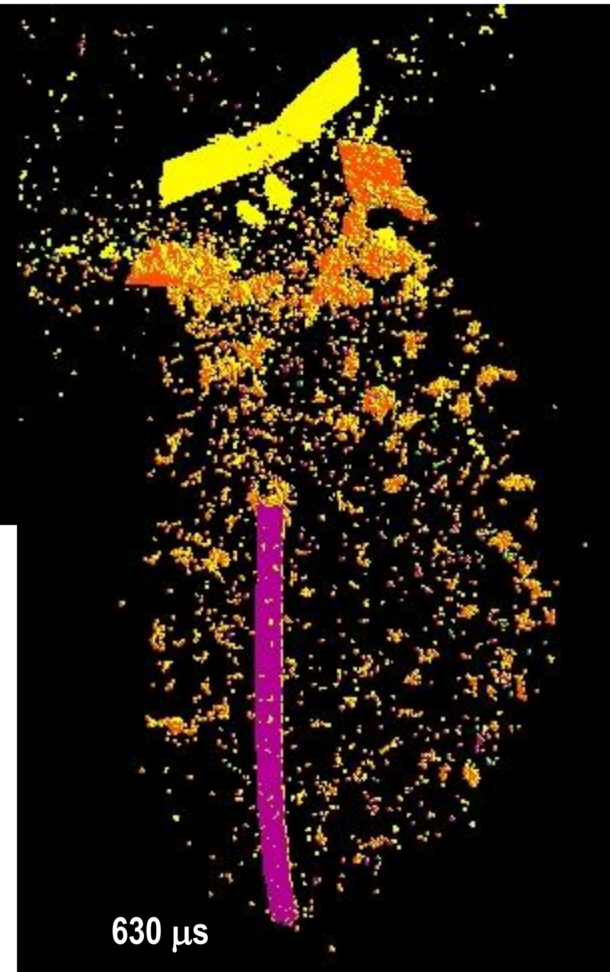


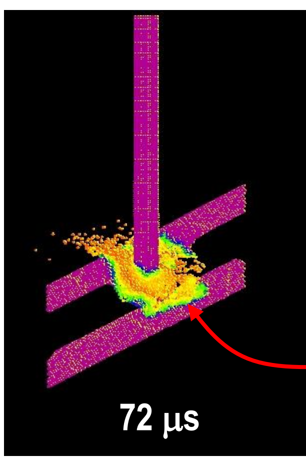
Final position of penetrator
(true prediction)



Armor/anti-armor:
Long rod penetrator & BAD







Colors indicate damage

Rear target is damaged before rod arrives

Some key theoretical milestones

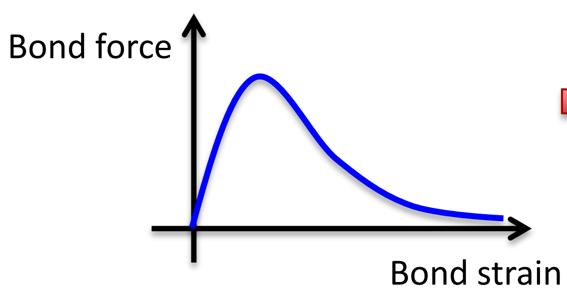
- PD equations are well posed (Du, Gunzburger, Lehoucq, & Zhou, 2013).
- PD equations can be derived from statistical mechanics (Lehoucq & Sears).

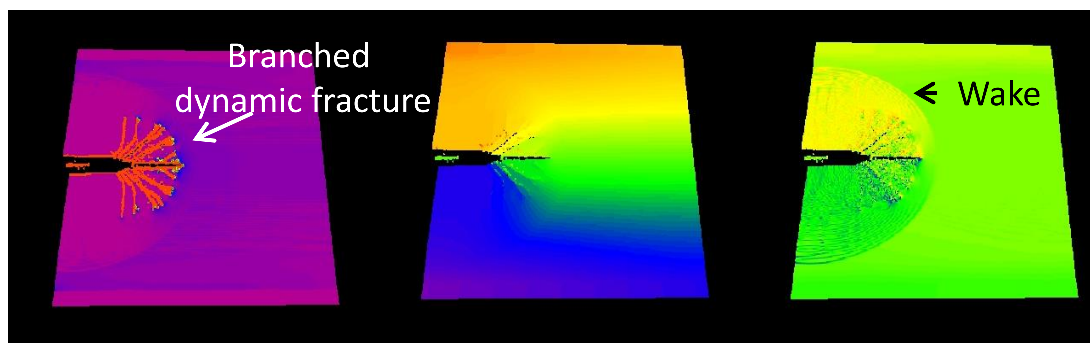
$$\frac{\partial}{\partial t}\langle \alpha \rangle = \left\langle \sum_i \frac{\partial \alpha}{\partial \mathbf{x}_i^\mu}\mathbf{v}_i^\mu \right\rangle - \left\langle \sum_i \frac{\partial \alpha}{\partial \mathbf{p}_i^\mu}\frac{\partial U}{\partial \mathbf{x}_i^\mu}\right\rangle$$

$$\frac{\partial}{\partial t}\boldsymbol{\pi}^\nu + \frac{\partial}{\partial \mathbf{x}^\mu}(\mathbf{v}^\mu\boldsymbol{\pi}^\nu) = \frac{\partial}{\partial \mathbf{x}^\mu}\boldsymbol{\sigma}_K^{\mu\nu} + \int_{\mathbb{R}^3}[\mathbf{T}^\nu(\mathbf{x},\mathbf{x}') - \mathbf{T}^\nu(\mathbf{x}',\mathbf{x})]d\mathbf{x}'$$

- As $\delta \to 0$:
  - For a <u>convex</u> material, the solution to the PD equations converges that of the local PDEs (Emmrich & Weckner, 2007).
  - For a <u>nonconvex</u> material, it converges to a smooth field plus one or more dynamic Griffith cracks (Lipton, 2014).

Nonconvex strain energy

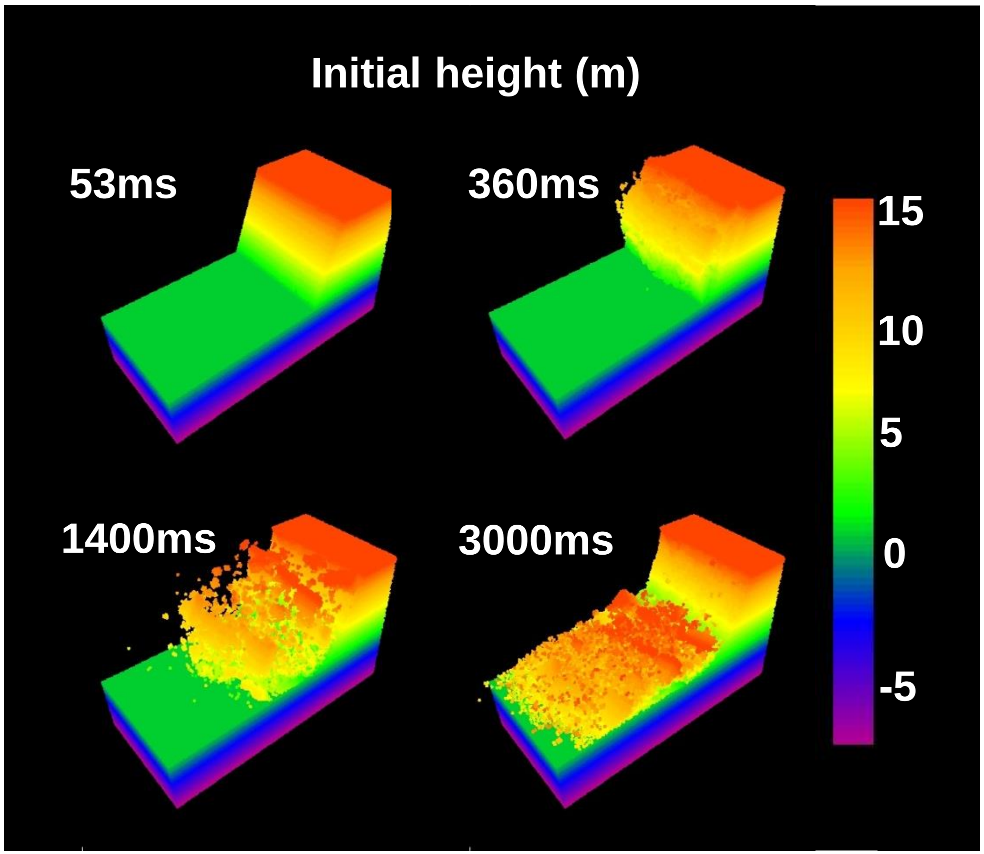




Bond strain Displacement Velocity

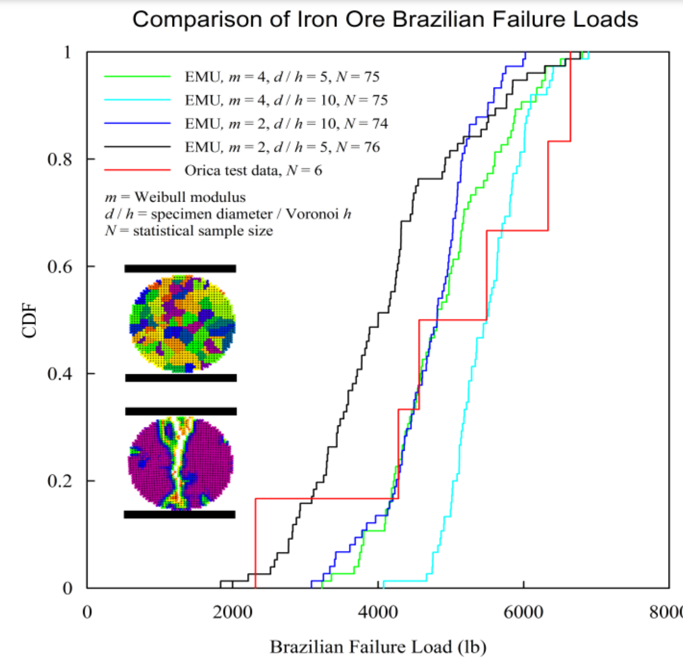
Success stories: Bench blasting

- Peridynamics correctly reproduces fragment size and velocity distributions in rock blasting (Orica USA Corp).



Predicted motion of fragments at four times

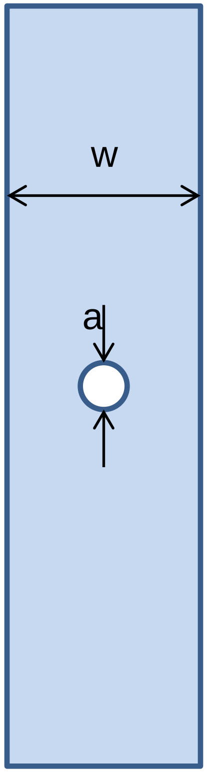
Actual bench blasting



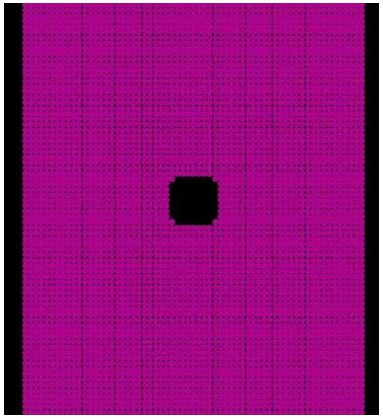
J. Bishop & J. Holland (1500)

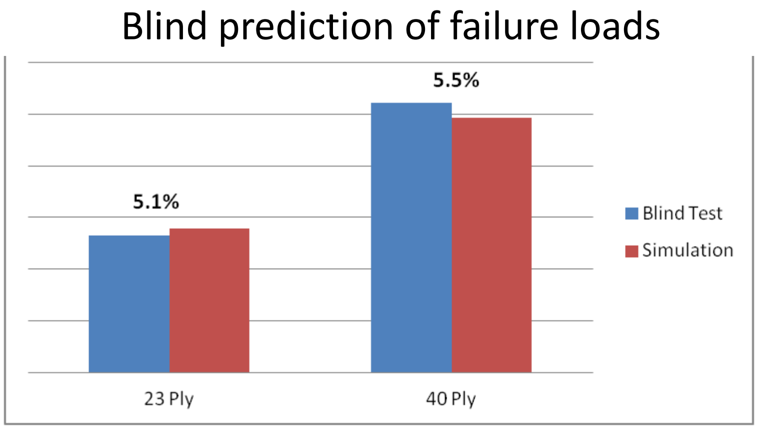
Success stories: Composite size effect

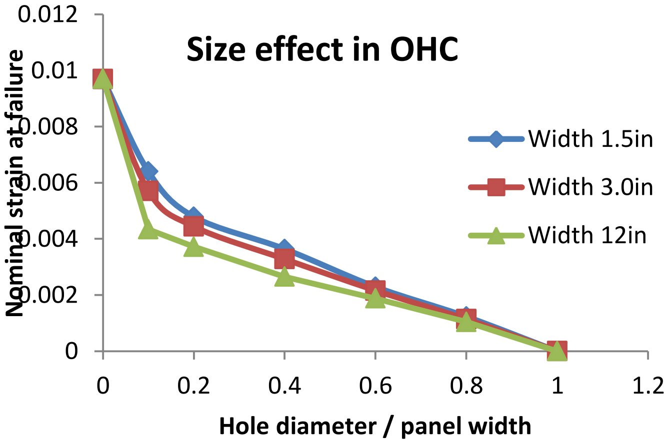
- Thanks to nonlocality, peridynamics correctly reproduces the size effect in composites: smaller samples are stronger (Boeing).



VIDEO

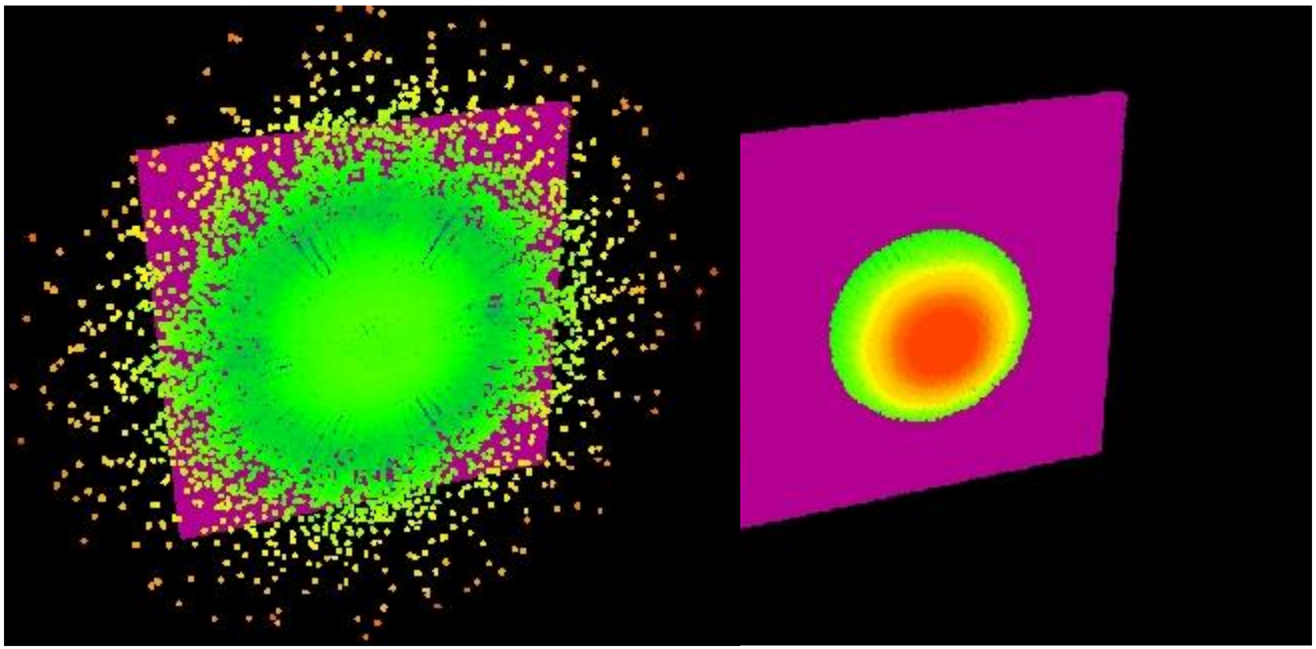






Success stories: Bird strike

- Bird simulant (gelatin) vs. heavy plate
- A material model that includes Eulerian fluid response and Lagrangian bond forces helps reduce the “spray” that is sometimes seen with SPH.



PD – Fluid only

PD – Fluid + bond forces

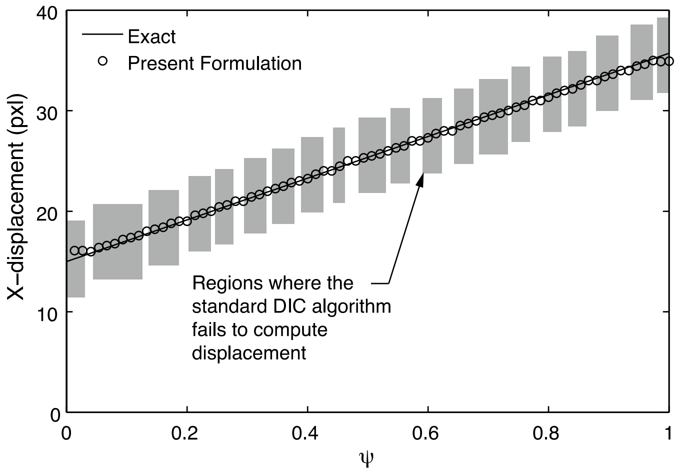
Test - LG 997

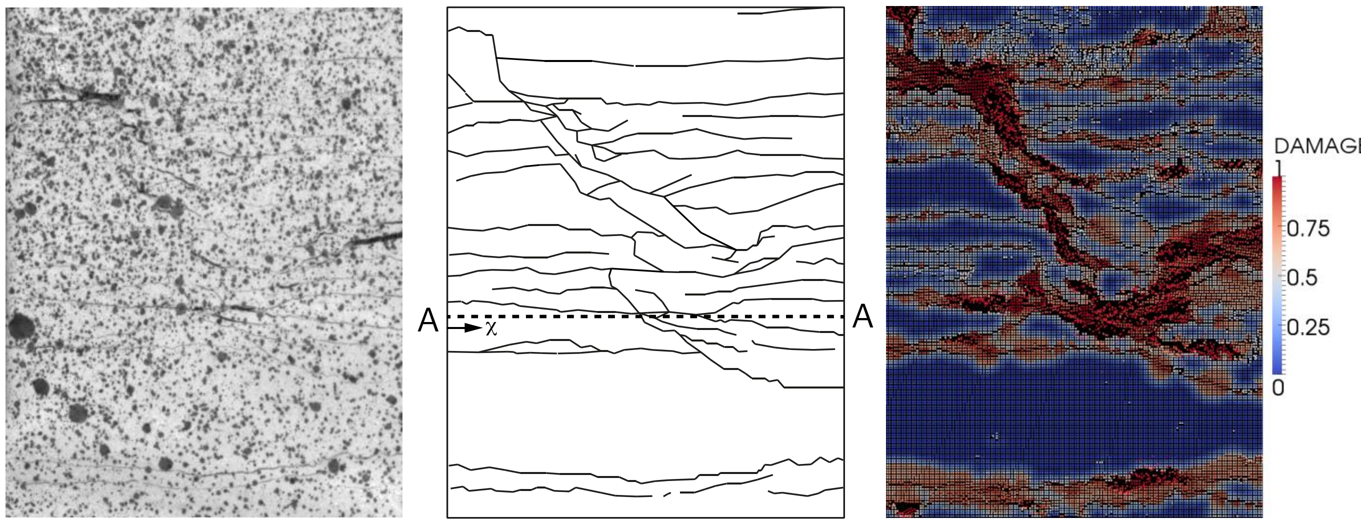
SPH

Olivares, NIS Document 09-039 (2010)

Success stories:
Peridynamics-Based Digital Image Correlation*

- Capable of resolving fragmentation (this is not possible with other methods)
- Near-crack strain is orders of magnitude more accurate



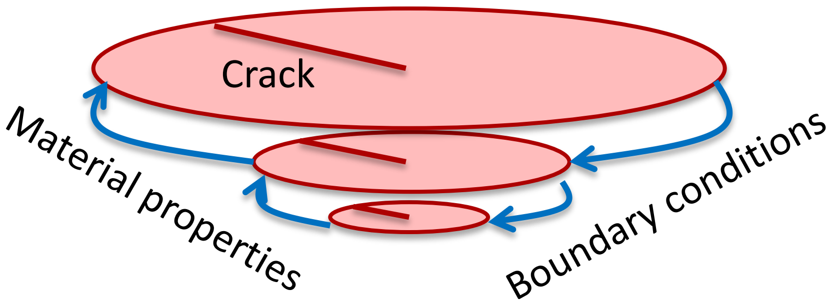


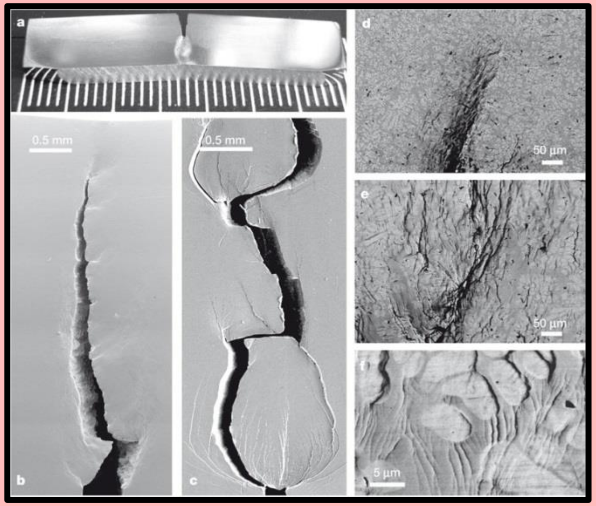
Digital Image Fracture Network Peridynamics Damage

*Dan Turner

Multiscale peridynamics helps to reveal the structure of brittle cracks

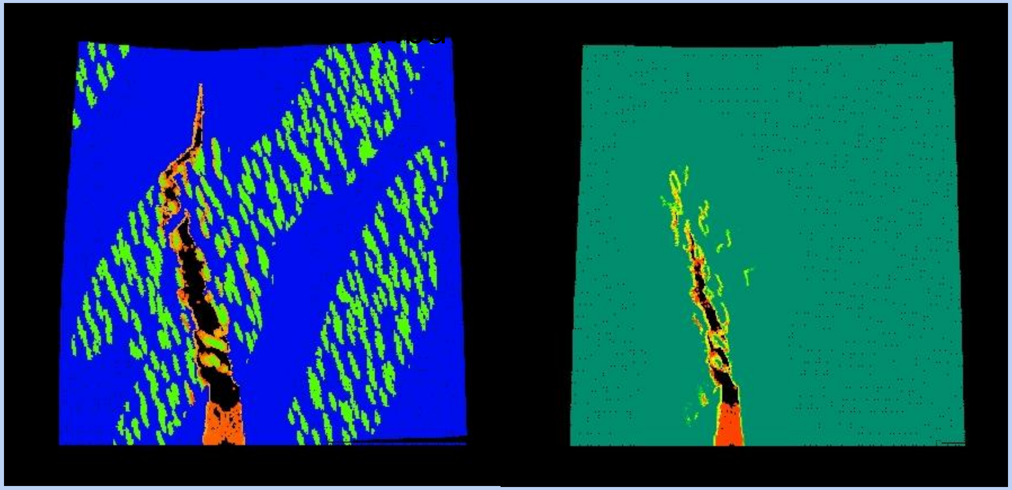
- Material design requires understanding of how morphology at multiple length scales affects strength.
- This is a key to material reliability.





Metallic glass fracture (Hofmann et al, Nature 2008)

Multiscale model of crack growth through a brittle material with



Peridynamics strengths and weaknesses

Strengths

- Offers potentially great generality in fracture modeling.
  - Cracks nucleate and grow spontaneously.
  - Cracks follow from the basic field equations.
- Any material model from the local theory can be used.
  - Plus a lot more!
- Compatible with molecular scale long-range forces.
  - MD is a special case.
  - Cauchy theory is a limiting case.
- Length scale can be exploited for multiscale modeling.

Weaknesses

- Slow due to many interactions.
  - Local-nonlocal coupling will help.
  - Need smarter integration methods.
- Surface effects
  - Correction methods are available, none totally satisfactory.
  - PALS material model will help solve this.
- Boundary conditions are different from the local theory.
- Particle discretization has known limitations.
  - FE methods are under development.

Thrust areas and needed research

- **Production software**
  - Unify Peridigm/Sierra/Emu
  - Address usability & interface issues
  - V&V
  - Material model library
- **Solvers and numerical methods**
  - SPH, kernel methods connection
  - Next gen platforms
  - Eulerian & ALE capability
- **Material/damage modeling**
  - Ductile failure
  - Continuum damage mechanics
  - Quasistatic material failure
  - Nonlocality: fundamental aspects
  - Digital image correlation (DIC)
  - Nonlocal deformation measures
- **Multiscale**
  - Scalable multiscale methods
  - Coarse graining
  - Atomistic-to-continuum coupling
  - General tool for material failure
- **Math and theory**
  - Boundary conditions
  - Quantify uncertainty esp. in fracture
  - Contact algorithms
  - Material stability
- **Multiphysics**
  - Math and numerics for multiphysics
  - Geological applications
  - Fluid-structure interaction
  - Diffusion, chemical reactions
  - Electromagnetic fields
  - Electronics & MEMS reliability
  - Friction