SAND2011-5650C

# Coarse Graining in Peridynamics

**Stewart Silling**

Multiphysics Simulation Technologies Department

Sandia National Laboratories
Albuquerque, New Mexico, USA

LAMMPS Users' Workshop 2011

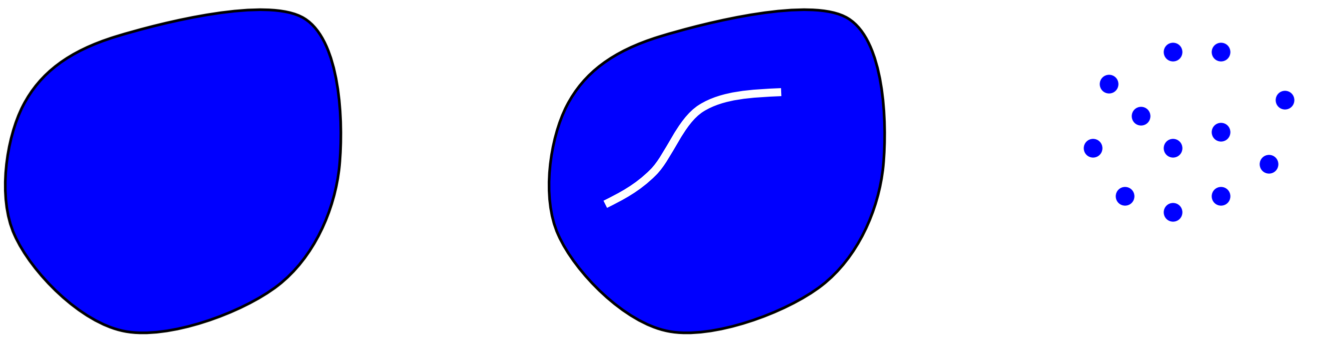
August 10, 2011

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.

Sandia National Laboratories

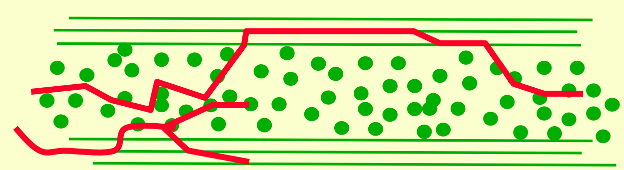
# Purpose of peridynamics

- To unify the mechanics of continuous and discontinuous media within a <u>consistent</u> modeling method.



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.



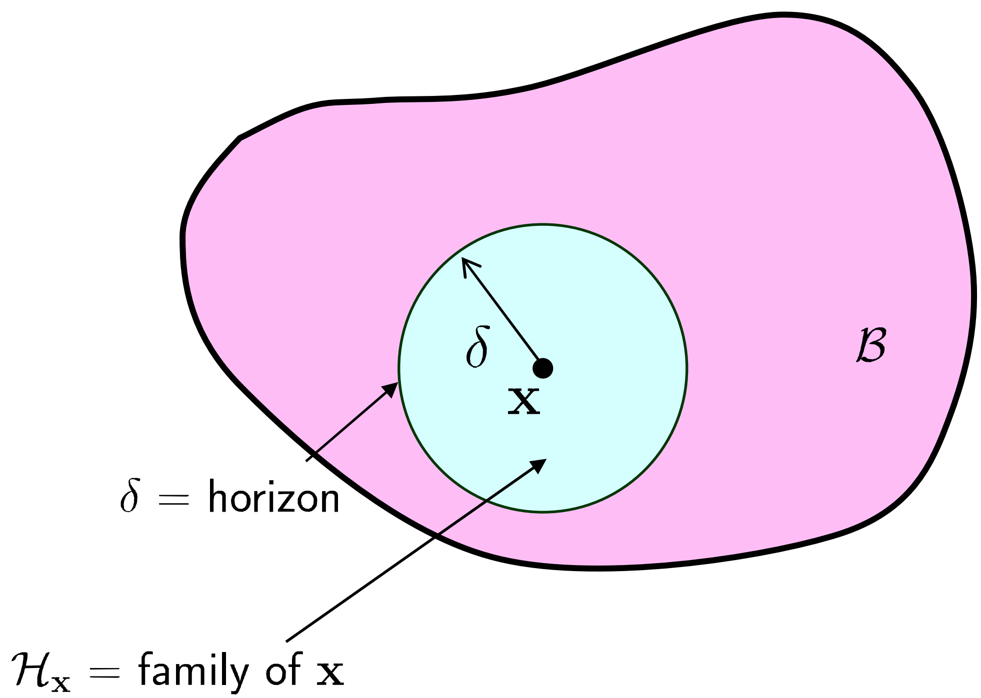
Complex crack path in a composite



Sandia National Laboratories

# Peridynamics basics: Horizon and family

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



# Peridynamics basics: Bonds and bond forces

- The vector from $\mathbf{x}$ to any point $\mathbf{q}$ in its family in the reference configuration is called a *bond*.

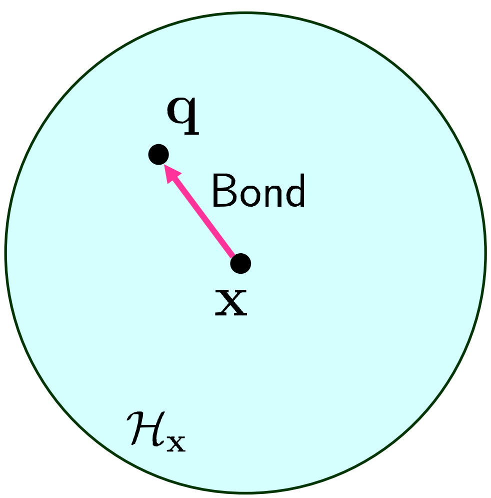
$$\boldsymbol{\xi} = \mathbf{q} - \mathbf{x}$$

- Each bond has a *pairwise force density* vector that is applied at both points:

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

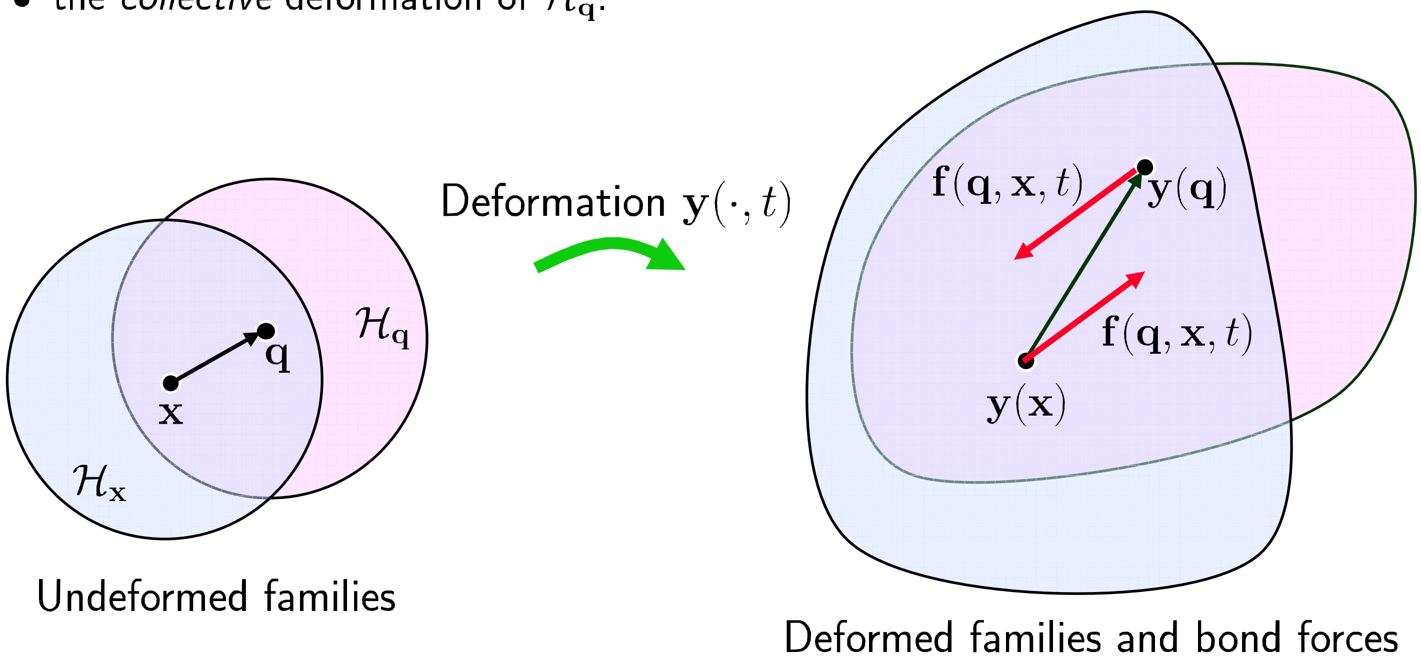
- Equation of motion:

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{q}, \mathbf{x}, t)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}, t).$$



# Peridynamics basics: Material modeling

- Each 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 $\mathcal{H}_{\mathbf{q}}$.



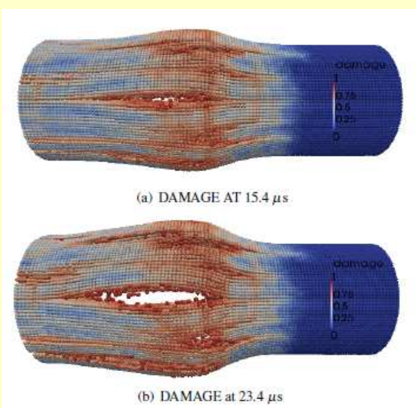
# EMU (and LAMMPS) numerical method

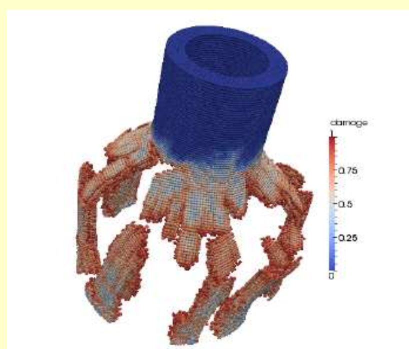
- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x},t)$$

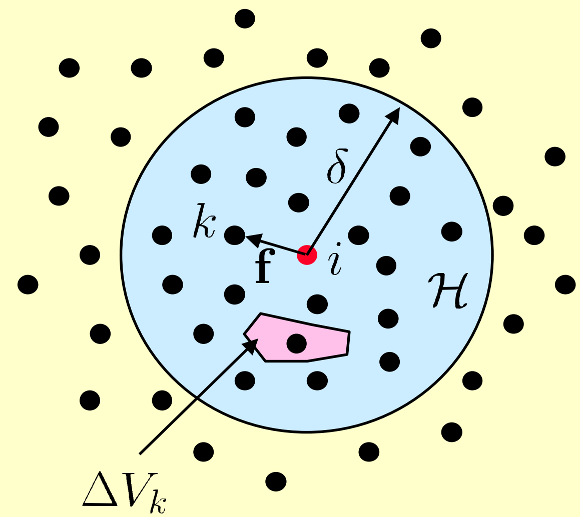
$$\downarrow$$

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



Method is also available in Sierra (D. Littlewood)




Discretized model in the reference configuration

# Linearized peridynamics

- General (nonlinear) equilibrium equation:

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

- Suppose $|\mathbf{u}| \ll \delta$ where $\mathbf{u}$ is the displacement field. Equilibrium equation becomes

$$\mathbf{L}(\mathbf{x}) = \int_{\mathcal{N}} \mathbf{C}(\mathbf{x}, \mathbf{q}) \big( \mathbf{u}(\mathbf{q}) - \mathbf{u}(\mathbf{x}) \big) \, dV_{\mathbf{q}}$$

  where $\mathbf{C}$ is the tensor-valued *micromodulus* function and $\mathcal{N}$ has twice the radius of $\mathcal{H}$.

- $\mathbf{C}$ can be derived from the material model.
- $\mathbf{C}$ has the following symmetry:

$$\mathbf{C}^T(\mathbf{x}, \mathbf{q}) = \mathbf{C}(\mathbf{q}, \mathbf{x}) \qquad \forall \mathbf{x}, \mathbf{q}.$$

- Linearized equilibrium equation is same as in Kunin's nonlocal theory (1983).

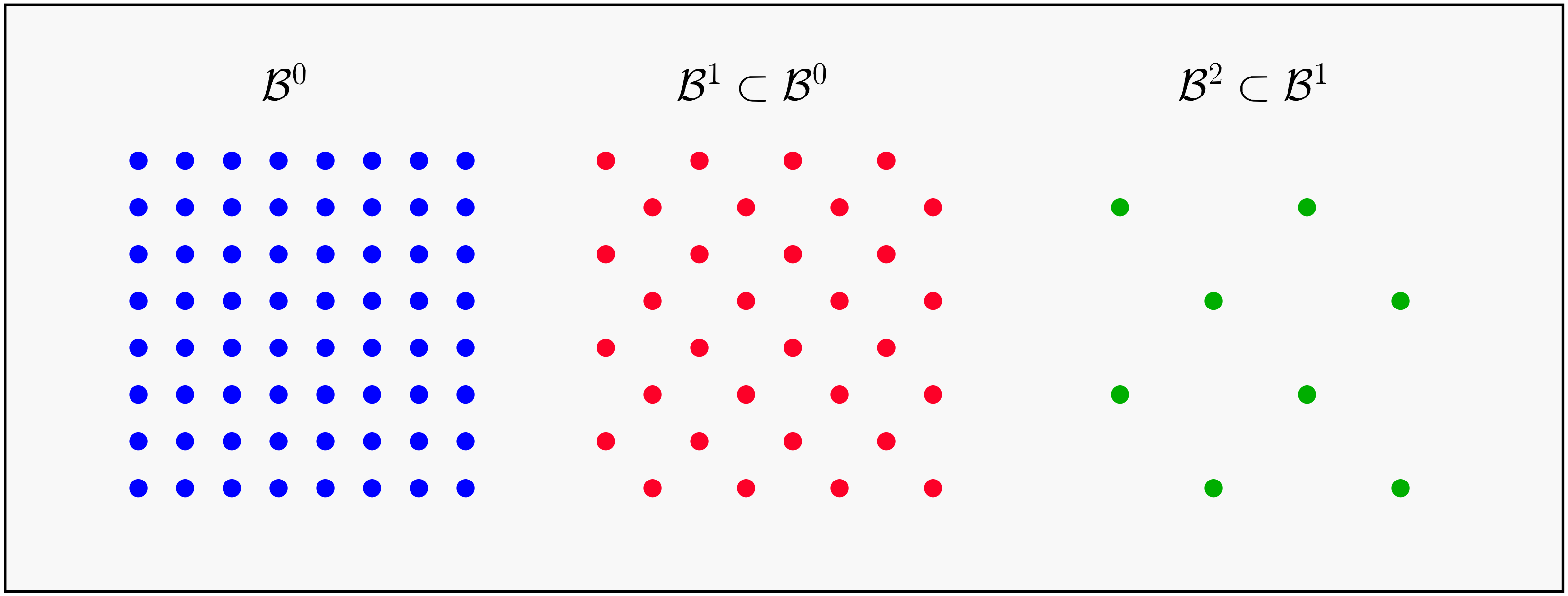
SS, Linearized theory of peridynamic states, J. Elast. (2010)



Sandia National Laboratories

# Coarse-graining: Reduce the number of degrees of freedom

- Start with a detailed "level 0" body $\mathcal{B}^0$.
- Level 0 can be either continuous or discrete.
- Choose a sequence of $M$ coarsened levels: $\mathcal{B}^M \subset \mathcal{B}^{M-1} \subset \cdots \subset \mathcal{B}^1 \subset \mathcal{B}^0$.

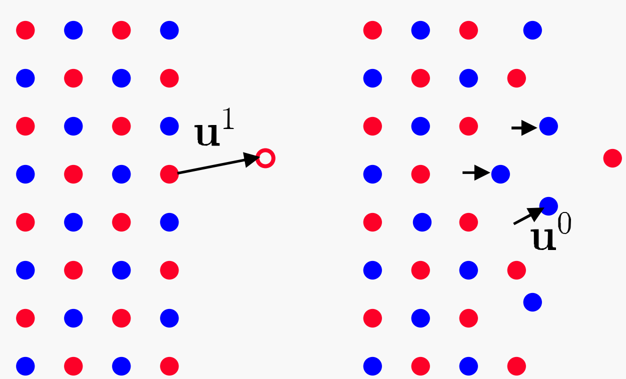





Sandia National Laboratories

# Each level's displacements are determined by the next higher level

- Assumption: If $\mathbf{u}^M$ is prescribed, the excluded DOFs in $\mathbf{u}^{M-1}$ "float" (change their equilibrium displacements).




$\mathcal{B}^0$ re-equilibrates in response to prescribed displacements in $\mathcal{B}^1$

- Let $\mathbf{S}^M$ be the solution operator that gives $\mathbf{u}^{M-1}$ in terms of $\mathbf{u}^M$:

$$\mathbf{u}^{M-1}(\mathbf{x}) = \int_{\mathcal{B}^M} \mathbf{S}^M(\mathbf{x}, \mathbf{q})\mathbf{u}^M(\mathbf{q})\, dV_{\mathbf{q}}.$$



Sandia National Laboratories

# Each level has the same mathematical structure

- Can express the forces in level $M$ in terms only of its own displacements:

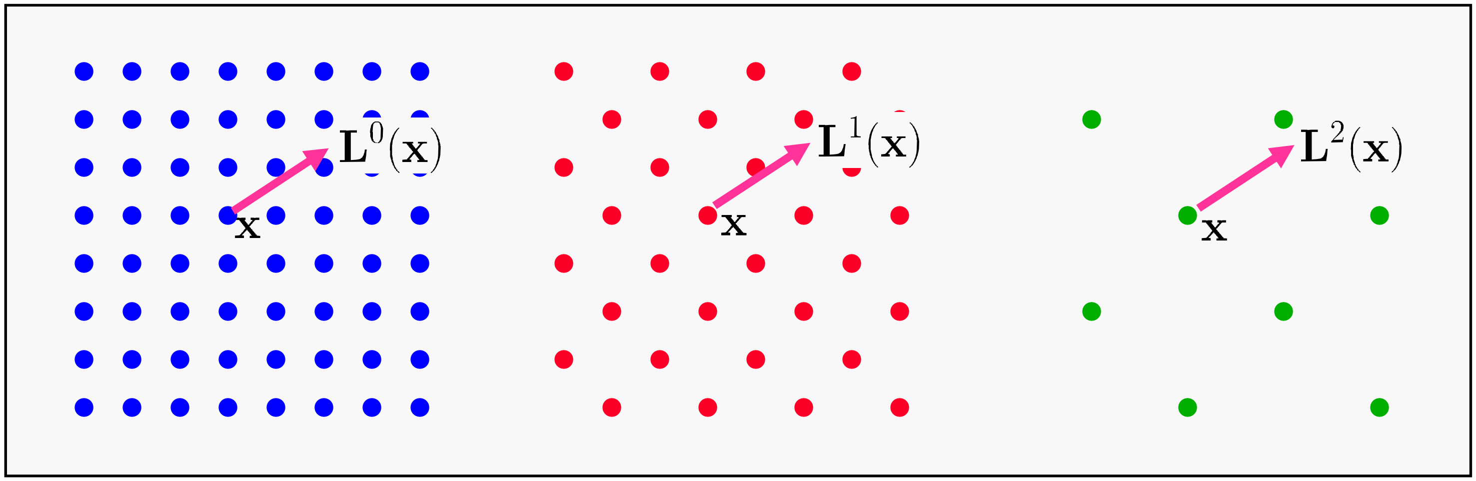
$$\mathbf{L}^M(\mathbf{x}) = \int_{\mathcal{B}^M} \mathbf{C}^M(\mathbf{x},\mathbf{q})(\mathbf{u}^M(\mathbf{q}) - \mathbf{u}^M(\mathbf{x}))\, dV_{\mathbf{q}}$$

where the level $M$ micromodulus is found from

$$\mathbf{C}^M(\mathbf{x},\mathbf{q}) = \int_{\mathcal{B}^{M-1}} \mathbf{C}^{M-1}(\mathbf{x},\mathbf{p})\mathbf{S}^M(\mathbf{p},\mathbf{q})\, dV_{\mathbf{p}}.$$

- If loads or displacements in $\mathcal{B}^M$ are prescribed, the forces are invariant through the levels:

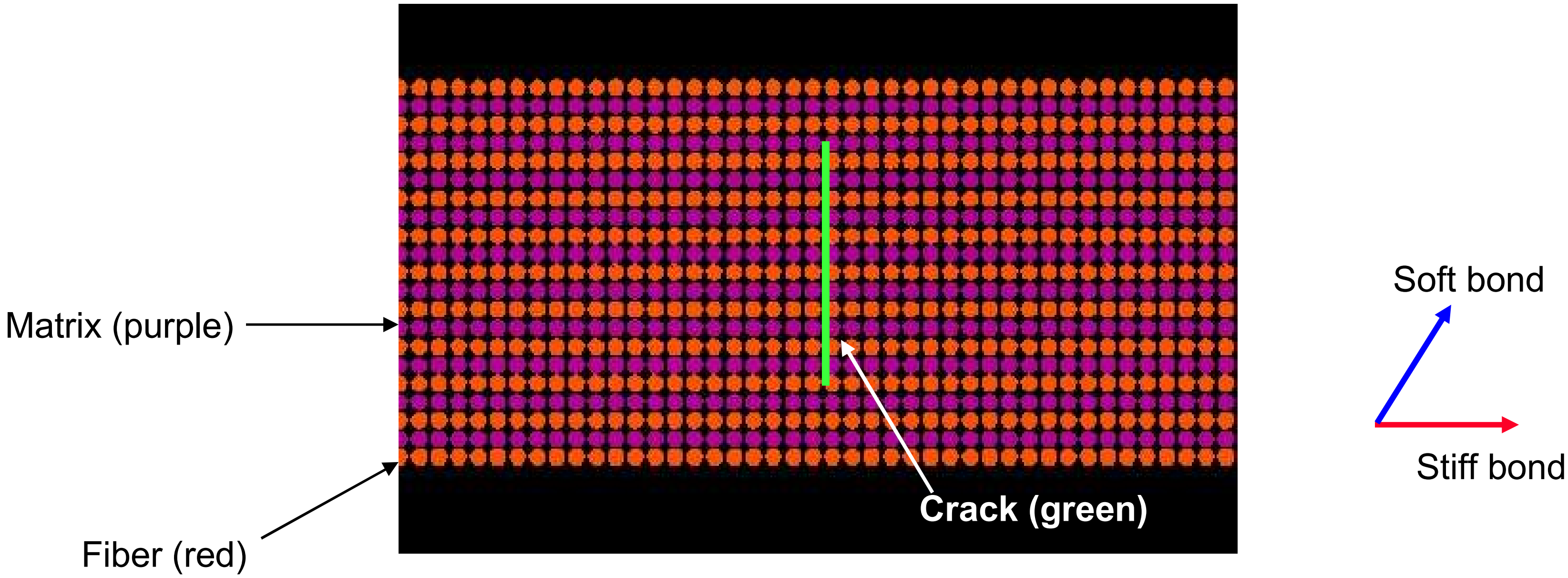
$$\mathbf{L}^0 = \mathbf{L}^1 = \cdots = \mathbf{L}^{M-1} = \mathbf{L}^M$$





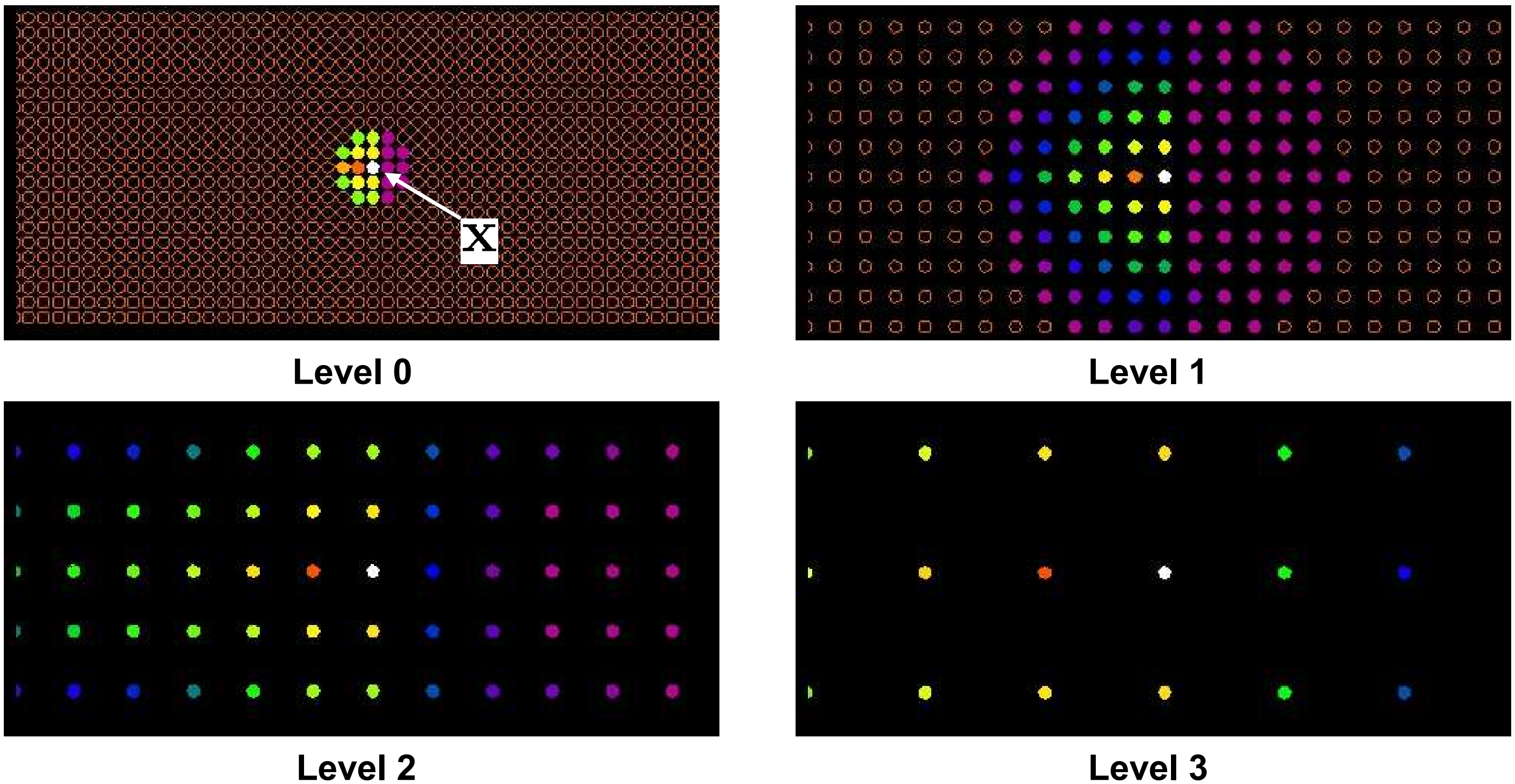

Sandia National Laboratories

# Example: Composite with a crack




- Crack is inserted into the level 0 model: bonds crossing the crack are ignored.
- $\mathbf{C}^0(\mathbf{x}, \mathbf{q}) = \mathbf{0}$ whenever $\mathbf{x}$ and $\mathbf{q}$ are on opposite sides of the crack.

# Composite bar with defect: Coarsened micromodulus

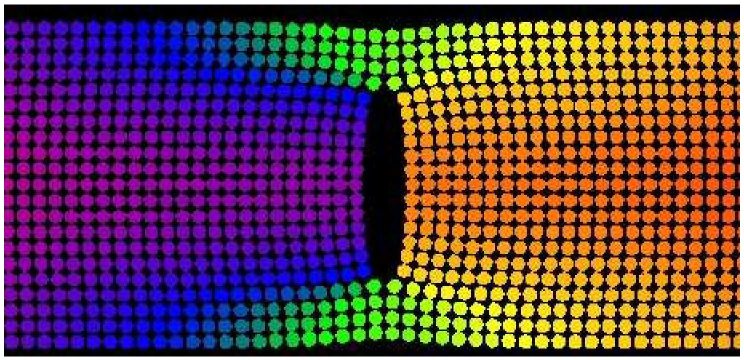



- Figures show contours of $\log |\mathbf{C}^m(\mathbf{x}, \cdot)|$ where $\mathbf{x}$ is the white dot, $m = 0, 1, 2, 3$.
- This $\mathbf{x}$ is near the crack surface.
- The effect of the crack on the micromodulus is visible in all levels.

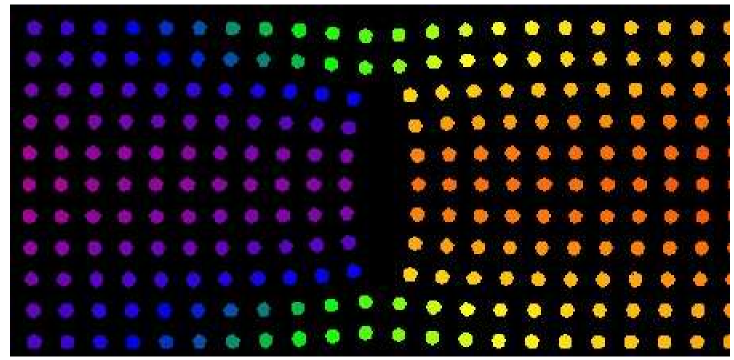


Sandia National Laboratories

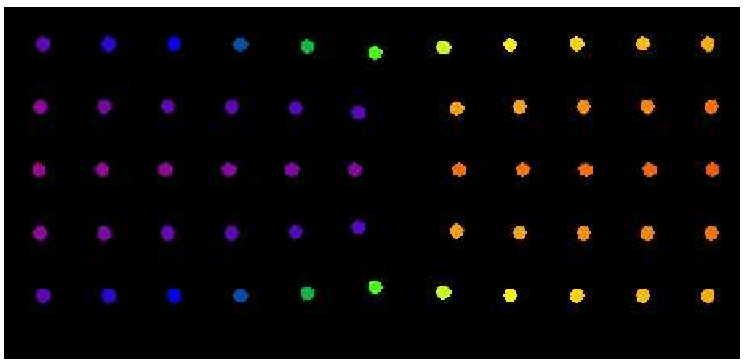
# Composite bar with defect: Displacements



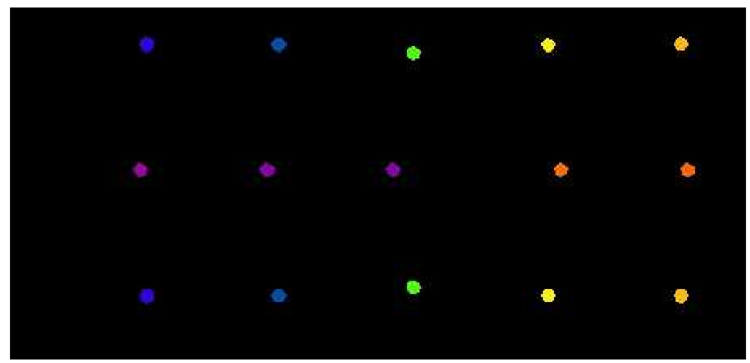
Level 0



Level 1



Level 2



Level 3

- The same boundary value problem is solved at each level $m$, where $m = 0, 1, 2, 3$.
- Figures show contours of $u_1^m$.
- Displacements at all nodes and total force on ends agree between levels.

# Discussion

- Any system of particles interacting through a multibody potential can be represented as a peridynamic body (i.e., level 0).
    - Need to re-linearize when displacements become large.

- Coarse graining method accomplishes the following:
    - Two-way coupling (coarsening + refinement): consistent multiscale method.
    - Contribution of features at smaller length scales are incorporated into larger length scales.

- Many issues remain regarding how to make the method efficient.

SS, A coasening method for linear peridynamics, Int. J. Multiscale Computation Engineering (to appear).

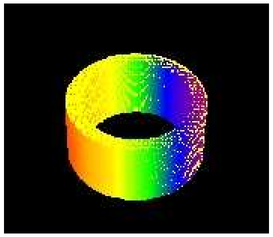


Sandia National Laboratories

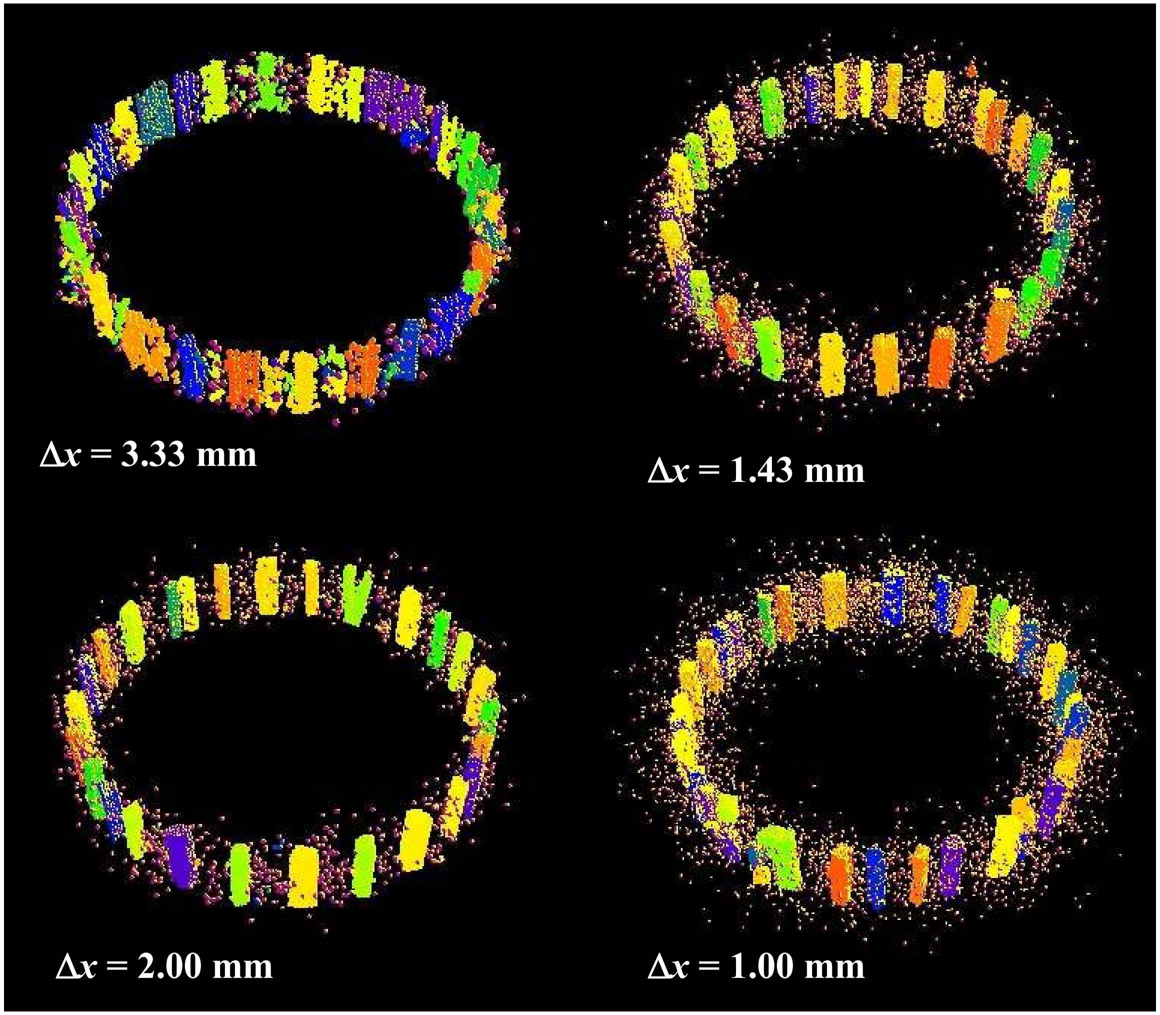
# Backup slides

# Typical macroscale applications involve fracture

$$\delta = 3\Delta x$$



Expanding brittle cylinder




Colors are just for visualization