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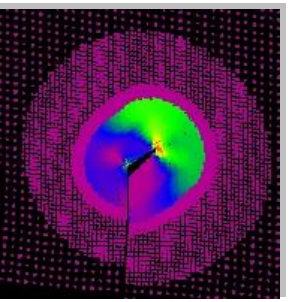

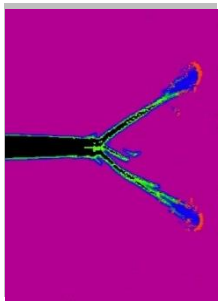

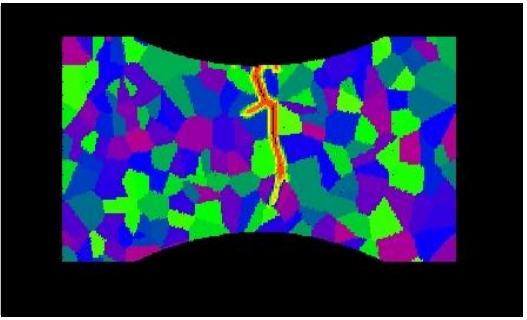

Peridynamics as a multiscale method

Stewart Silling
Sandia National Laboratories
Albuquerque, New Mexico

SIAM Annual Meeting
Chicago, IL
July 8, 2014

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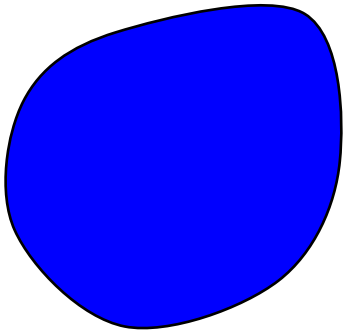
Outline

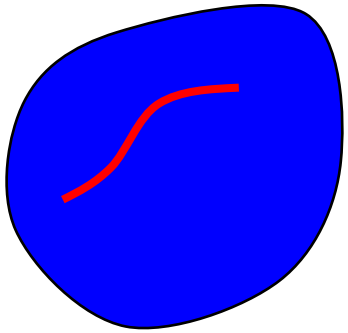
- Peridynamics background and examples
- Concurrent hierarchical multiscale method
- Calibrating a bond damage model using MD
- Coarse graining

Purpose of peridynamics*

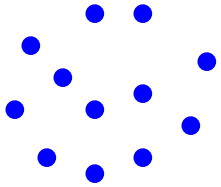
- To unify the mechanics of continuous and discontinuous media within a single, consistent set of equations.



Continuous body



Continuous body with a defect



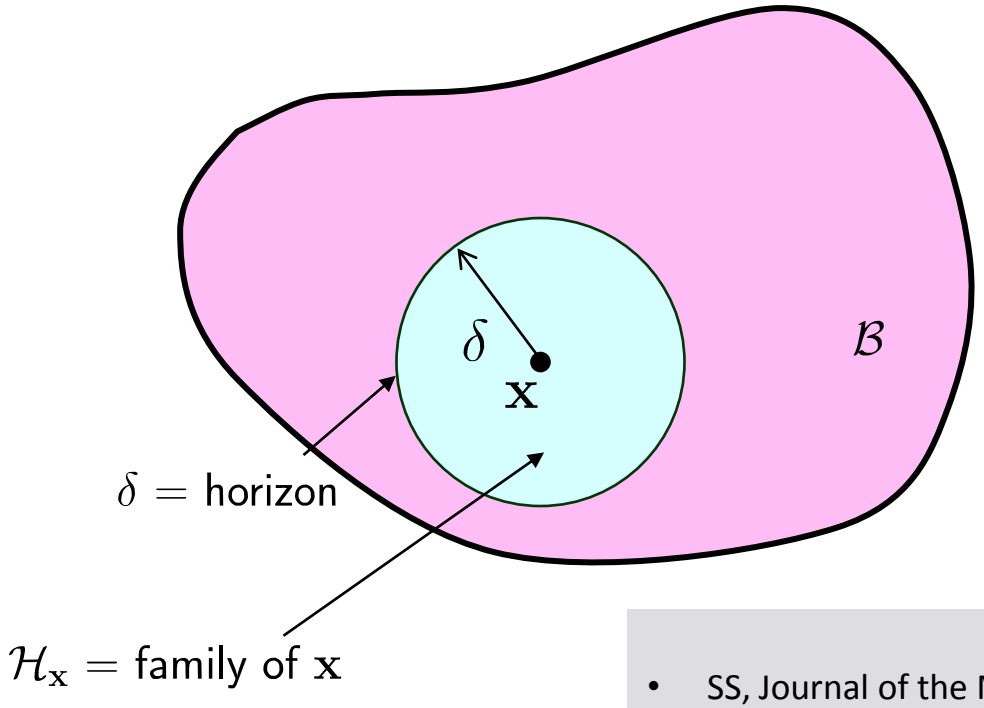
Discrete particles

- 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

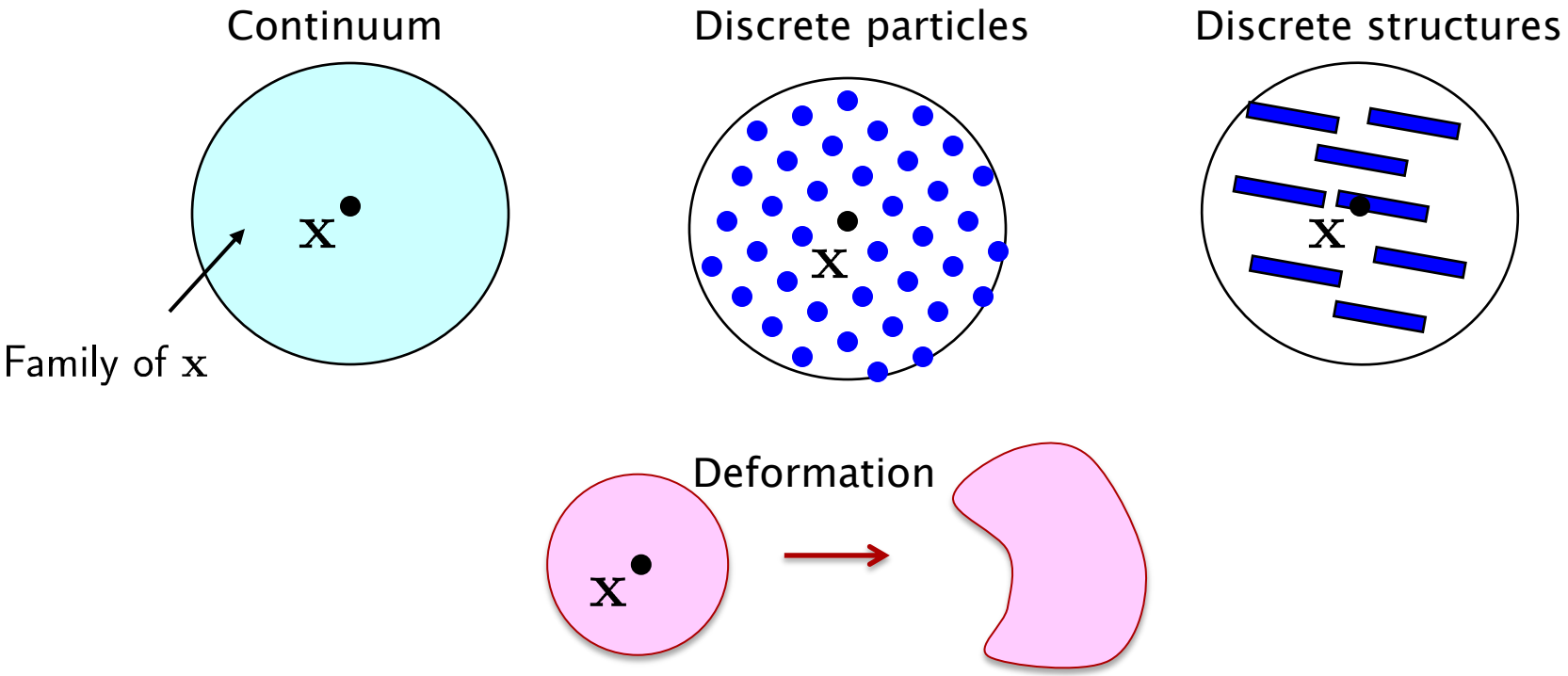
- Any point $\mathbf{x}$ interacts directly with other points within a distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}_{\mathbf{x}}$.



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 $\mathbf{x}$ is determined by the deformation of its family.

Potential energy minimization yields the peridynamic equilibrium equation

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- 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.

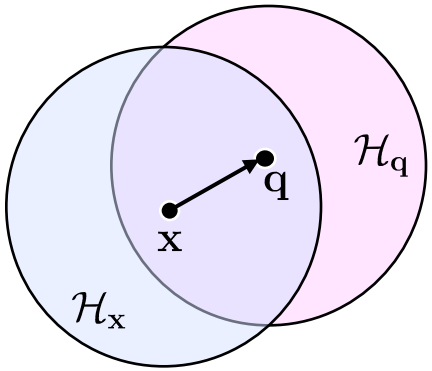
- Euler-Lagrange equation is the equilibrium equation:

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

  for all $\mathbf{x}$. $\mathbf{f}$ is the *pairwise bond force density*.

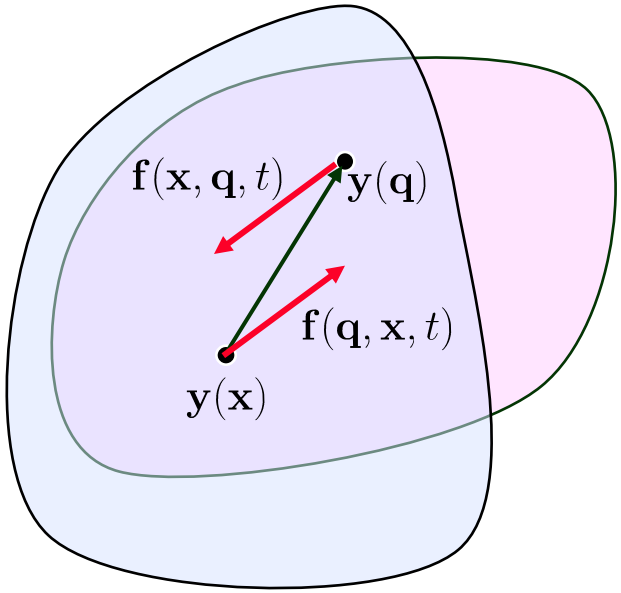
Peridynamics basics: Material model determines bond forces

- 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

Deformation $\mathbf{y}(\cdot, t)$



Deformed families and bond forces

Peridynamic vs. local equations

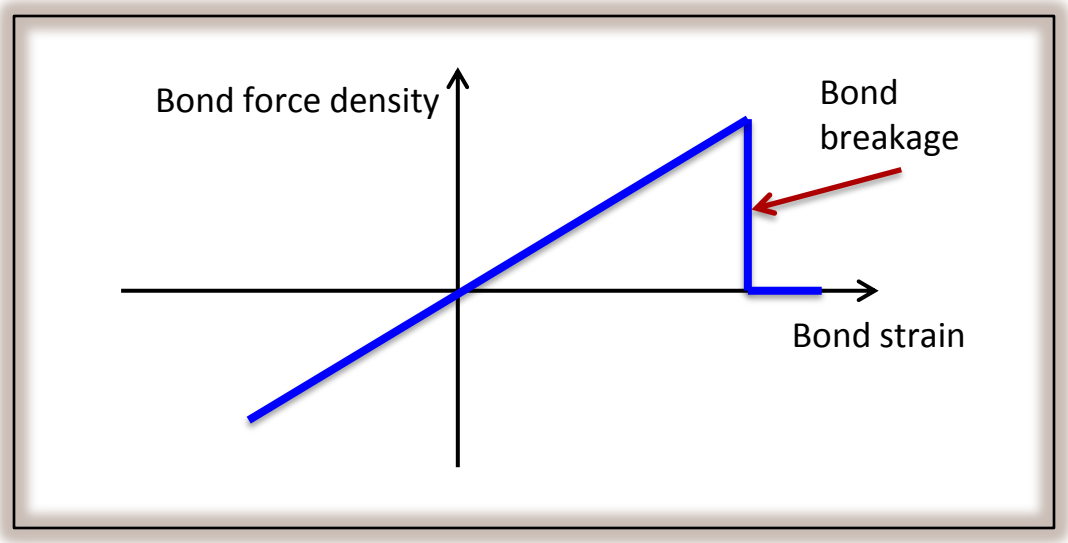
- The structures of the theories are similar, but peridynamics uses nonlocal operators.

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

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

Bond based material models

- 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.
- Damage can be modeled through bond breakage.
- Bond response is calibrated to:
  - Bulk elastic properties.
  - Critical energy release rate.



Linearized theory

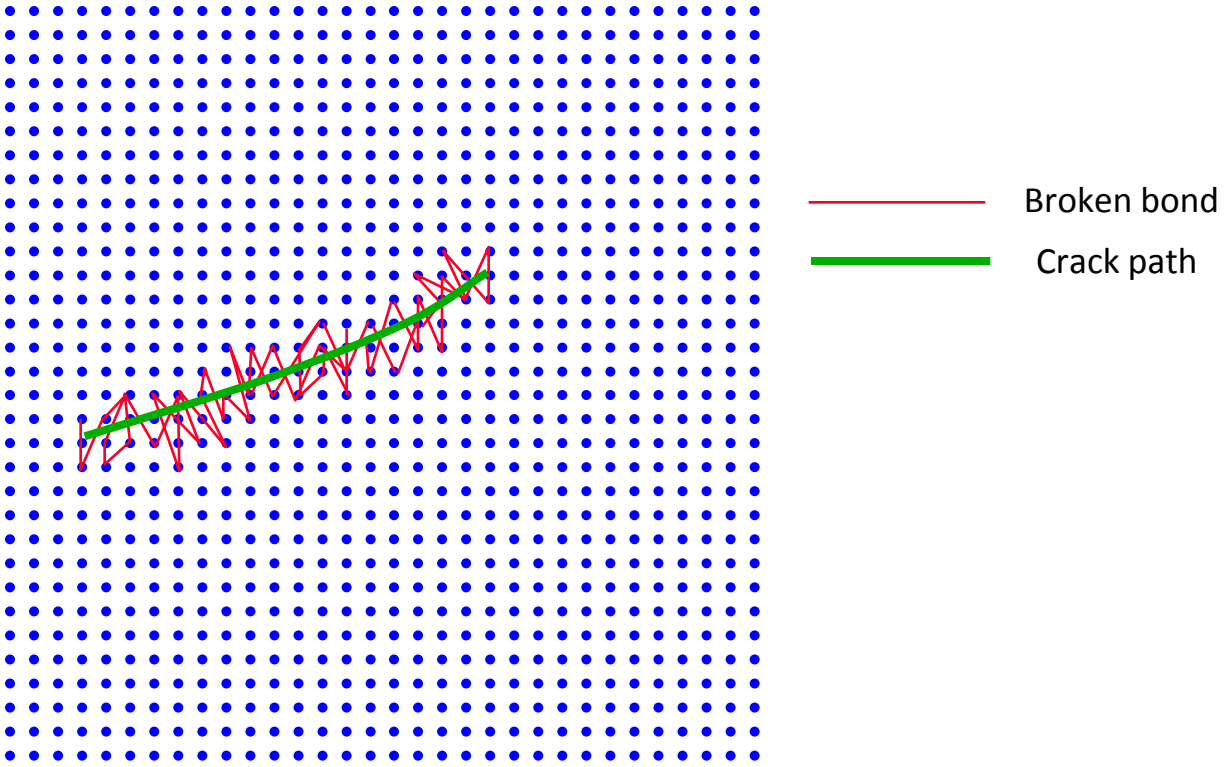
- For small displacements (possibly superposed on a large deformation):

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

  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.

Autonomous crack growth



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

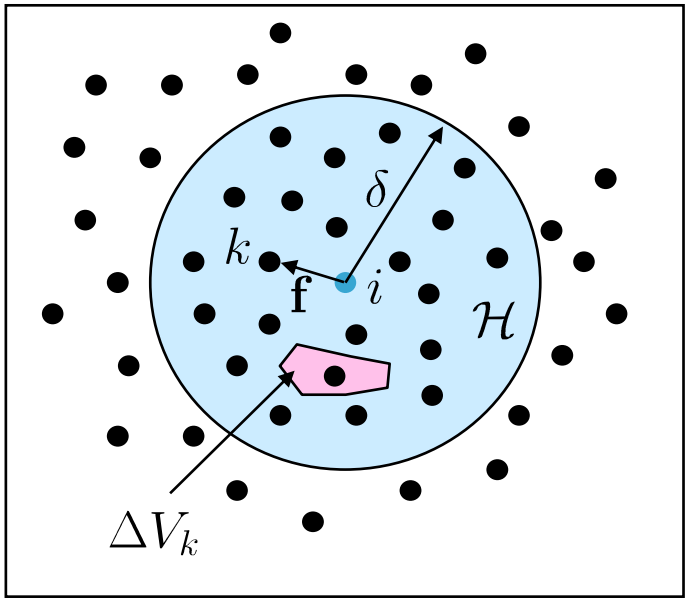
EMU numerical method

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

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t) \quad \longrightarrow \quad \rho\ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\, \Delta V_k + \mathbf{b}_i^n$$

- Linearized model:

$$\rho\ddot{\mathbf{u}}_i = \sum_{k\in\mathcal{H}_i} \mathbf{C}_{ik}(\mathbf{u}_k - \mathbf{u}_i)\Delta V_k + \mathbf{b}_i$$



Peridynamics fun facts

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- Molecular dynamics is a special case of peridynamics
  - Any multibody potential can be made into a peridynamic material model (Seleson & Parks, 2014).
- Classical (local) PDEs are a limiting case of peridynamics as $\delta \to 0$ (SS & Lehoucq, 2008).
- Any material model from the classical theory can be included.
  - e.g., Strain-hardening viscoplastic (Foster & Chen, 2010.)
  - Classical material models with the Emu discretization are similar to
    - RKPM (Bessa, Foster, Belytschko, & Liu, 2014).
    - SPH (Ganzenmüller, Hiermaier, & May, 2014).
- Waves are dispersive
  - Material properties can be deduced from dispersion curves (Weckner & SS, 2011).
- It's possible to model crack nucleation and growth without damage (!).
  - Use nonconvex bond energy (Lipton, 2014).

Examples: Membranes and thin structures (videos)

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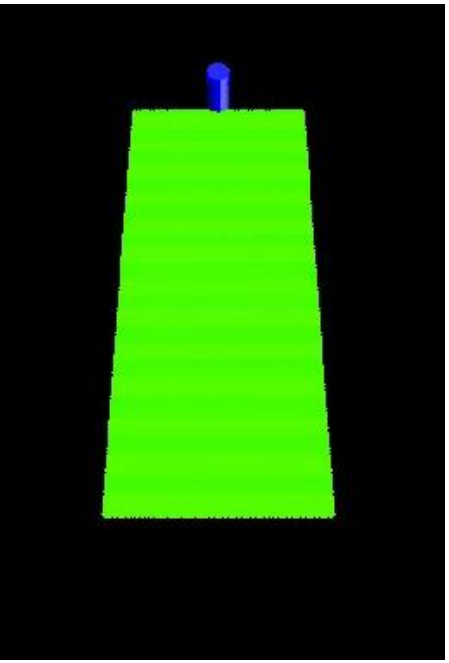
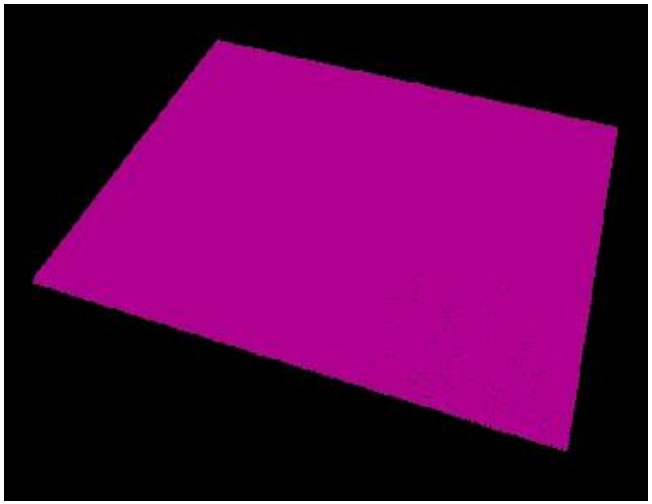
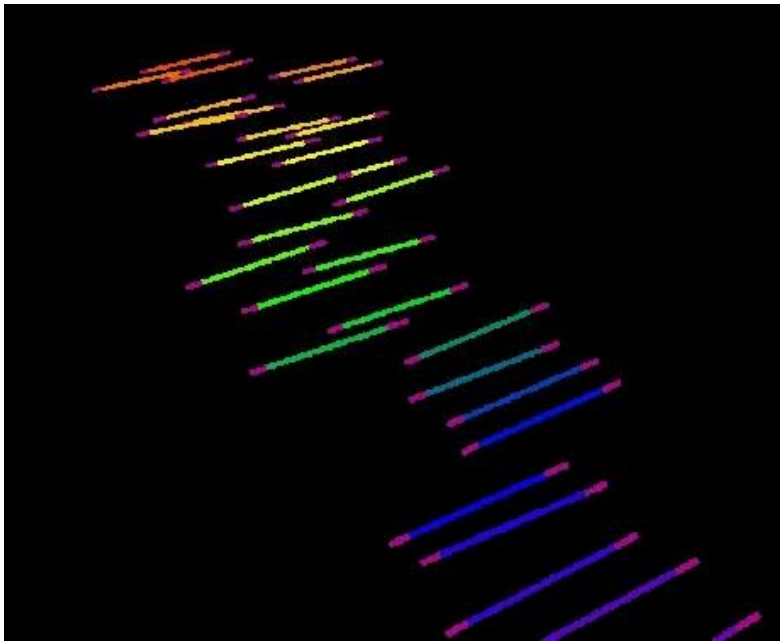


Oscillatory crack path



Crack interaction in a sheet



Self-assembly

Dynamic crack branching

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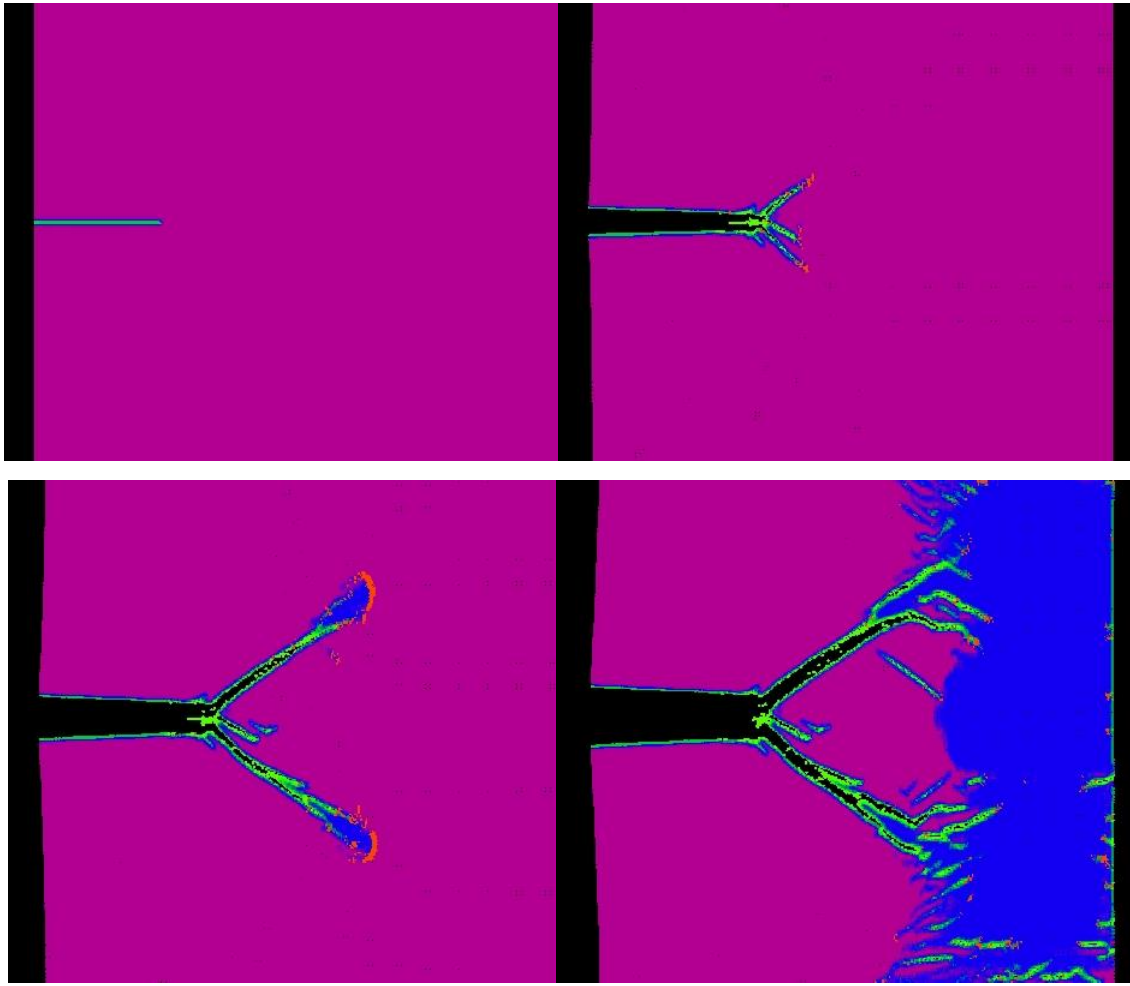
- Similar to previous example but with higher strain rate applied at the boundaries.
- Red indicates bonds currently undergoing damage.
    - These appear ahead of the visible discontinuities.
- Blue/green indicate damage (broken bonds).
- More and more energy is being built up ahead of the crack – it can't keep up.
    - Leads to fragmentation.



More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Dynamic crack branching (video)

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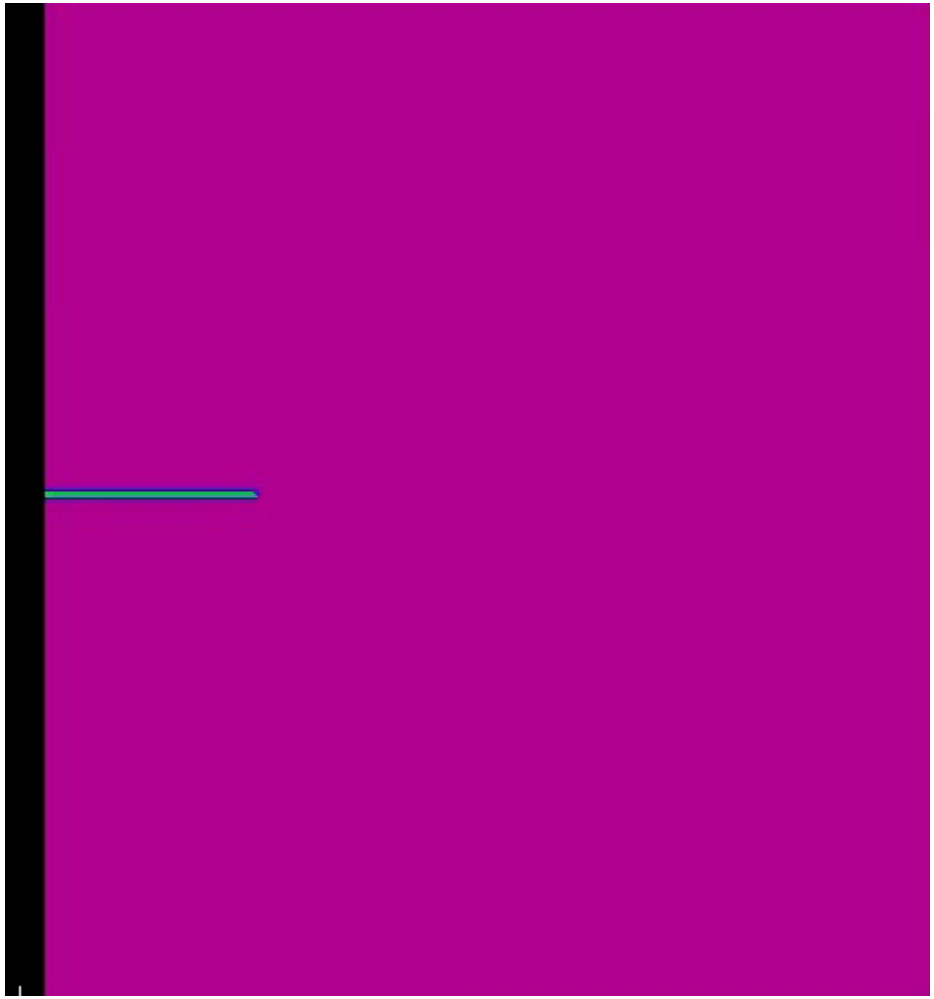

More on dynamic fracture: see Ha & Bobaru (2010, 2011)

Some peridynamic multiscale methods and results

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- 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).
- Coarse-graining (SS, 2011).
- Two-scale evolution equation for composites (Alali & Lipton, 2012).
- PFHMM method for atomistic-to-continuum coupling (Rahman, Foster, & Haque, 2014).

Concurrent multiscale method for defects

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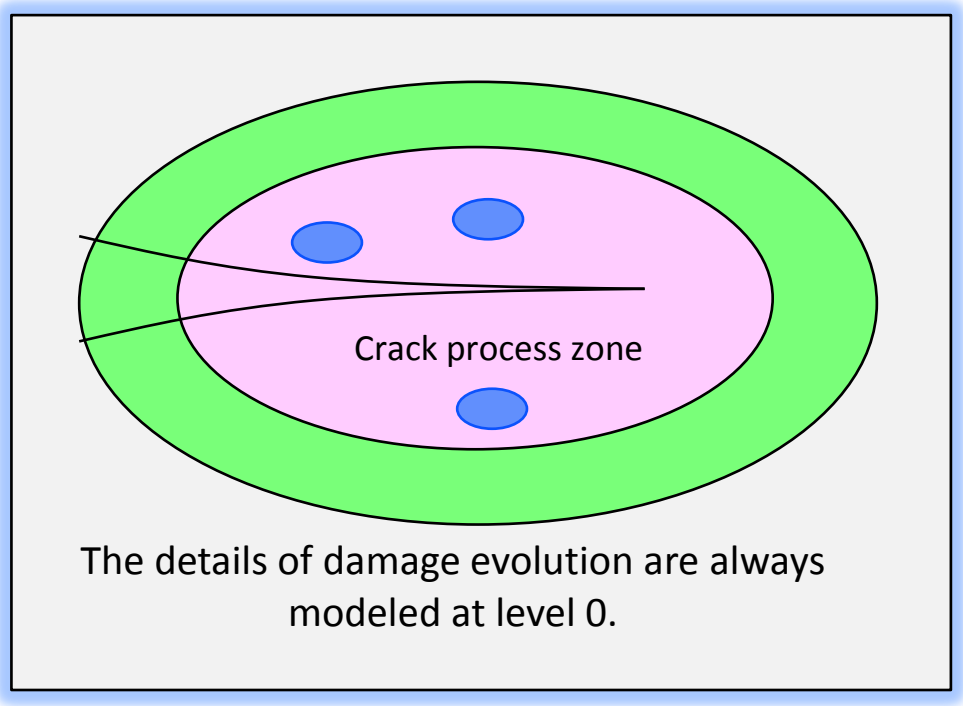
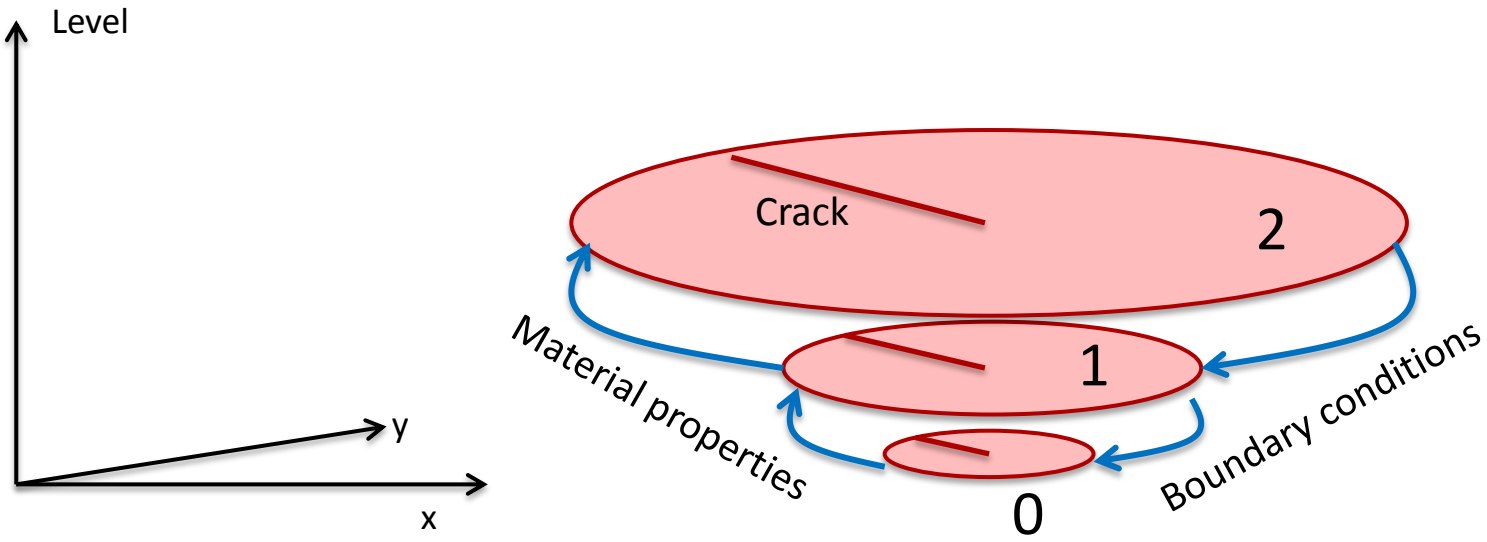
- Apply the best practical physics at the smallest length scale (near a crack tip).
- Scale up hierarchically to larger length scales.
- Each level is related to the one below it by the same equations.
  - Any number of levels can be used.
- Adaptively follow the crack tip.



Concurrent solution strategy

- The equation of motion is applied only within 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

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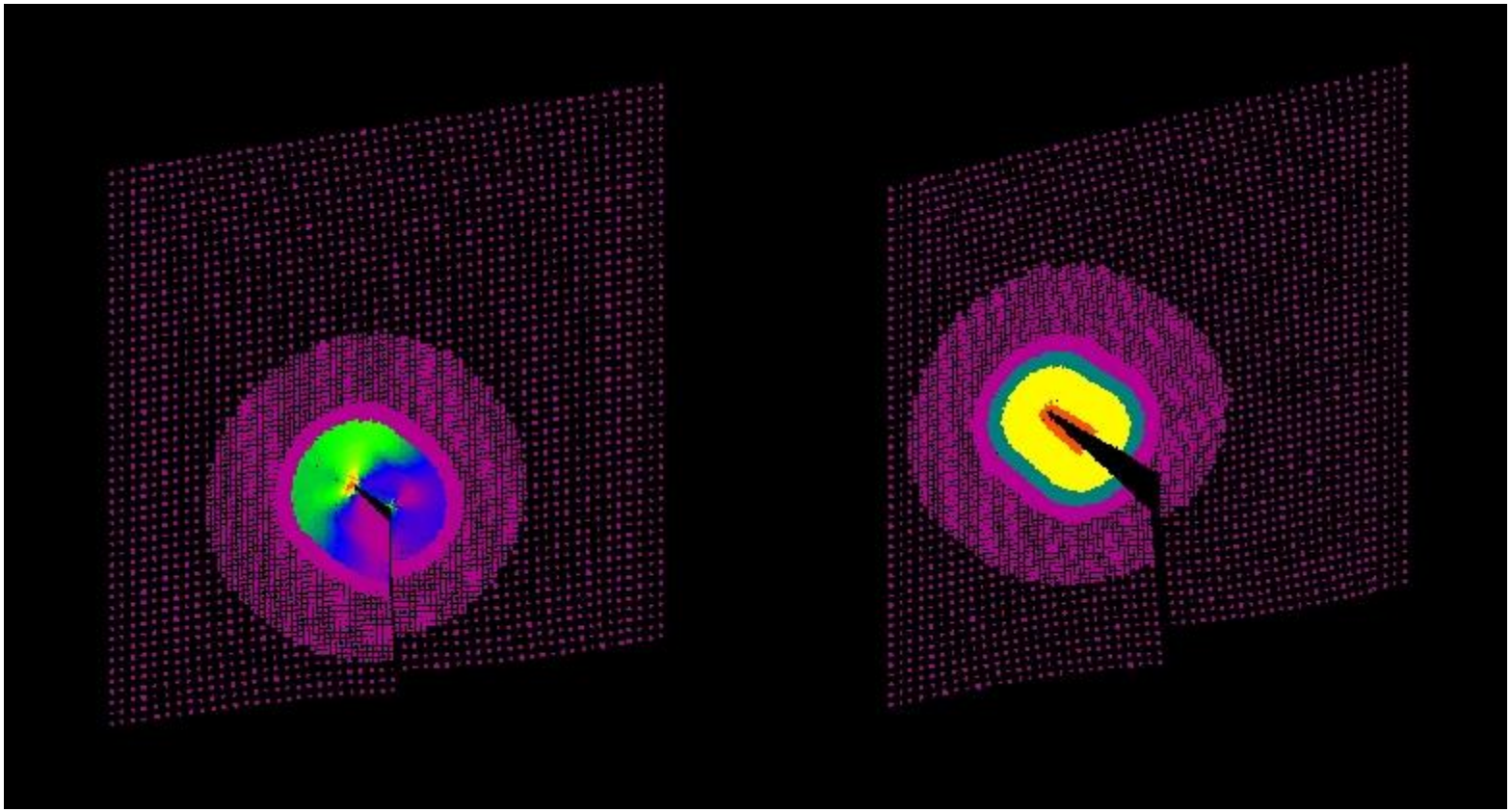
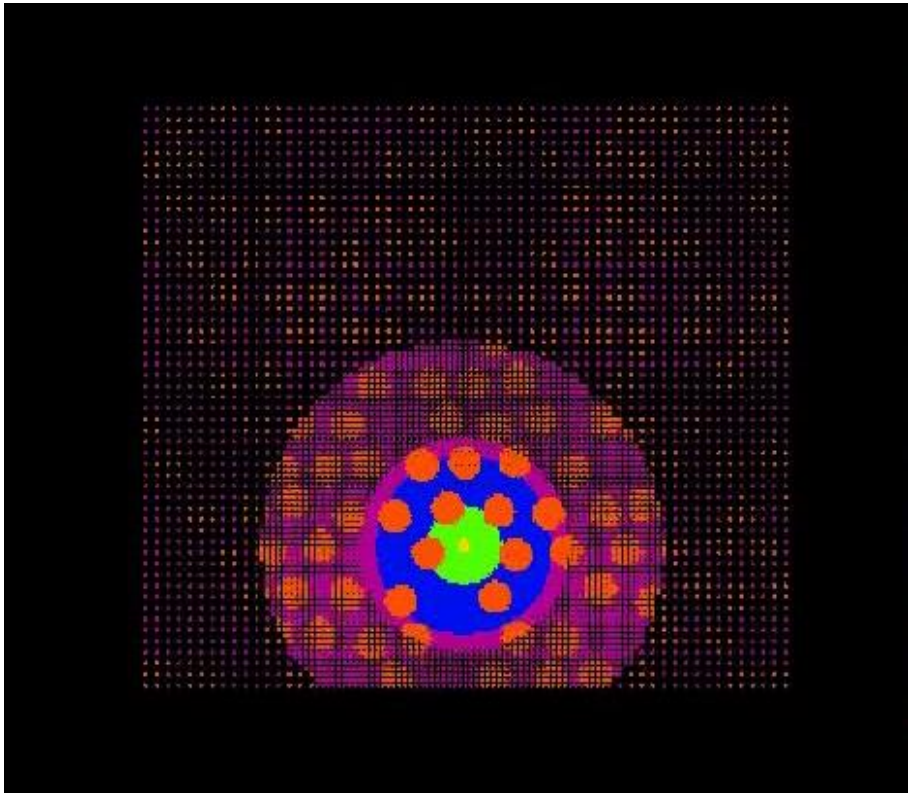


Bond strain

Damage process zone

Multiscale crack growth in a heterogeneous medium (video)



Branching in a heterogeneous medium

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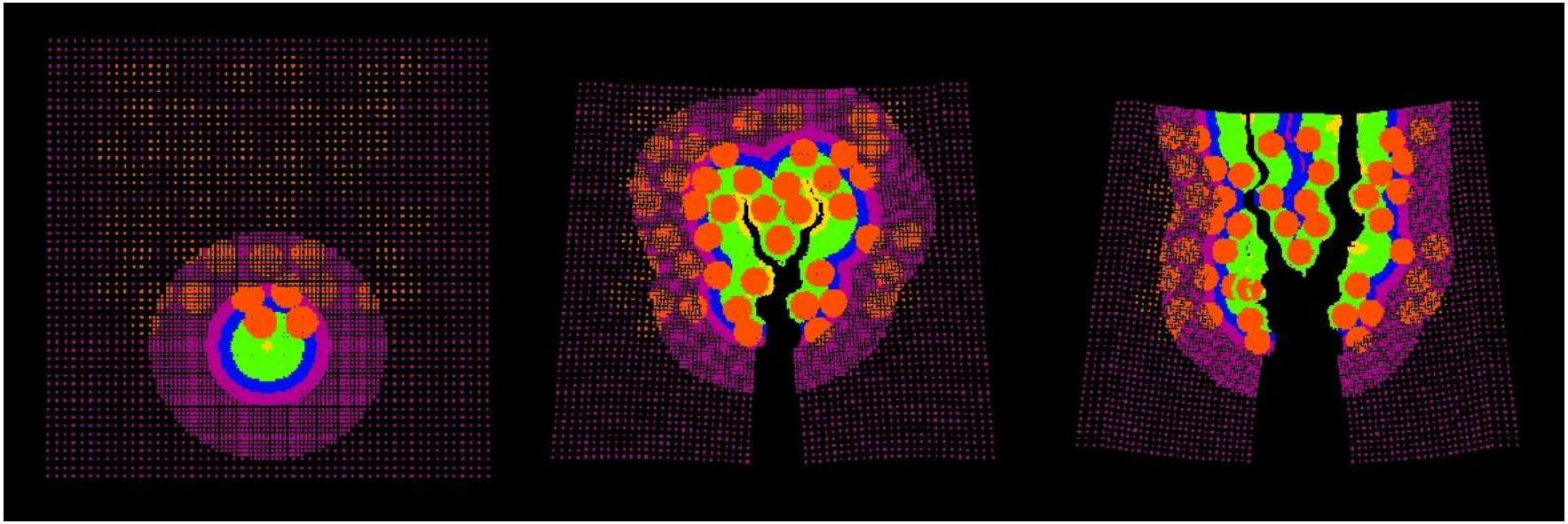
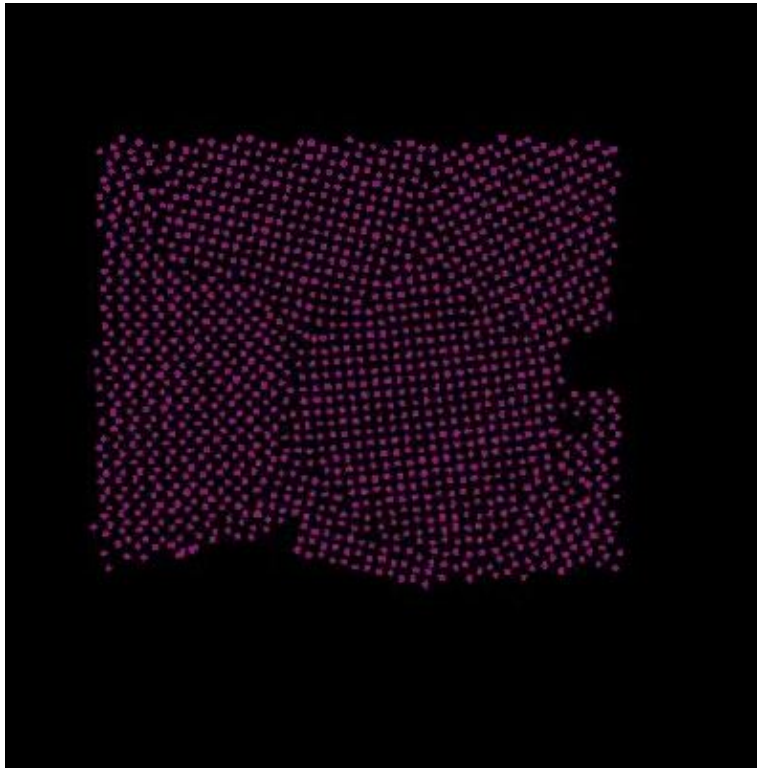
- Crack grows between randomly placed hard inclusions.



Level 0: calibrating a peridynamic model using molecular dynamics

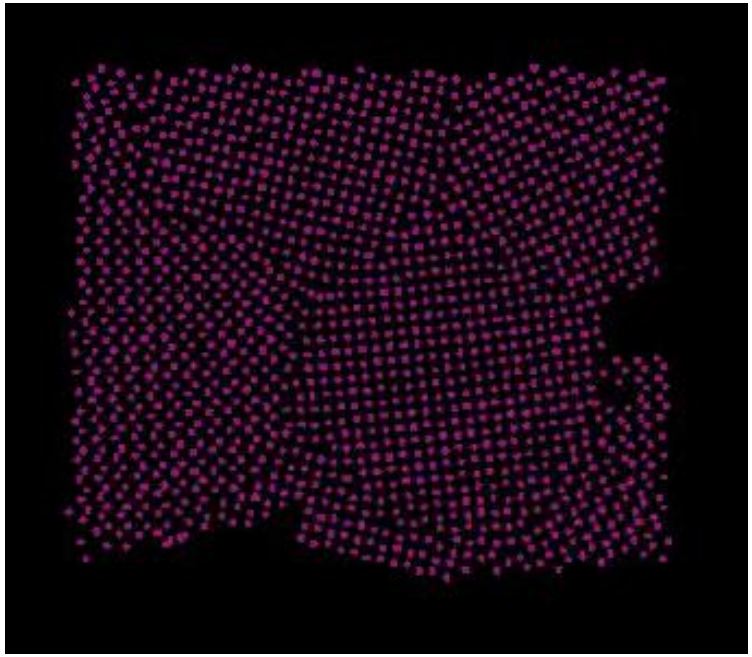
- The concurrent multiscale method, in spite of subcycling the lower levels, is still not efficient enough to use MD in level 0 for growing cracks.
- Instead: Use MD to calibrate a continuum model.

- Video show smoothed atomic positions in a LAMMPS model of Al polycrystal (courtesy David Newsome, CFD Research Corp.)
- Yellow-red: bond strains > 1.0.



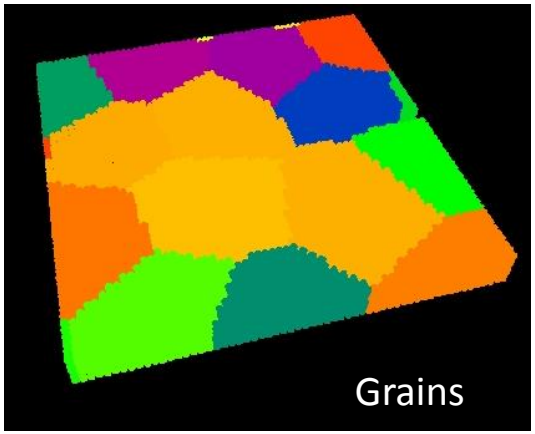
Peridynamic mesoscale simulations using properties determined from MD

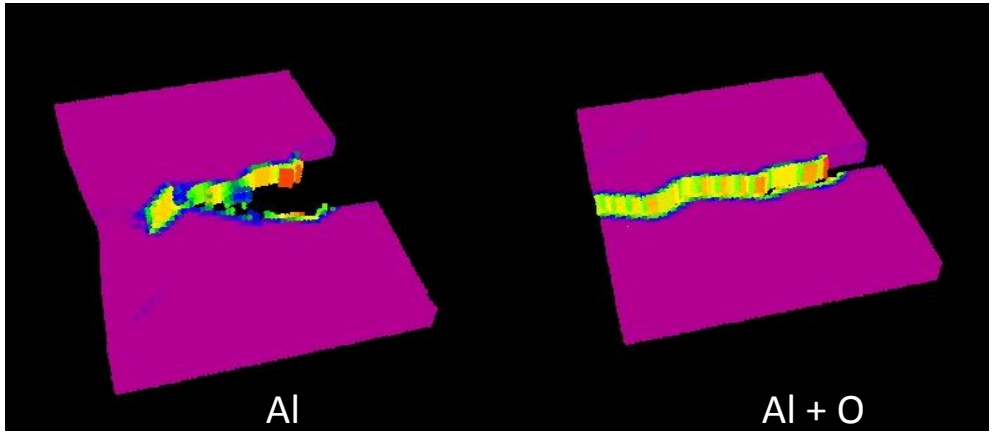
- Continuum model of a polycrystal shows the effect of embrittlement due to oxide.



Time-averaged atomic positions (LAMMPS).
Colors = peridynamic bond strain.

Calibrated peridynamic bond interactions

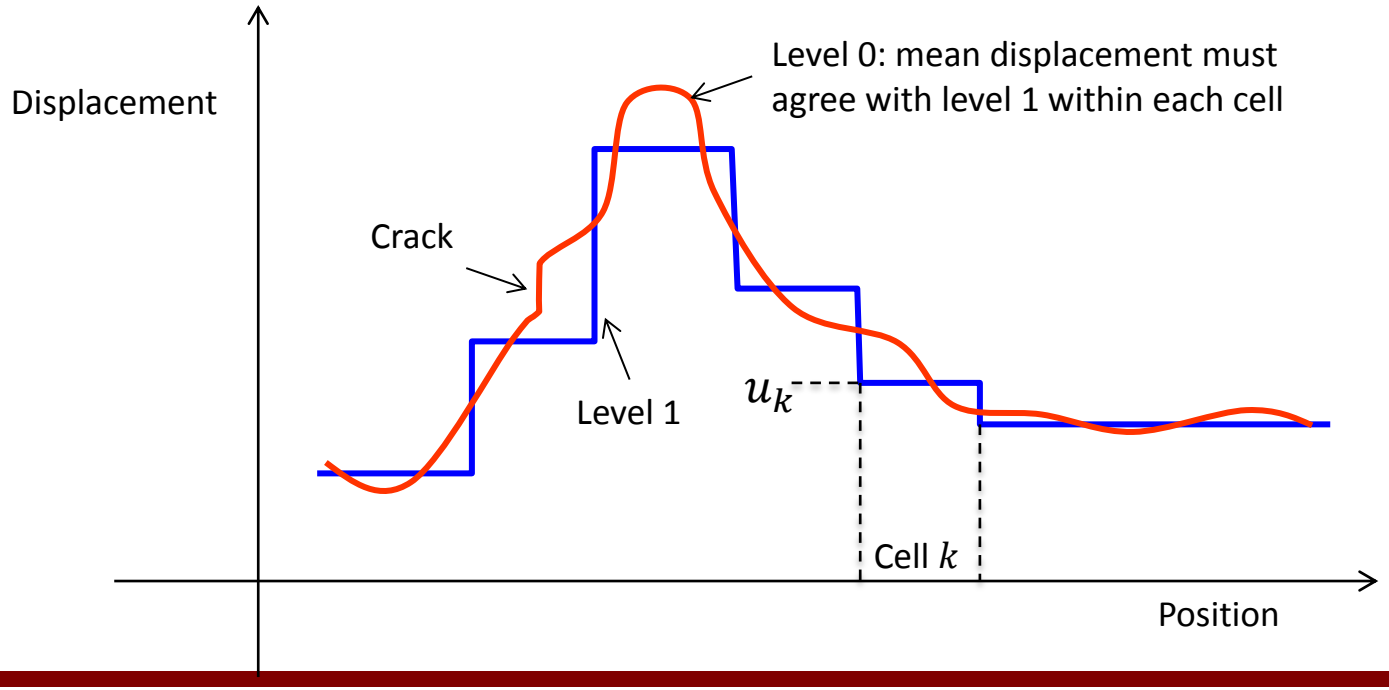




Colors indicate damage (broken bonds)

Coarse-graining to get higher-level material properties

- How can we rigorously derive higher-level material properties from lower levels?
- Divide the level 0 region into K cells $\mathcal{B}_k$.
- The mean displacement in each cell is a coarse-grained DOF u_k.



Coarse-graining, ctd.

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- Define the constrained potential energy by

$$\Phi = \int_{\mathcal{B}} (W - bu)\, dx - \sum_{k=1}^{K} \lambda_k \left(\int_{\mathcal{B}} (\phi_k u\, dx - u_k \right)$$

where $\phi_k(x) = 1/\text{vol}\ \mathcal{B}_k$ in cell k, 0 elsewhere. The λ_k are Lagrange multipliers.

- The Euler-Lagrange equation is

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

where k is the cell that contains x.

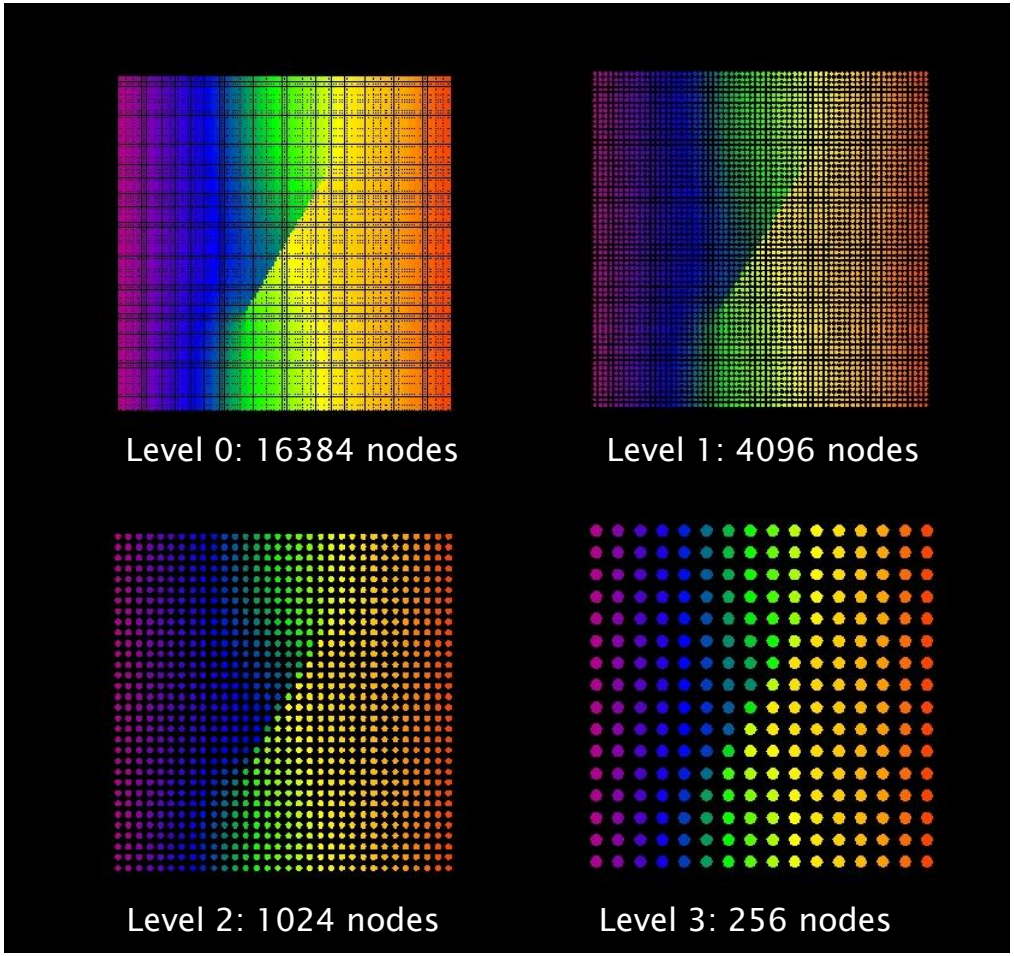
- So, λ_k is the force density required to constrain the mean displacements.
- The coarse-grained micromodulus is

$$C_{ki} = \lambda_k / u_i$$

if we set $0 < u_i << 1$, all other cell displacements 0.

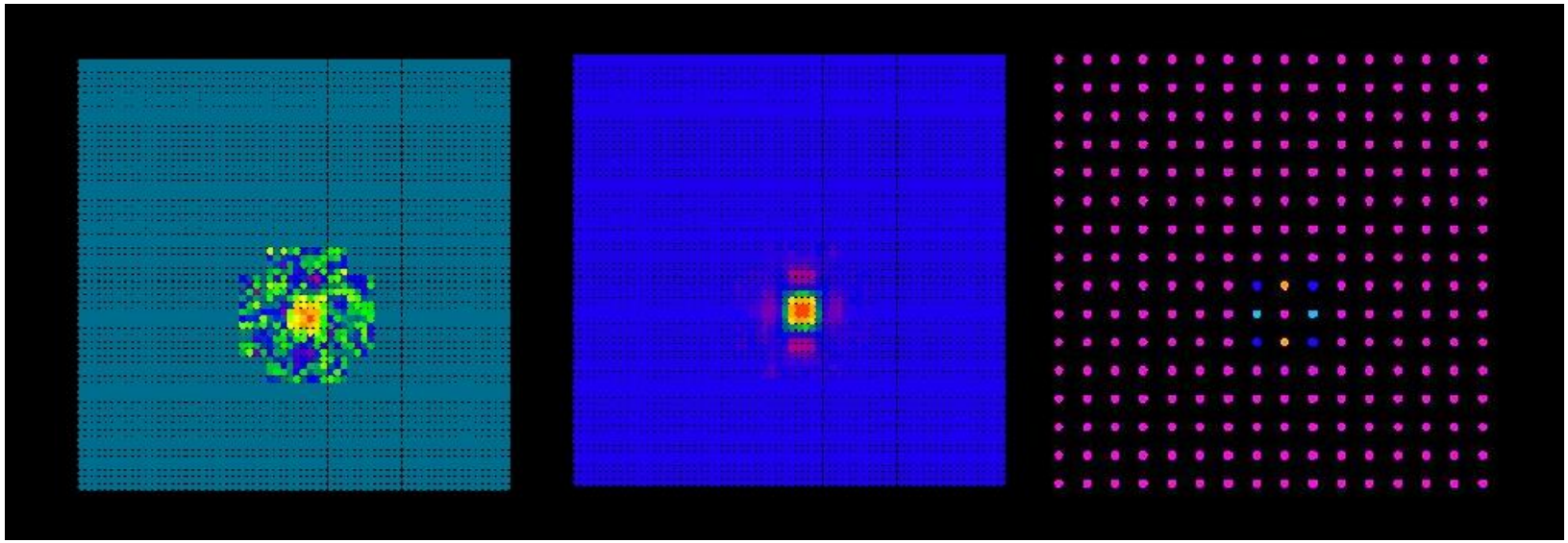
Coarse graining verification: crack in a plate

- Example: Solve the same problem in four different levels – results are the same.
- The crack is hidden rather than smeared out.



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

Defining damage from coarse-grained material properties

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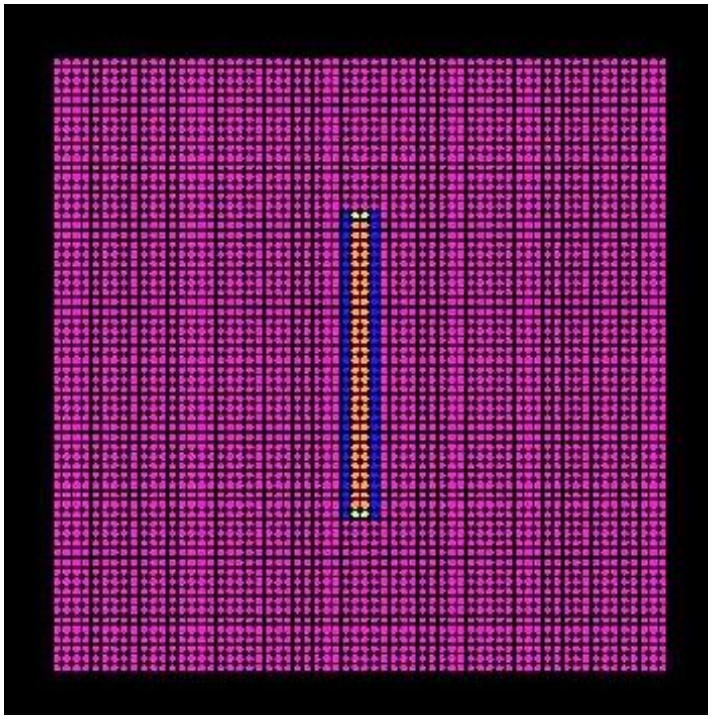
- Define bonds to be damaged if their coarse-grained micromodulus is less than a tolerance.
- This allows damage to be determined without deforming the MD grid.



Level 1 damage contours deduced from coarse-grained properties

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:

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

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

Coarse graining a damage criterion

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- 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.

Summary

- Concurrent multiscale:
  - Adaptively follow crack tips.
  - Apply the best practical physics in level 0.
  - MD time step is impractical. Instead…
- Calibrate a peridynamic damage model from an MD simulation.
  - Derives continuum damage parameters (“parameter passing”).
- 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.