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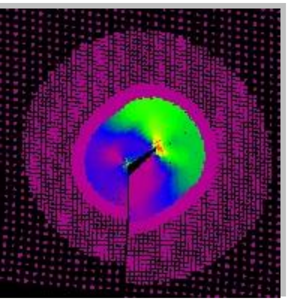

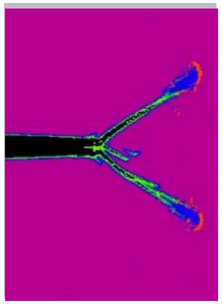

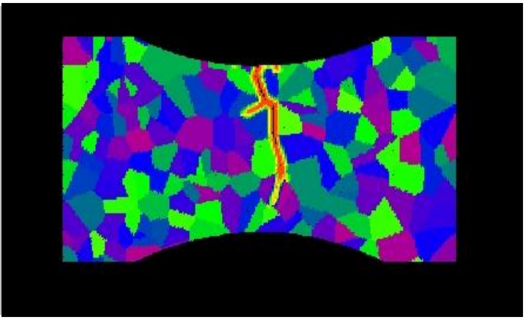

Upscaling Material Properties and Damage in Peridynamics

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Conference on Recent Developments in Continuum Mechanics and Partial Differential Equations

Lincoln, Nebraska

April 18, 2015

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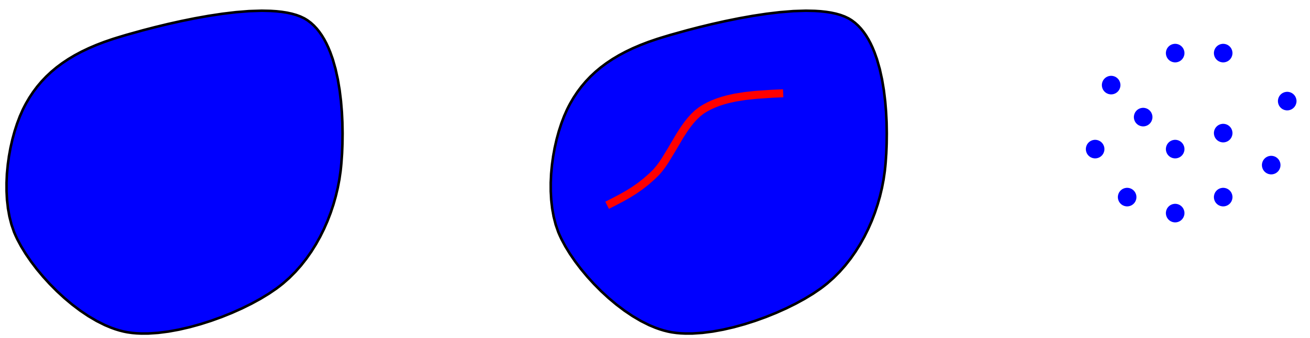
Outline

- Peridynamics background
  - Linearized model
- Peridynamics and multiscale
  - Concurrent hierarchical multiscale method
- Upscaling for multiscale material properties
  - Constrained minimization
  - Crack example
  - Time-dependent form
  - Implications for molecular dynamics

Purpose of peridynamics*

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



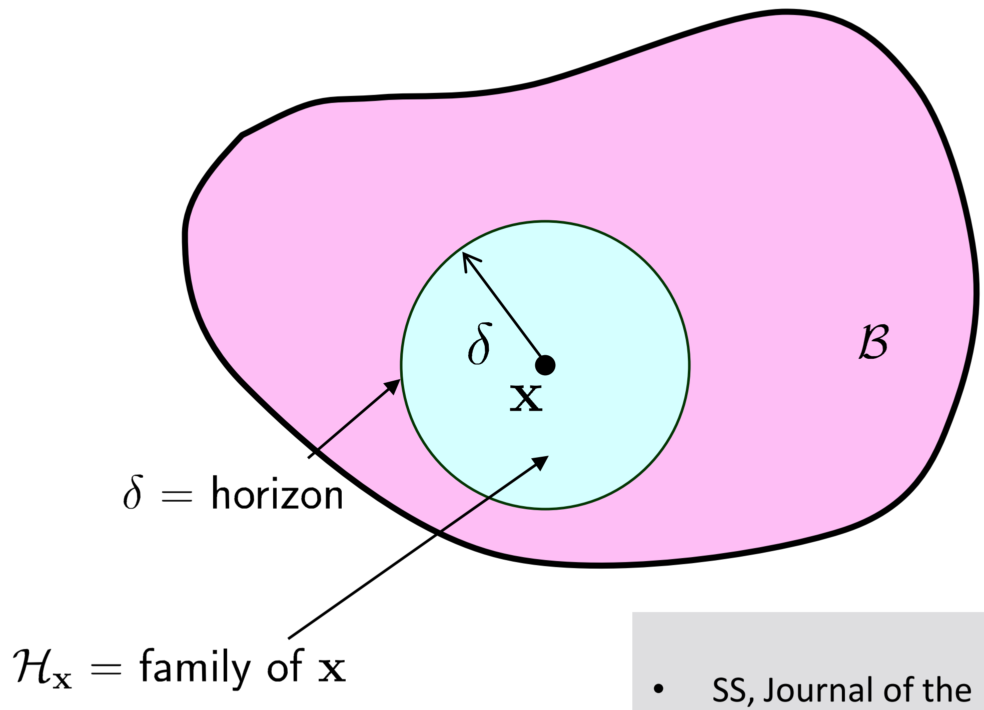
Continuous body　　Continuous body with a defect　　Discrete particles

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

* Peri (near) + dyn (force)

Peridynamics basics: Horizon and family

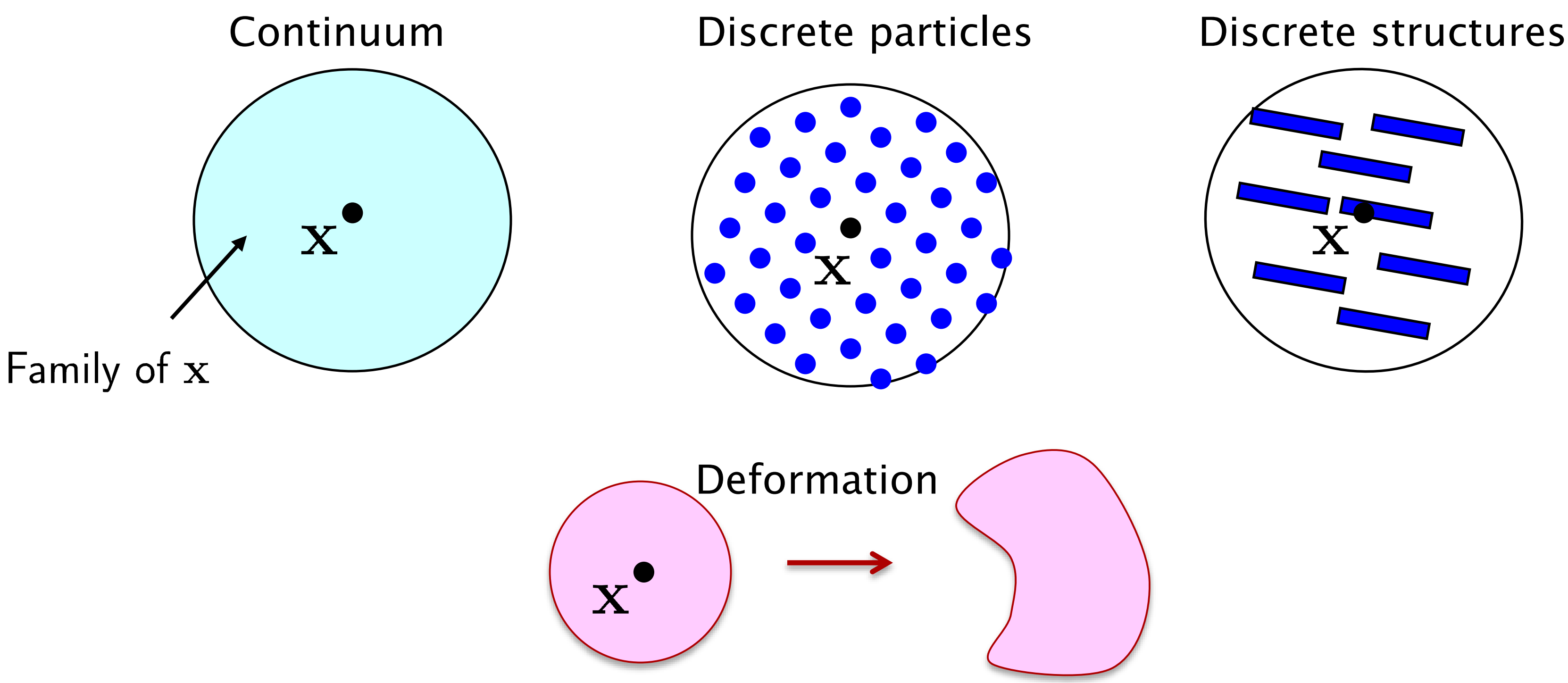
- Any point $\mathbf{x}$ interacts directly with other points within a distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}_{\mathbf{x}}$.



General references

- SS, Journal of the Mechanics and Physics of Solids (2000)
- SS and R. Lehoucq, Advances in Applied Mechanics (2010)
- Madenci & Oterkus , *Peridynamic Theory & Its Applications* (2014)

Point of departure: Strain energy at a point



- Key assumption: the strain energy density at **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 $\mathbf{x}$. $\mathbf{f}$ is the *pairwise bond force density*.

Peridynamic vs. local equations

- The structures of the theories are similar, but peridynamics uses nonlocal operators.
  - Notation: State<bond>=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	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + q + r$	$\dot{\varepsilon} = \boldsymbol{\sigma}\cdot\dot{\mathbf{F}} + q + r$

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

Linearized theory

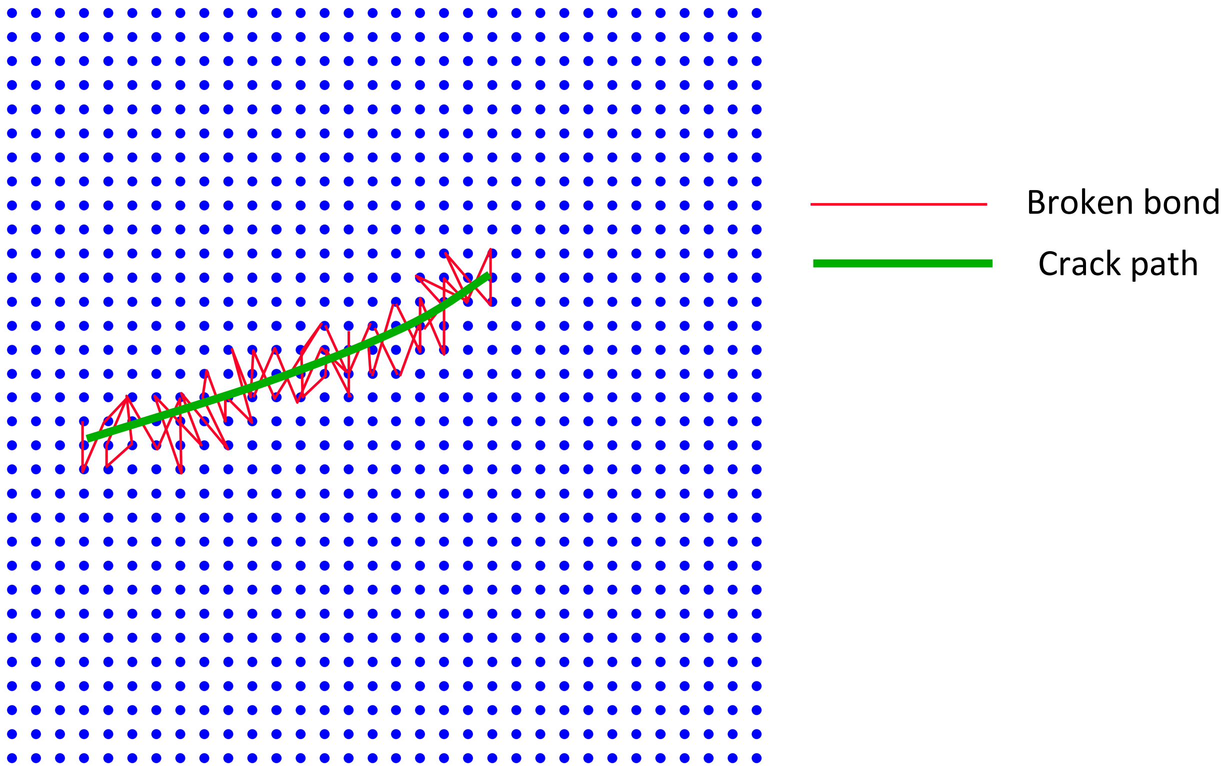
- For small displacements (possibly superposed on a large deformation):

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

  where $\mathbf{C}$ is the tensor-valued *micromodulus* field.

- Equation is formally the same as in Kunin's nonlocal theory.
- Can still have bond breakage.
- Most of the following discussion uses the linearized theory.
- Will see how to get $\mathbf{C}$ by multiscale methods.

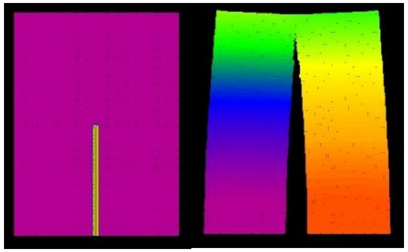
Bond breakage leads to autonomous crack growth

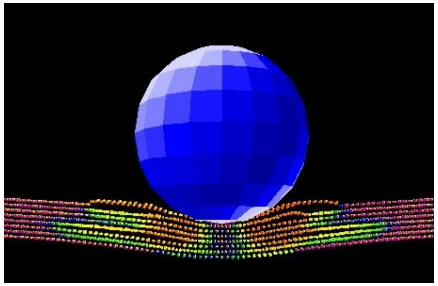


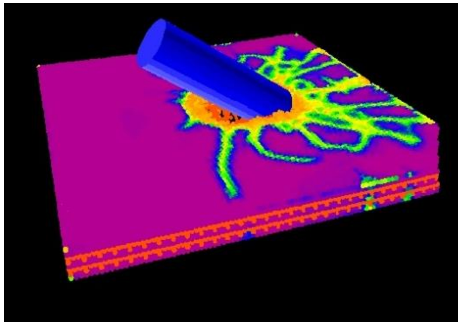
- When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.

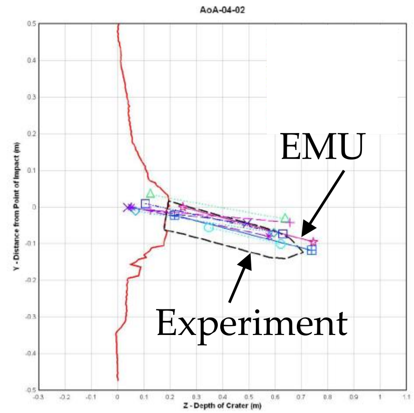
Examples of application of peridynamics

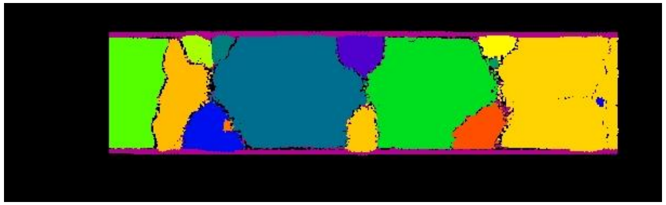
- Single crack brittle energy balance
- 3-point bend test
- Dynamic fracture
    - Crack growth velocity
    - Trajectory
    - Branching
- Impact into concrete and aluminum
    - Residual velocity
    - Penetration depth
    - Crater size
- Fatigue
    - S-N curves for aluminum and epoxy
    - Paris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



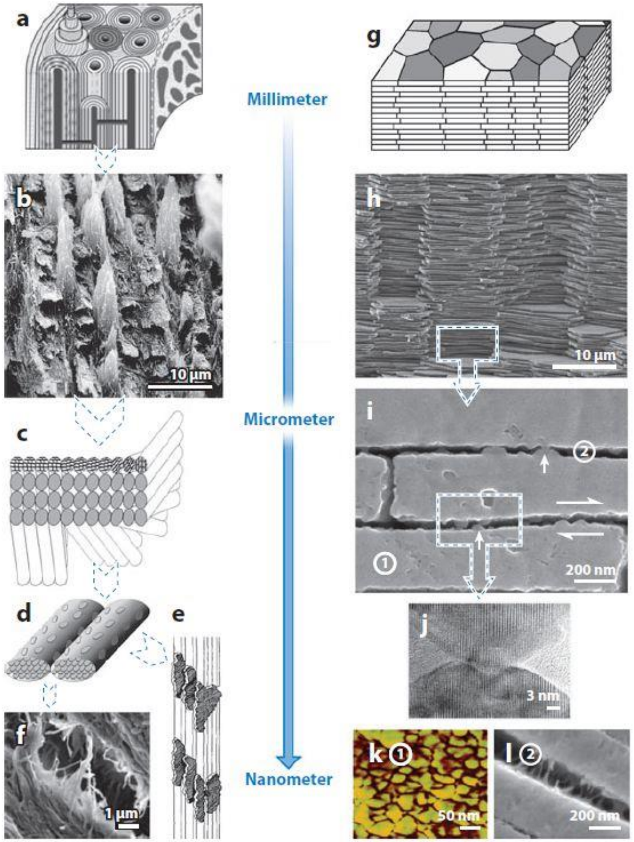




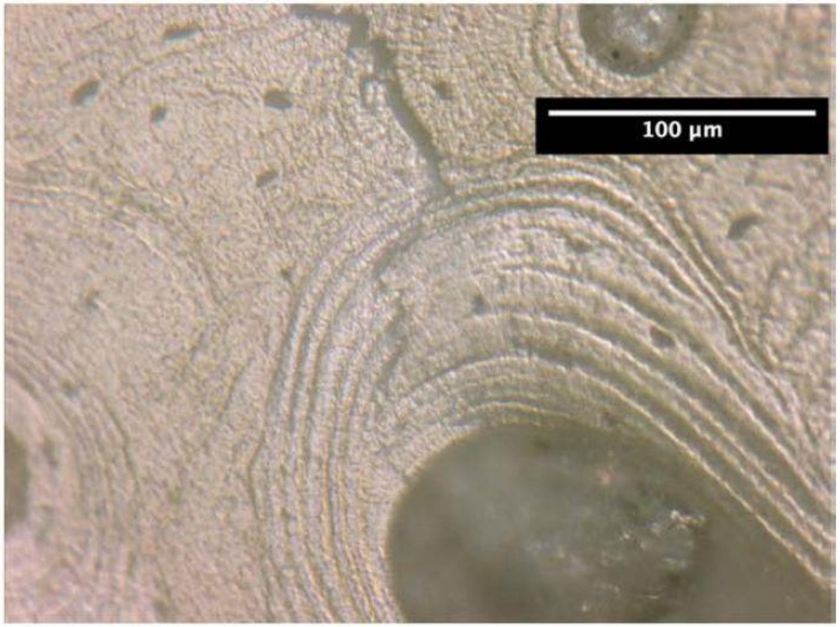




Bone: A composite material with many length scales



Bone contains a heirarchy of structures at many length scales. Image: Wang and Gupta, *Ann. Rev. Mat. Sci.* 41 (2011) 41-73



Bone structure helps delay, deflect crack growth. Image: Chan, Chan, and Nicolella, *Bone* 45 (2009) 427–434

Peridynamics as a multiscale method

- The basic equations have a fundamental length scale (the horizon).
- Changing the horizon in a consistent way could provide a way to connect length scales.

Some previous work on multiscale peridynamics

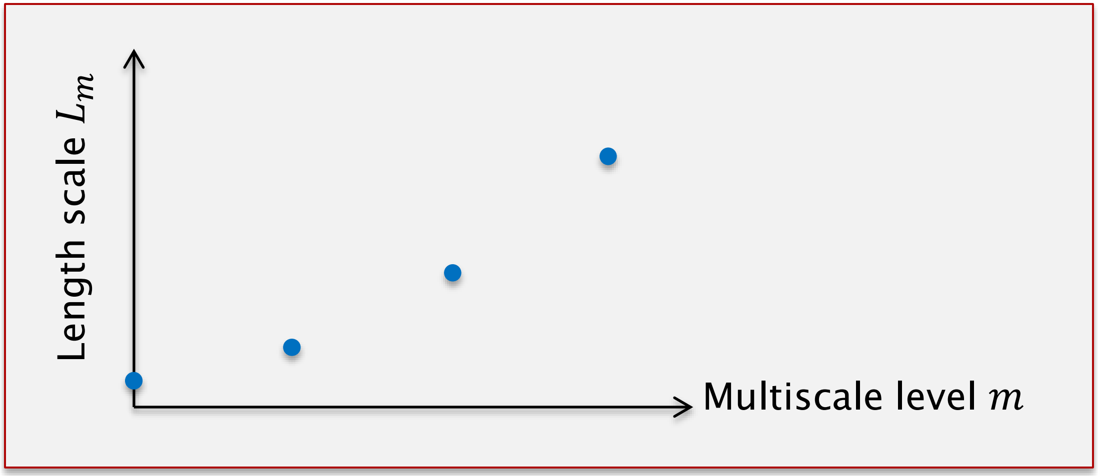
- Derivation of peridynamic equations from statistical mechanics (Lehoucq & Sears, 2011).
- Higher order gradients to connect MD to peridynamic (Seleson, Parks, Gunzburger, & Lehoucq, 2005).
- Adaptive mesh refinement (Bobaru & Hu, 2011).
- Two-scale evolution equation for composites (Alali & Lipton, 2012).
- PFHMM method for atomistic-to-continuum coupling (Rahman, Foster, & Haque, 2014).

Scalable multiscale methods

- How to couple multiple physics across wide variations in length/time scales when many length scales are naturally present in the problem?
- Idea:
  - Hierarchy of levels m each with length scale $L_m = L_0 2^m$
  - L_0 is the smallest physically operative length scale.
  - Each level is coupled to the adjacent levels by the same equations:

$$\dot{y}_m = f(y_{m-1}, y_m, y_{m+1})$$

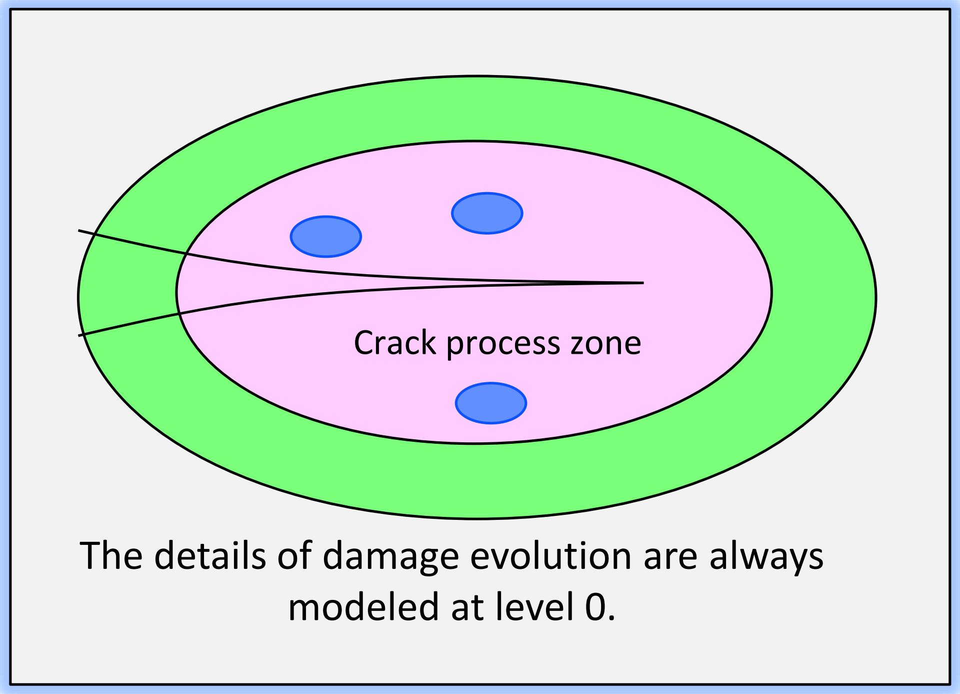
where f is independent of m.



- Avoids reinventing the wheel at each level.

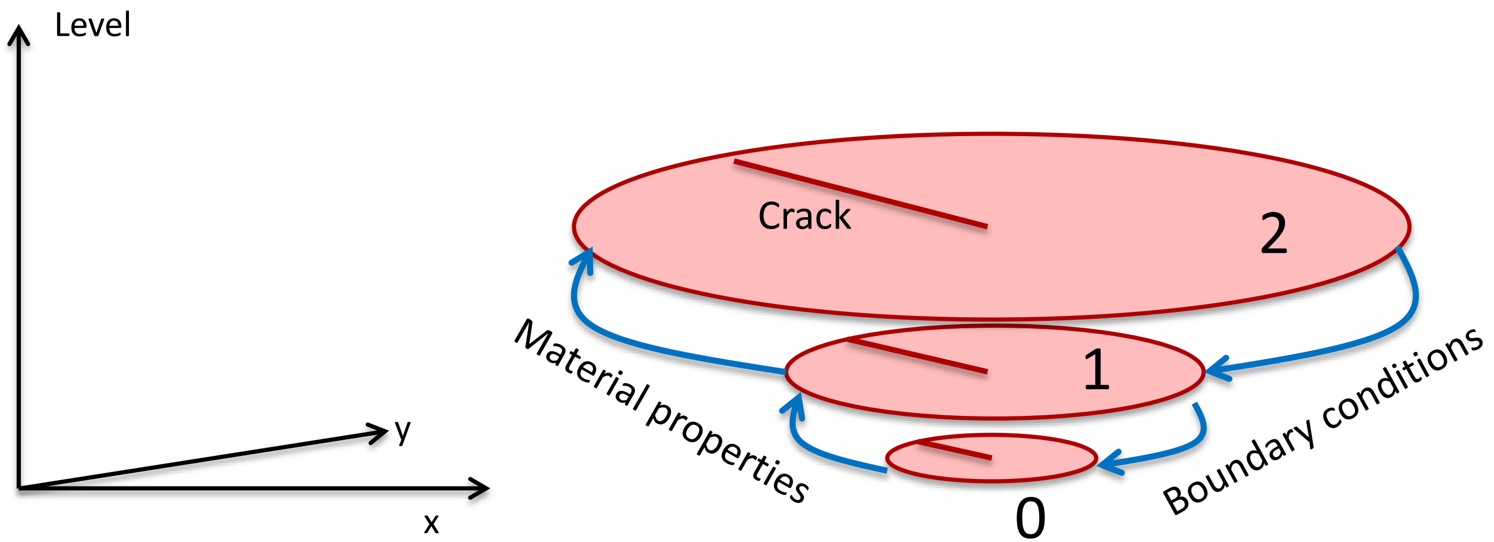
Concurrent multiscale method for defects

- Apply the best practical physics at the smallest length scale (near a crack tip).
- Scale up hierarchically to larger length scales.
- Each level is related to the one below it by the same equations.
    - Any number of levels can be used.
- Adaptively follow the crack tip.



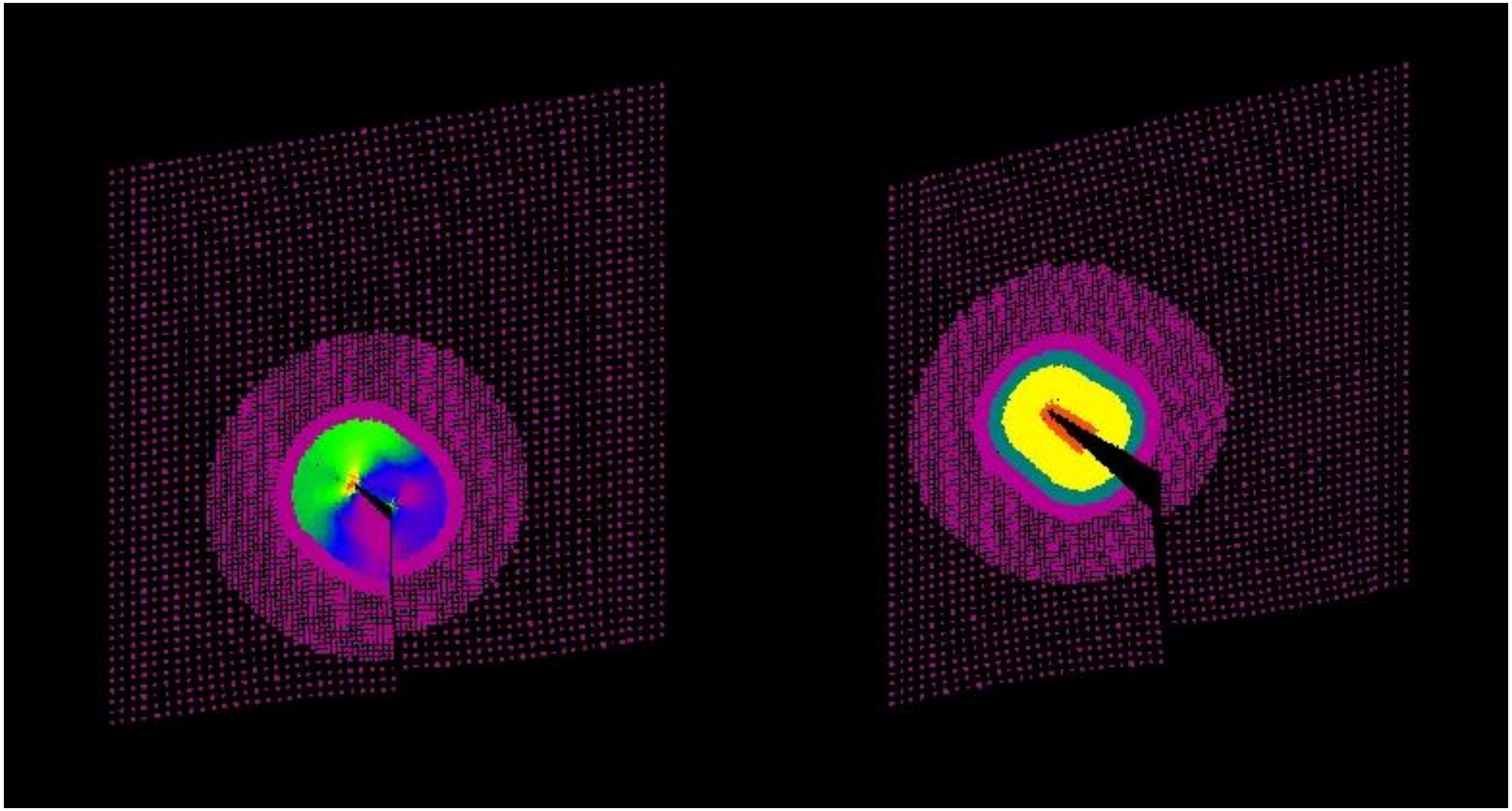
Concurrent solution strategy

- The equation of motion is applied only <u>within</u> each level.
- Higher levels provide boundary conditions on lower levels.
- Lower levels provide coarsened material properties (including damage) to higher levels.



Schematic of communication between levels in a 2D body

Concurrent multiscale example: shear loading of a crack

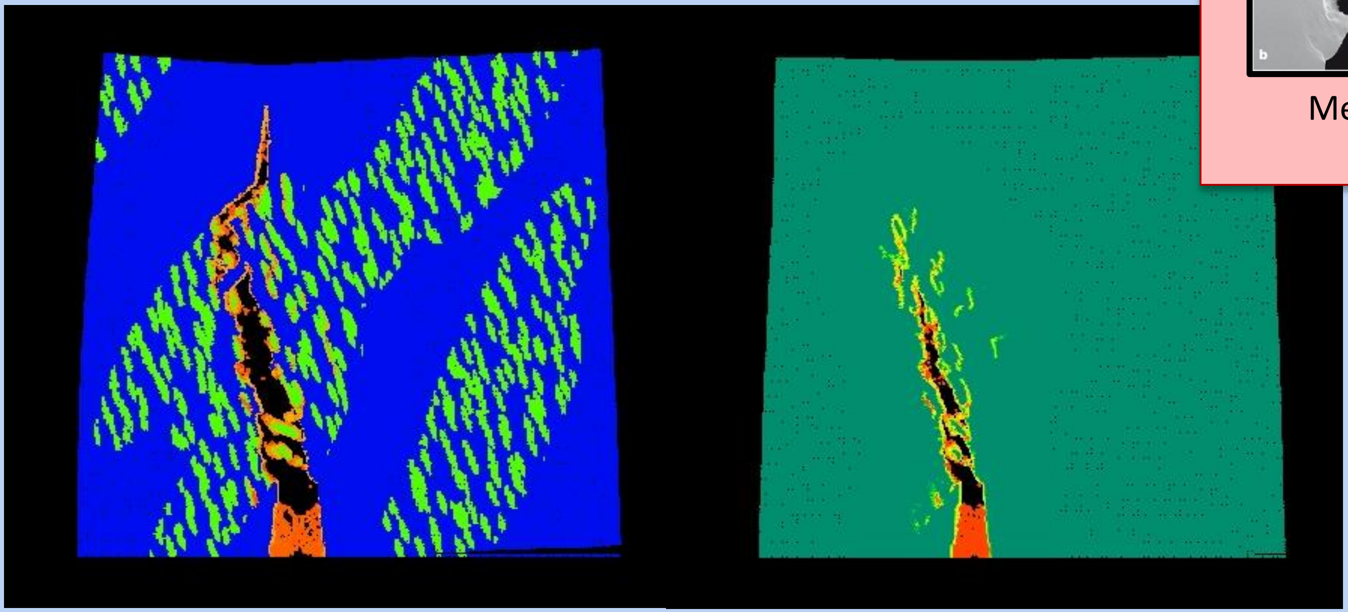


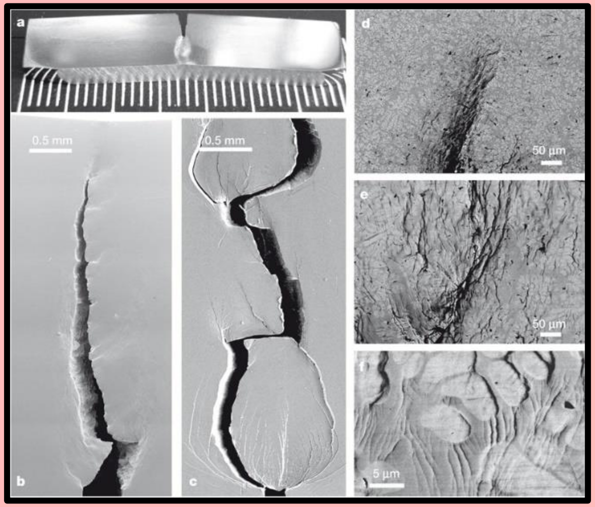
Bond strain	Damage process zone

Multiscale modeling reveals 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.

Multiscale model of crack growth through a brittle material with distributed defects





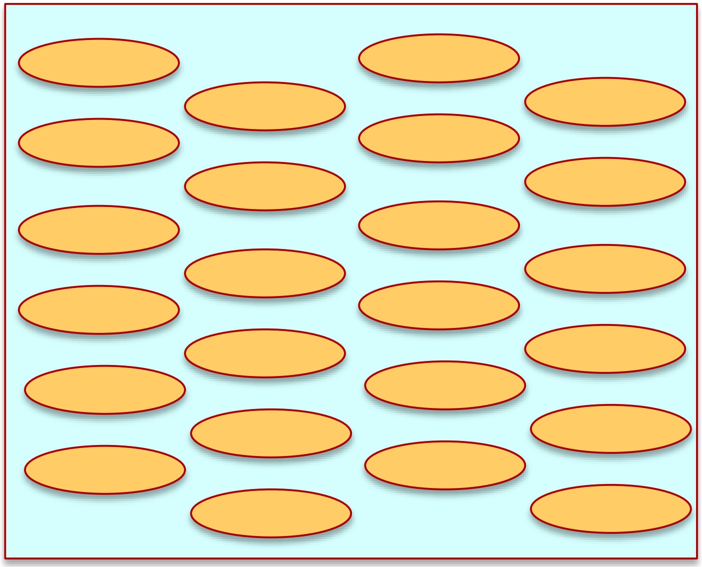
Metallic glass fracture (Hofmann et al, Nature 2008)

Upscaling of material properties

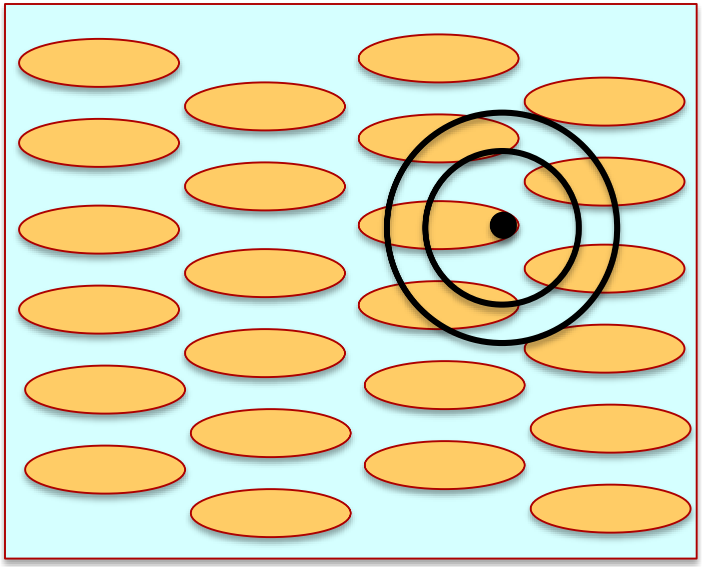
- Suppose we have an accurate model in level 0.
  - How can we obtain material properties in level 1?
  - This is called “upscaling” or “coarse-graining”.
  - Will next describe a method for doing this based on constrained optimization.

What are the elastic moduli of a heterogeneous material?

- This is an imprecise question in the classical (local) theory.
- Only becomes meaningful in the limit of a very large volume.
- Try to find a peridynamic approach to upscaling that does not assume this.



We will try to find the micromodulus for different multiscale levels



- Level 0:

$$\int_{\mathcal{H}^0} C^0(q,x)(u^0(q)-u^0(x))\,dV_q + b(x) = 0$$

- Level 1:

$$\int_{\mathcal{H}^1} C^1(q,x)(u^1(q)-u^1(x))\,dV_q + b(x) = 0$$

- Level m:

$$\int_{\mathcal{H}^m} C^m(q,x)(u^m(q)-u^m(x))\,dV_q + b(x) = 0$$

- Upscaling: Find C^1 from C^0, C^2 from C^1, ...

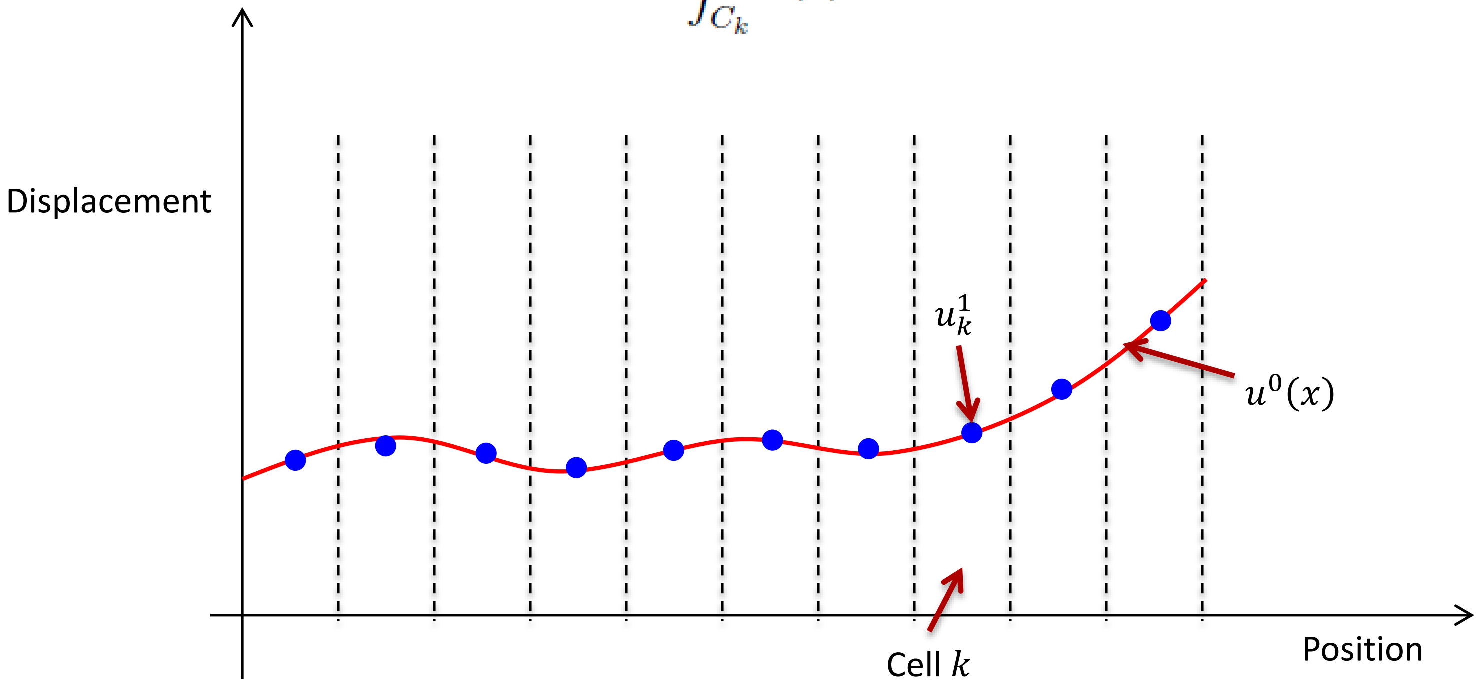
Level 1 DOFs

- Divide the region into K "cells" C_k.
- The mean level 0 displacement within each cell is the level 1 DOF:

$$u_k^1 = \int_{C_k} \varphi(x) u^0(x)\, dx$$

where

$$\int_{C_k} \varphi(x) = 1.$$



Level 1 DOF as a constraint

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- Pretend all the u_k^1 values are given.
- In effect, this places a constraint on the u^0 function.
- Constrained potential energy functional:

$$\Phi = \int_{\mathcal{B}} (W^0(x) - u^0(x)b(x))\,dx - \sum_{k=1}^{K} \lambda_k \left(\int_{C_k} \varphi(x)u^0(x)\,dx - u_k^1 \right)$$

where $\lambda_1, \lambda_2, \ldots, \lambda_K$ are Lagrange multipliers.

Force balance on cell k

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- Resulting constrained equilibrium equation:

$$L^0(x) + b(x) + \lambda_k \varphi(x) = 0$$

where k is whichever cell contains x and L^0 is the level 0 internal force operator:

$$L^0(x) = \int_{\mathcal{H}_\mathbf{x}} \Big(\underline{T}[x]\langle q - x \rangle - \underline{T}[q]\langle x - q \rangle \Big) \, dq.$$

- Observe that the constraint acts like a body force distributed over cell k.
- Integrate the equilibrium equation over cell k, recall $\int \varphi = 1$, set $b \equiv 0$:

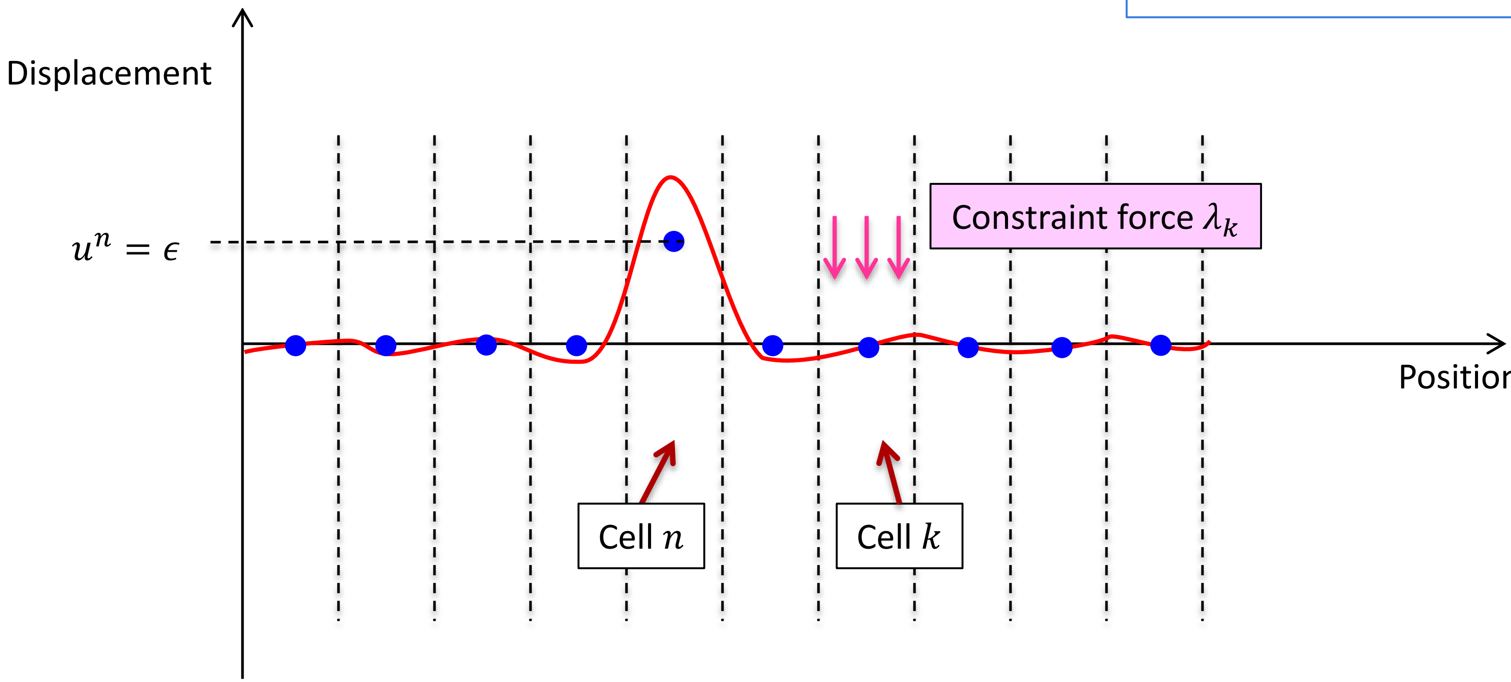
$$\int_{C_k} L^0(x) \, dx + \lambda_k = 0.$$

Interaction forces from other cells + constraint force = 0

Level 1 micromodulus

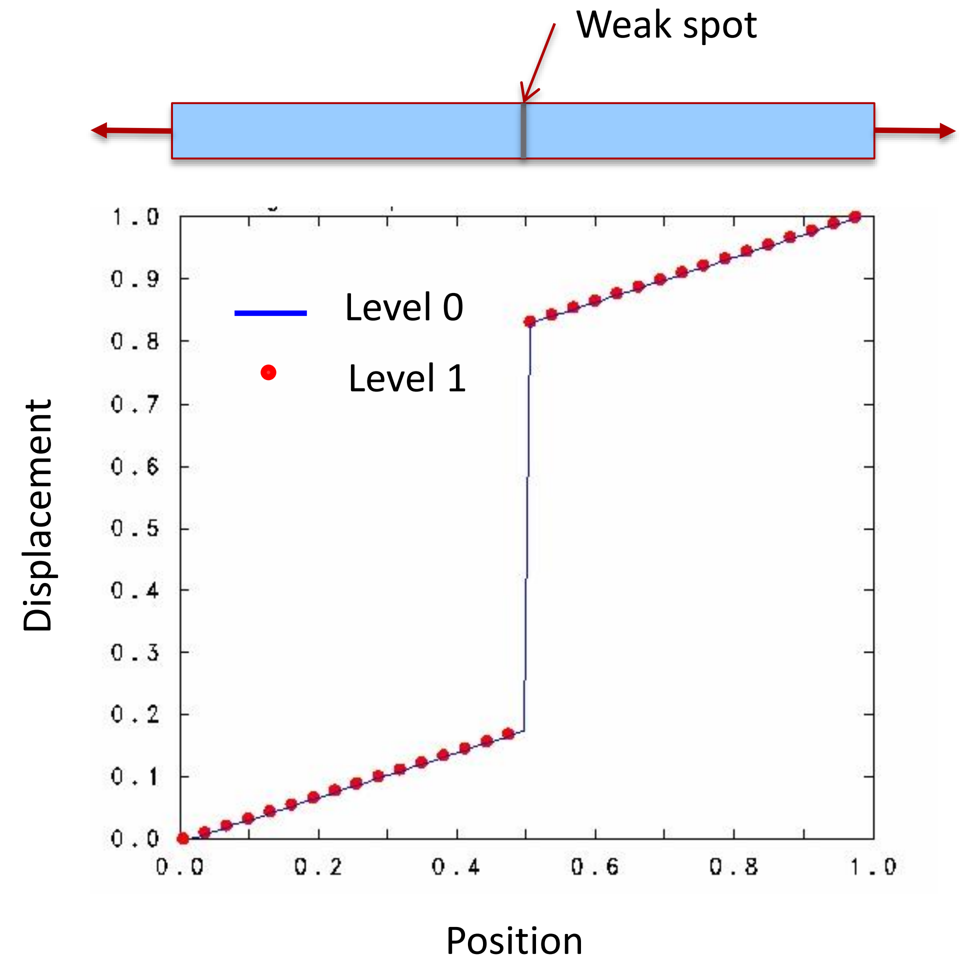
- Set all $u_k^1 = 0$ except for cell n: $u_n^1 = \epsilon \ll 1$.
- Solve the constrained equilibrium equation for $u^0(x)$ and the $\lambda_1, \lambda_2, \ldots, \lambda_K$.
- The upscaled micromodulus is

$$c_{kn}^1 = \lambda_k/\epsilon. \quad \rightarrow \quad \boxed{\rho \ddot{u}_i^1 = \sum_{j \in H_i} c_{ij}^1 (u_j^1 - u_i^1)}$$



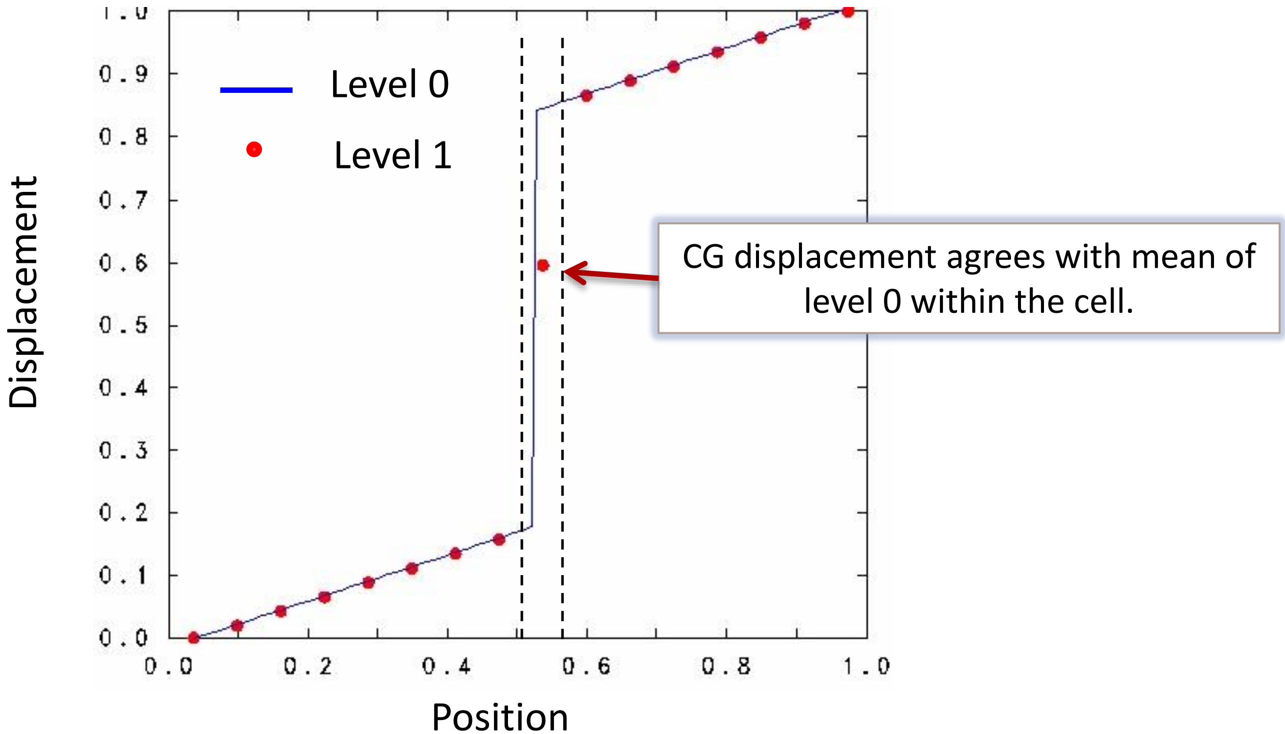
Example: Rod with a defect

- Upscaling method preserves the effect of a defect embedded within a cell.



Coarser level 1

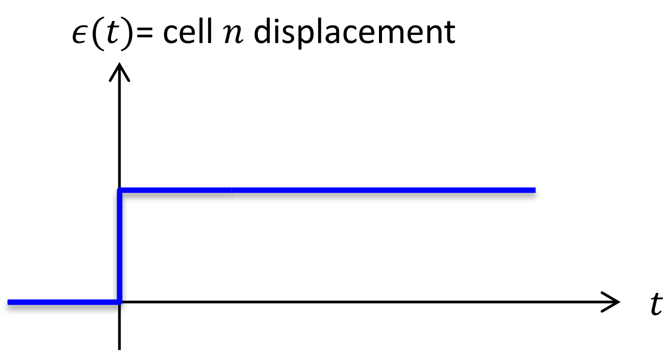
- If the defect is not exactly at a cell boundary, the method still produces the mean of the level 0 displacements within each cell.

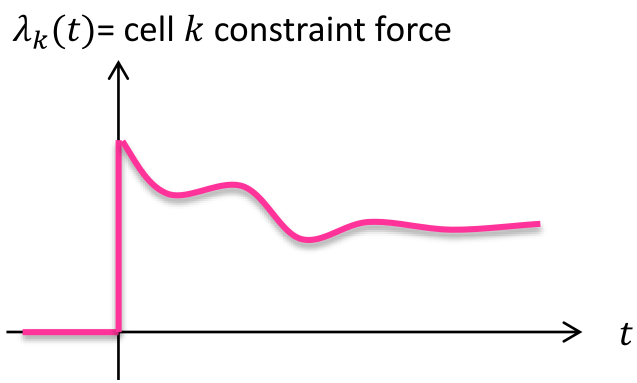


Time-dependent response

- Time-dependent bond force model for level 1:

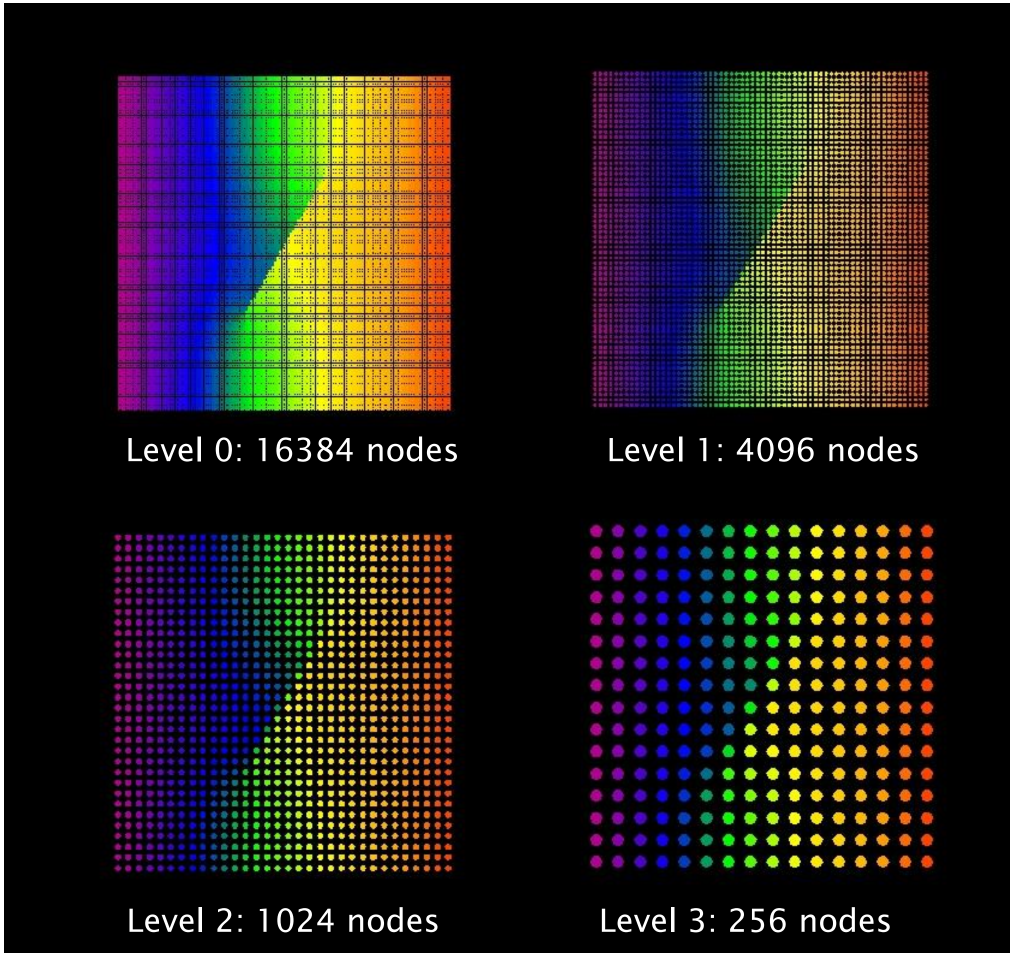
$$f(x_n, x_k) = \int_0^t \lambda_k(t-\tau)(\dot{u}(x_k,\tau) - \dot{u}(x_n,\tau))\, d\tau$$





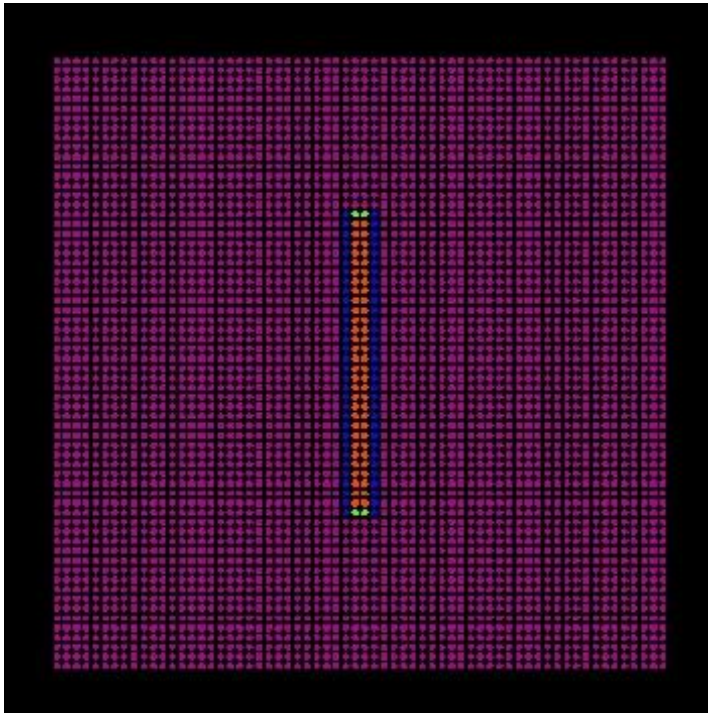
Coarse graining verification: crack in a plate

- Example: Solve the same problem in four different levels using the successively upscaled material properties – results are the same.



Defining damage from coarse-grained material properties

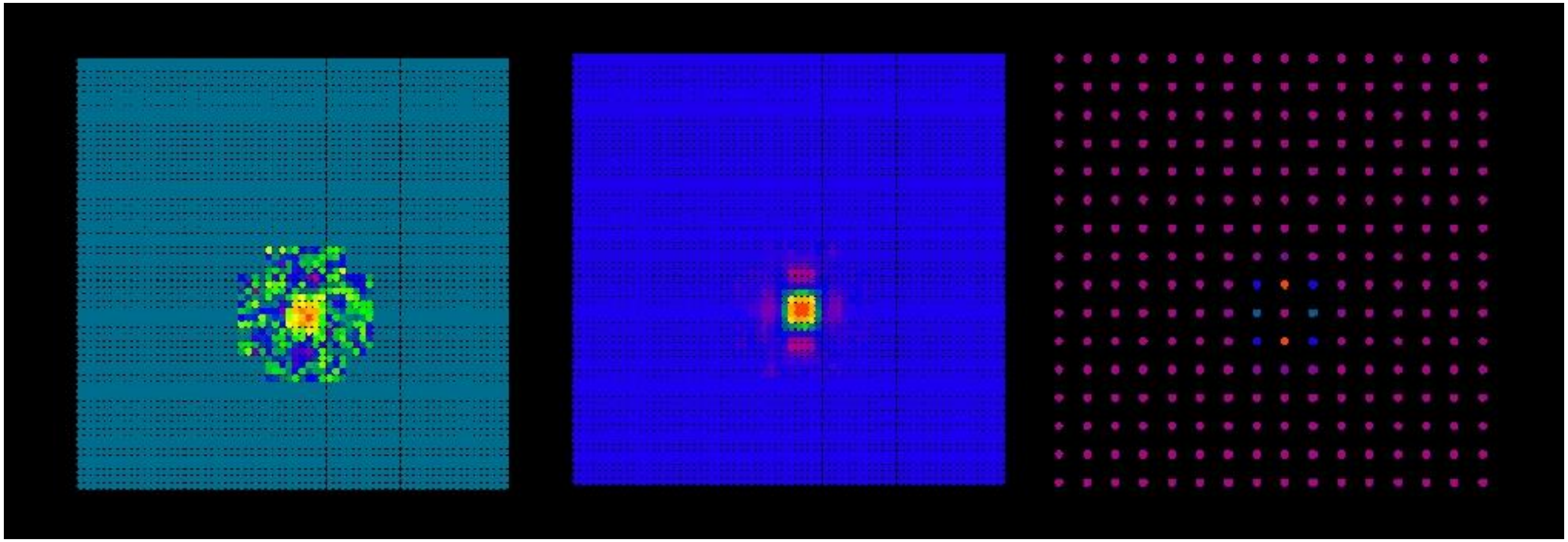
- Define bonds to be damaged if their coarse-grained micromodulus is less than a tolerance.
- This allows damage to be determined without deforming the MD grid.



Level 1 damage contours deduced from coarse-grained properties

Coarse graining MD directly into peridynamics

- The level 0 physics can be anything: PD, standard continuum, MD, MC(?), DFT(?)



Level 0: MD showing thermal oscillations

MD time-averaged displacements

Level 1: Coarse grained micromodulus

Summary

- Concurrent multiscale:
  - Adaptively follow crack tips.
  - Apply the best practical physics in level 0.
  - Also multiscale in time because of time step increase for higher levels.
- Coarse-graining:
  - Derives incremental elastic properties at higher levels.
  - Does not rely on a representative volume element (RVE).
- Methods are "scalable:" can be applied any number of times to obtain any desired increase in length scale.

Extra slides

Reconstruction

- The constrained minimization problem is:

$$\int_{\mathcal{H}_{\mathbf{x}}} C^m(x,q)(u^m(q) - u^m(x))\, dq + b + \lambda_k \phi_k = 0, \qquad \int_{\mathcal{B}_k} u^m \phi = u_k^{m+1}$$

- To get level $m+1$ from level m:

$$\begin{bmatrix} [C^m] & [\phi^m] \\ [\phi^m]^T & [0] \end{bmatrix} \begin{Bmatrix} \{u^m\} \\ \{\lambda^m\} \end{Bmatrix} = \begin{Bmatrix} \{0\} \\ \{u^{m+1}\} \end{Bmatrix}.$$

- Invert the matrix:

$$\begin{bmatrix} [\dots] & [R^m] \\ [R^m]^T & [\dots] \end{bmatrix} \begin{Bmatrix} \{0\} \\ \{u^{m+1}\} \end{Bmatrix} = \begin{Bmatrix} \{u^m\} \\ \{\lambda^m\} \end{Bmatrix}.$$

- $[R^m]$ is the *reconstruction matrix*.

Coarse graining a damage criterion

- Can we model level 1 damage processes without modeling level 0 explicitly?
- Suppose the level 0 damage depends only on the bond displacements

$$\underline{U}^0[x]\langle q - x\rangle := u^0(q) - u^0(x).$$

- Recall

$$\{u^0\} = [R^0]\{u^1\}.$$

- Can use this to find a *bond reconstruction state* $\underline{R}^0$ such that

$$\underline{U}^0[x] = \underline{R}^0[x] \bullet \underline{U}^1[x]$$

  where $\underline{U}^1[x]$ is the level 1 displacement state at x.

- We can then compute level 0 bond damage without solving for the level 0 displacements.

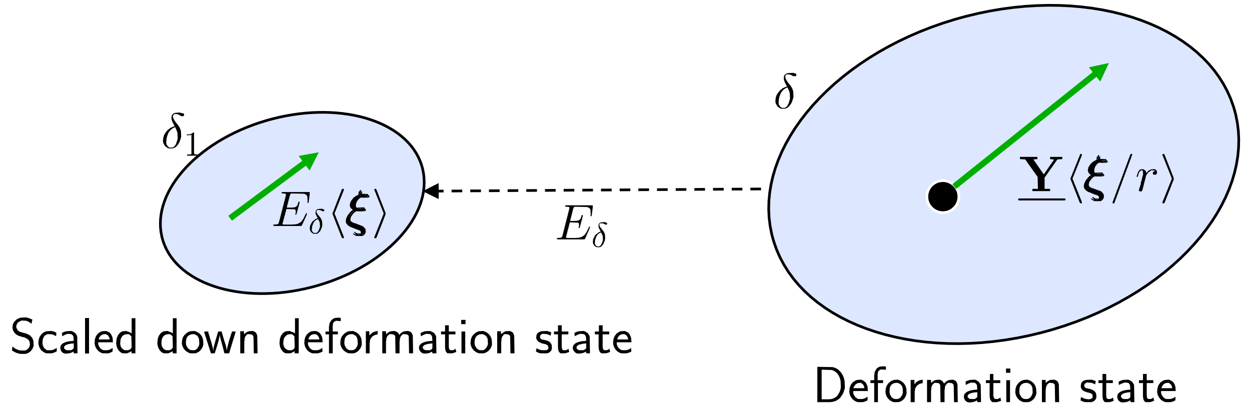
Rescaling an elastic material model

- Start with a material model W_1 which has some fixed horizon δ_1.
- Define a mapping that takes a new, larger horizon δ into the original:

$$(E_\delta(\underline{\mathbf{Y}}))\langle\boldsymbol{\xi}\rangle = r\underline{\mathbf{Y}}\langle\boldsymbol{\xi}/r\rangle, \qquad r = \frac{\delta_1}{\delta} \leq 1$$

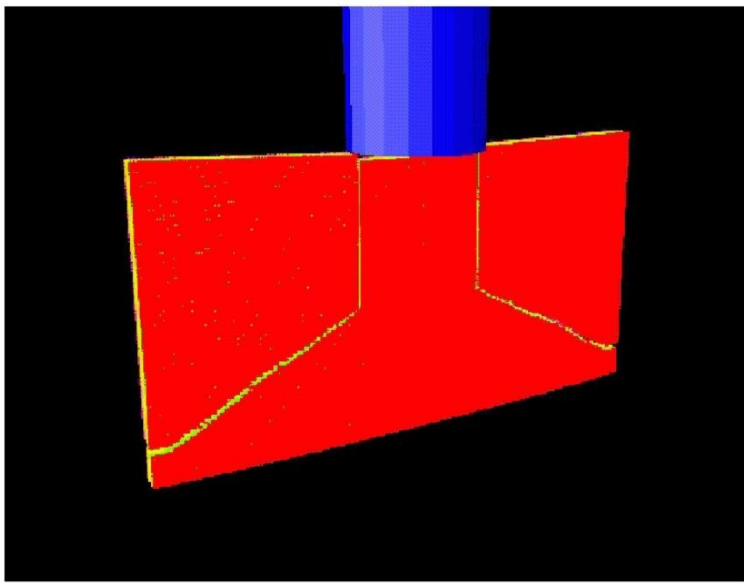
- Then set

$$W_\delta(\underline{\mathbf{Y}}) = W_1(E_\delta(\underline{\mathbf{Y}}))$$

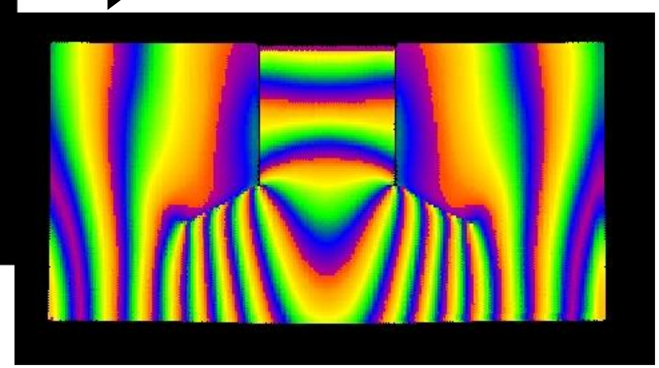


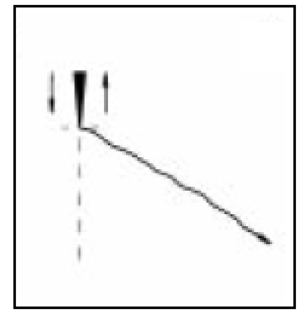
Example: Dynamic fracture

- Dynamic fracture in maraging steel (Kalthoff & Winkler, 1988)
- Mode-II loading at notch tips results in mode-I cracks at 70deg angle.
- 3D EMU model reproduces the crack angle.



EMU*





Experiment

S. A. Silling, Dynamic fracture modeling with a meshfree peridynamic code, in *Computational Fluid and Solid Mechanics 2003*, K.J. Bathe, ed., Elsevier, pp. 641-644.

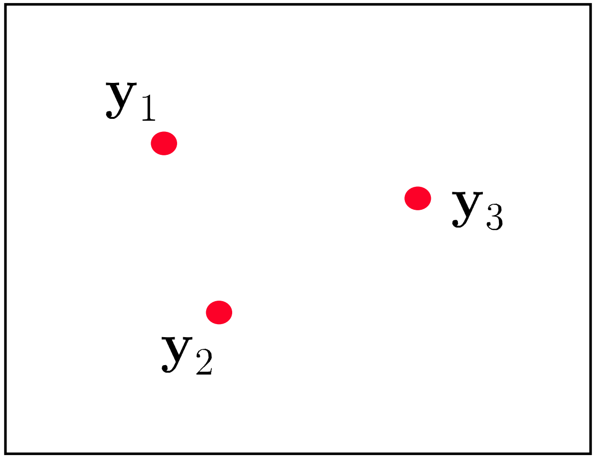
Discrete particles and PD states

- Consider a set of atoms that interact through an $N-$body potential:

$$U(\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N),$$

$\mathbf{y}_1, \ldots, \mathbf{y}_N$ = deformed positions, $\mathbf{x}_1, \ldots, \mathbf{x}_N$ = reference positions.

- This can be represented exactly as a peridynamic body.

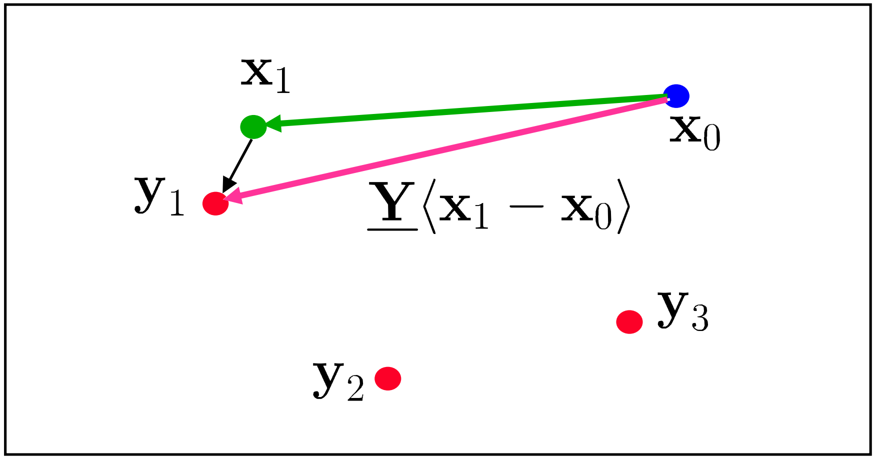


Discrete particles and PD states, ctd.

Define a peridynamic body by:

$$\hat{W}(\underline{\mathbf{Y}}, \mathbf{x}) = \Delta(\mathbf{x}-\mathbf{x}_0)U(\underline{\mathbf{Y}}\langle\mathbf{x}_1-\mathbf{x}_0\rangle, \underline{\mathbf{Y}}\langle\mathbf{x}_2-\mathbf{x}_0\rangle, \dots, \underline{\mathbf{Y}}\langle\mathbf{x}_N-\mathbf{x}_0\rangle),$$

$$\rho(\mathbf{x}) = \sum_i \Delta(\mathbf{x}-\mathbf{x}_i)M_i$$



Discrete particles and PD states, ctd.

After evaluating the Frechet derivative $\underline{\mathbf{T}}$, find

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \int \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'}$$

implies

$$M_i\ddot{\mathbf{y}}(\mathbf{x}_i,t) = -\frac{\partial U}{\partial \mathbf{y}_i}, \qquad i = 1,\dots,N$$

In other words, the PD equation of motion reduces to Newton's second law.