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Coarse Graining in Peridynamics

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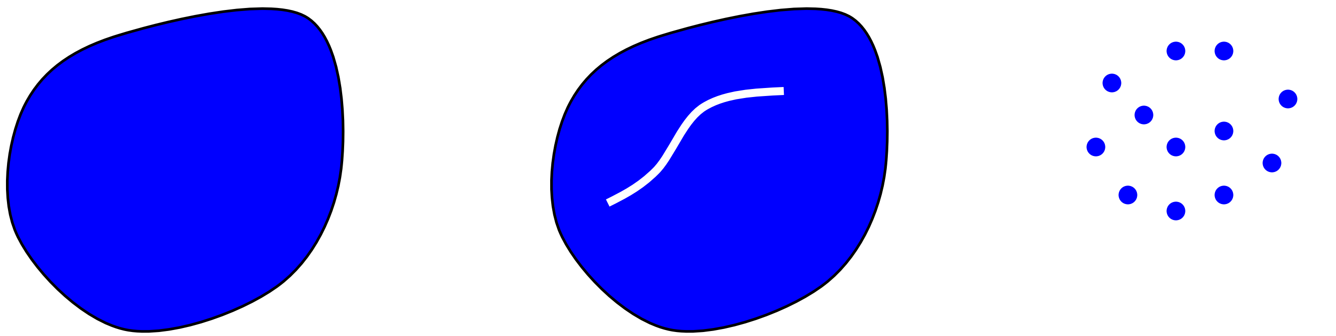
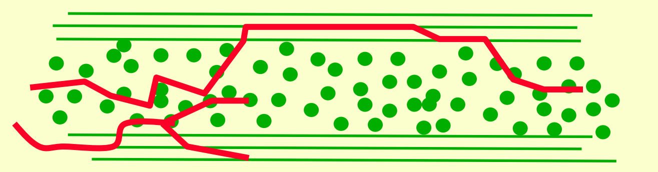
Purpose of peridynamics

- 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.



Complex crack path in a composite

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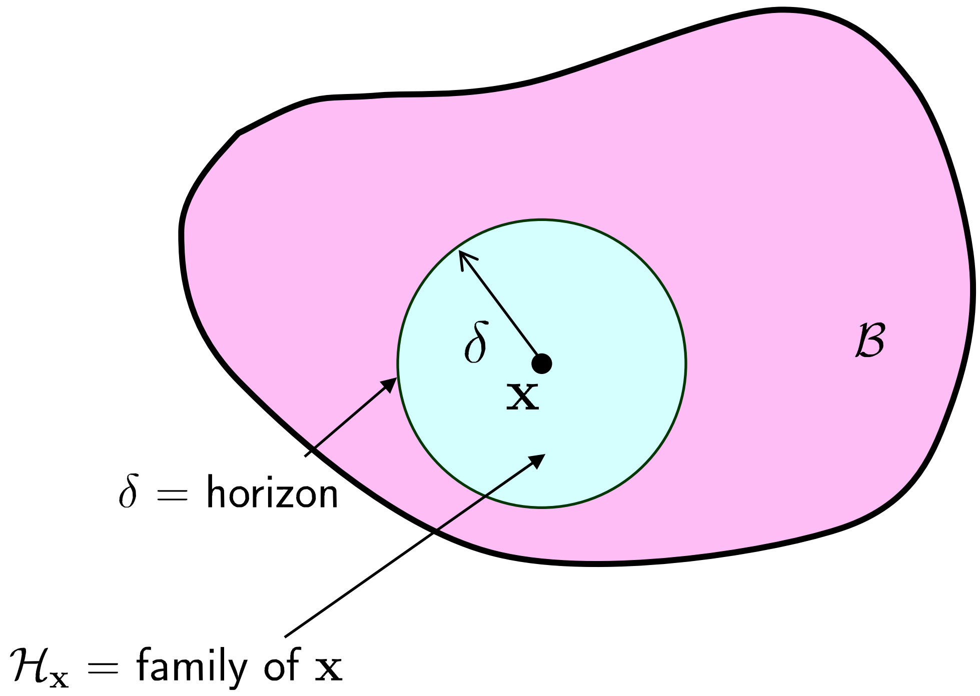
Peridynamics basics: Horizon and family

- 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 $\mathbf{x}$, $\mathcal{H}_\mathbf{x}$.



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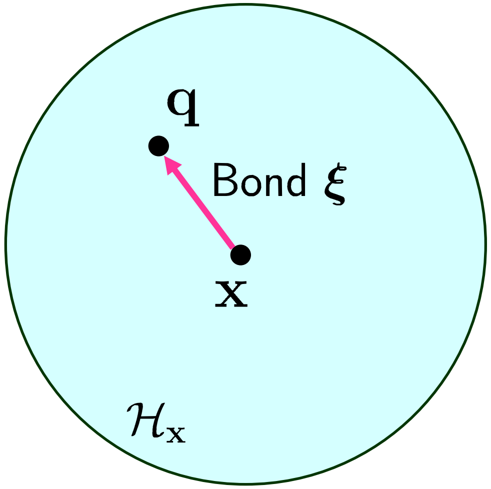
States

- A *state* is a function defined on all the bonds in $\mathcal{H}_{\mathbf{x}}$.
- Notation for states: $\underline{\mathbf{A}}\langle \boldsymbol{\xi} \rangle$.
- *Vector state:* $\underline{\mathbf{A}}\langle \cdot \rangle : \mathcal{H} \to \mathbb{R}^3$ where $\mathcal{H}$ is the set of all the bonds in $\mathcal{H}_{\mathbf{x}}$.



SS, Askari, Epton, Wecker, & Xu, Peridynamic States and Constitutive Modeling, J. Elast (2007)

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Vector states take the place of tensors

- The *deformation state* maps each bond to its deformed image:

$$\underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q},t)-\mathbf{y}(\mathbf{x},t).$$

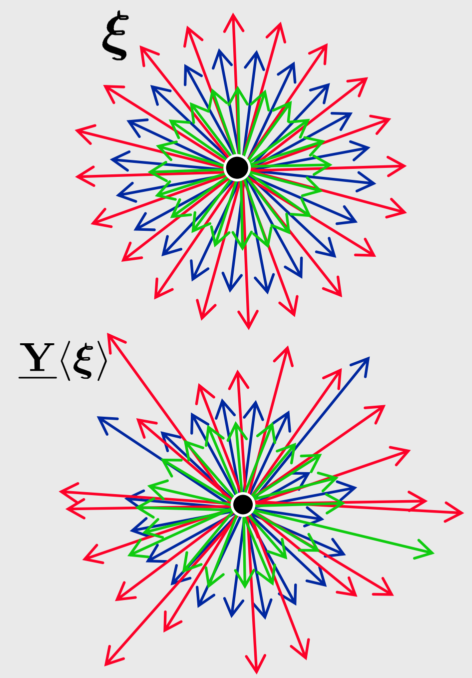
- The *force state* maps a bond to its *bond force*:

$$\underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle = \mathbf{t}(\mathbf{q},\mathbf{x},t).$$

- Constitutive model is a state-valued function of a state:

$$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$$

- Compare standard theory: $\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$.



Deformed bonds in $\mathcal{H}_{\mathbf{x}}$

Summary of nonlinear, state based PD

- Equation of motion:

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \mathbf{L}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t)$$

  where the internal force density at $\mathbf{x}$ is given by

$$\mathbf{L}(\mathbf{x},t) = \int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\, dV_{\mathbf{q}}$$

  and $\mathbf{b}$ is the body force density.

- Pairwise force density is given by

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

  where $\mathbf{t}$ is determined by the constitutive model:

$$\mathbf{t}(\mathbf{q},\mathbf{x},t) = \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}).$$

Force state at $\mathbf{x}$, t

Constitutive model

Elastic materials

- Strain energy density:

$$W(\mathbf{x},t) = \hat{W}(\underline{\mathbf{Y}}[\mathbf{x},t])$$

- Compare standard theory:

$$W(\mathbf{x},t) = \hat{W}(\mathbf{F}(\mathbf{x},t)), \qquad \mathbf{F} := \frac{\partial \mathbf{y}}{\partial \mathbf{x}}.$$

- Bond force:

$$\mathbf{t}(\mathbf{q},\mathbf{x},t) = \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{W}_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}})$$

where $\hat{W}_{\underline{\mathbf{Y}}}$ is the Fréchet derivative of $\hat{W}$ with respect to $\underline{\mathbf{Y}}$.

Linearized peridynamics

- Suppose $|\mathbf{u}| \ll \delta$. Equilibrium equation becomes

$$\mathbf{L}(\mathbf{x}) + \mathbf{b}(\mathbf{x}) = \mathbf{0}$$

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

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

- $\mathbf{C}$ involves the second Fréchet derivatives of strain energy density $\hat{W}_{\underline{\mathbf{YY}}}$:

$$\mathbf{C}(\mathbf{x},\mathbf{q}) = \int_{\mathcal{B}} \Big(\hat{W}_{\underline{\mathbf{YY}}}[\mathbf{x}]\langle \mathbf{p}-\mathbf{x}, \mathbf{q}-\mathbf{x}\rangle - \hat{W}_{\underline{\mathbf{YY}}}[\mathbf{p}]\langle \mathbf{x}-\mathbf{p}, \mathbf{q}-\mathbf{p}\rangle + \hat{W}_{\underline{\mathbf{YY}}}[\mathbf{q}]\langle \mathbf{x}-\mathbf{q}, \mathbf{p}-\mathbf{q}\rangle\Big)\ dV_{\mathbf{p}}$$

- $\mathbf{C}$ 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)

EMU (and LAMMPS) numerical method

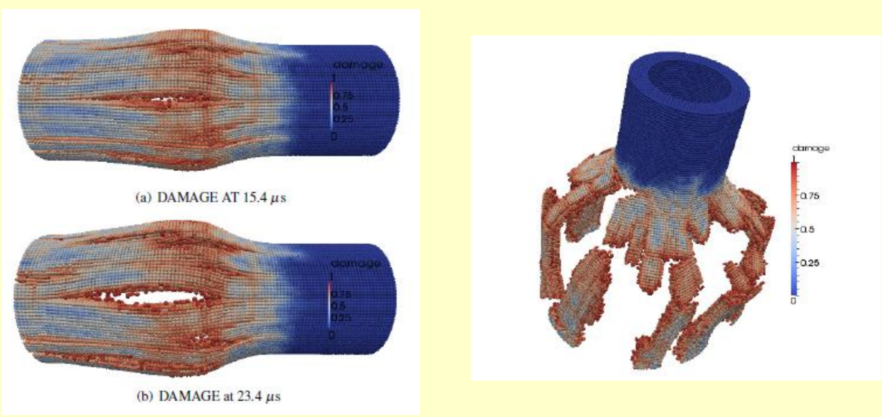
- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

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

$$\downarrow$$

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

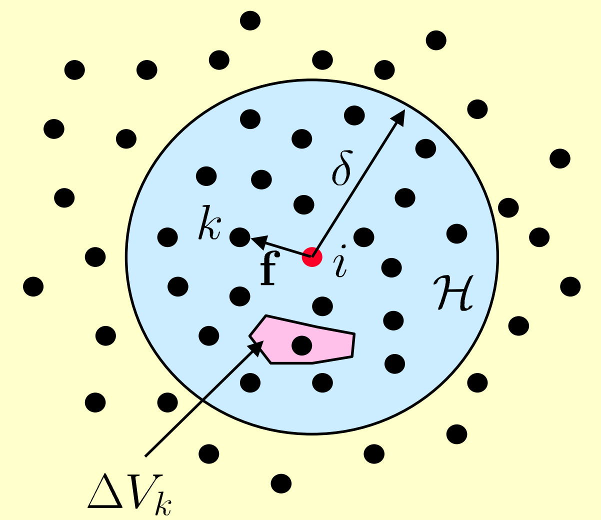
- Looks a lot like MD!
- LAMMPS implementation by M. Parks & . Seleson



(a) DAMAGE AT 15.4 μs

(b) DAMAGE at 23.4 μs

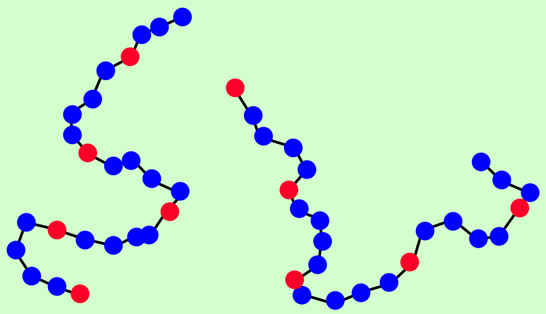
Method is also available in Sierra (D. Littlewood)



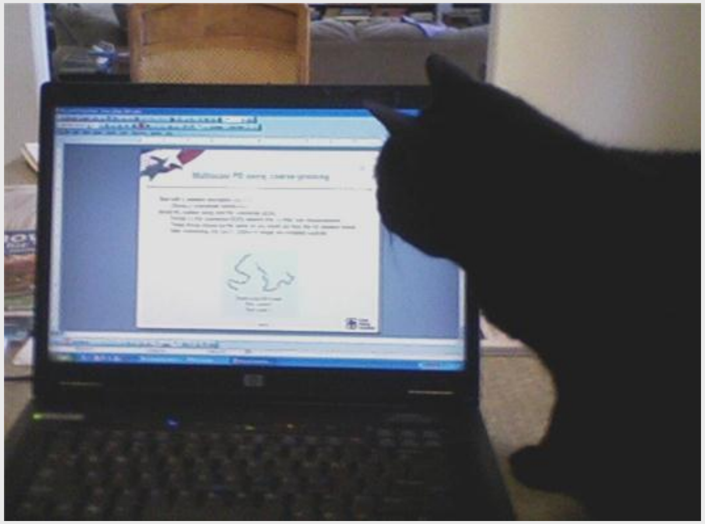
Discretized model in the reference configuration

Multiscale PD using coarse-graining

- Start with a detailed description (level 0).
  - Choose a *coarsened* subset (level 1).
- Model the system using only the coarsened DOFs…
  - Forces on level 1 DOFs depend only on their own displacements.
  - These forces should be the same as you would get from the full detailed model.
  - The level 0 DOFs no longer appear explicitly.

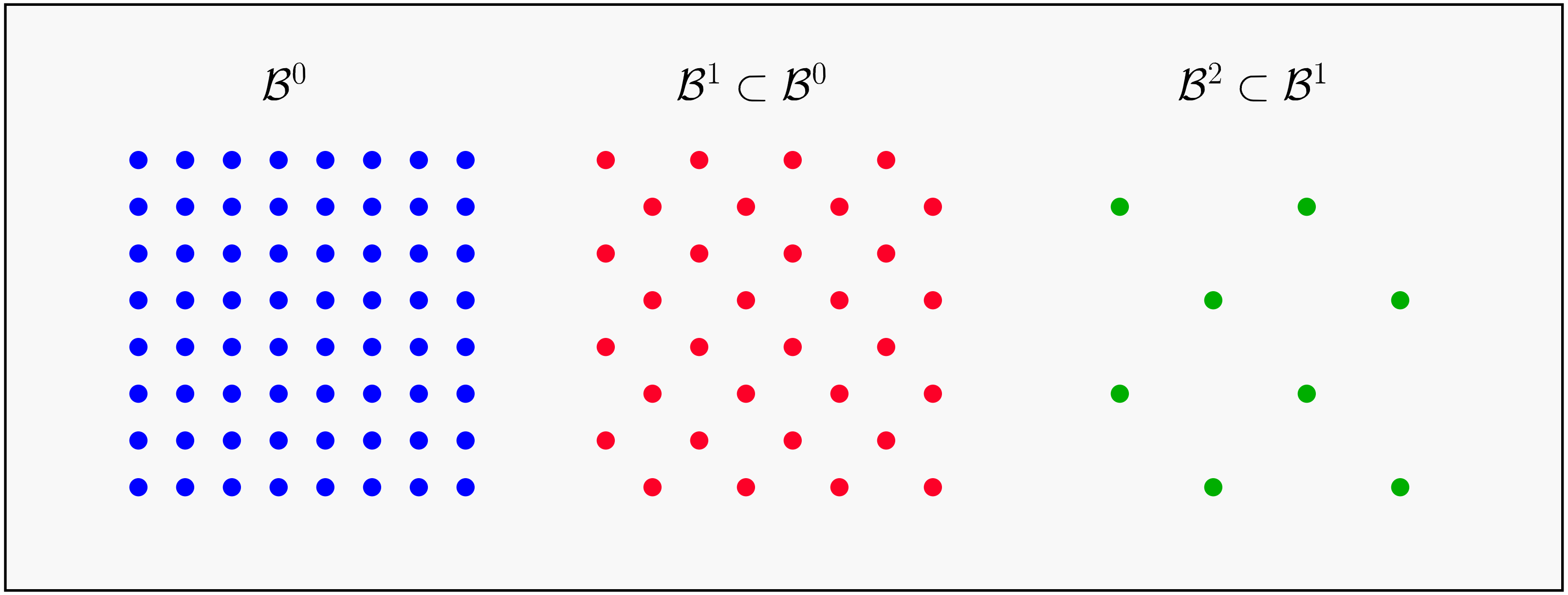


Small-scale MD model
Blue: Level 0
Red: Level 1



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: $\mathcal{B}^M \subset \mathcal{B}^{M-1} \subset \cdots \subset \mathcal{B}^1 \subset \mathcal{B}^0$.



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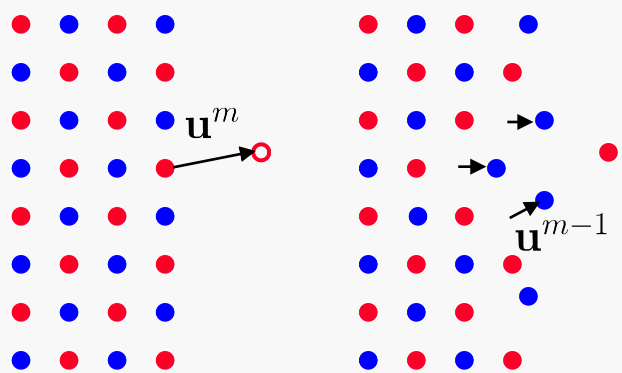
Each level's displacements are determined by the next higher level

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



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

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

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

Each level has the same mathematical structure

- Equilibrium equation for level m involves only the level m displacements:

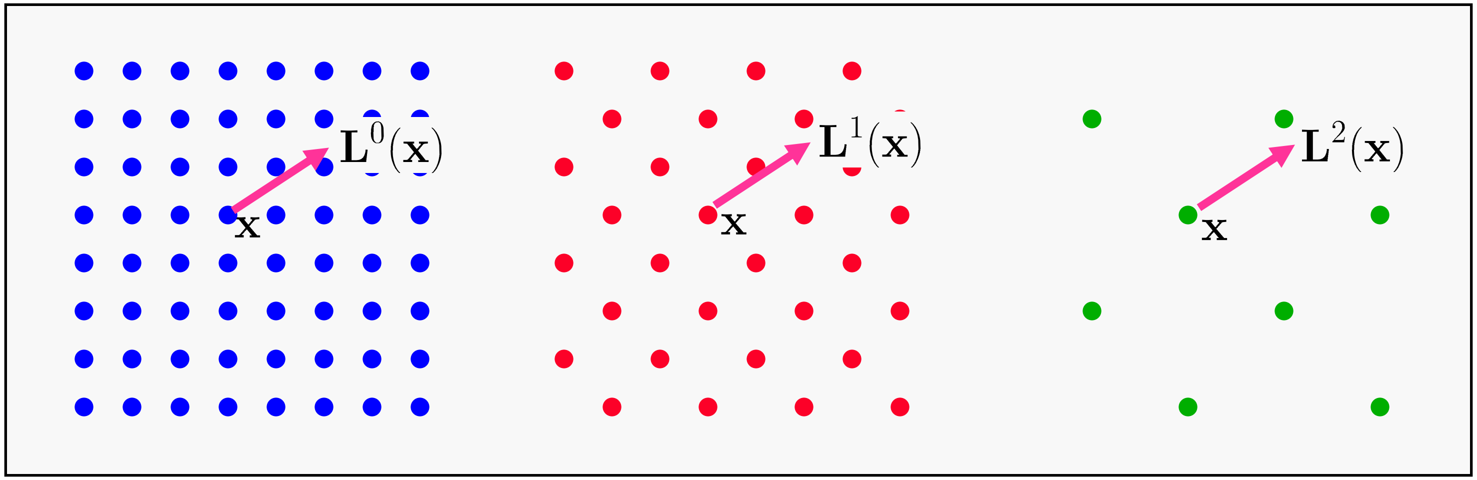
$$\mathbf{L}^m(\mathbf{x}) = \int_{\mathcal{B}^m} \mathbf{C}^m(\mathbf{x},\mathbf{q})(\mathbf{u}^m(\mathbf{q}) - \mathbf{u}^m(\mathbf{x}))\, dV_{\mathbf{q}} = \mathbf{0}$$

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:

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



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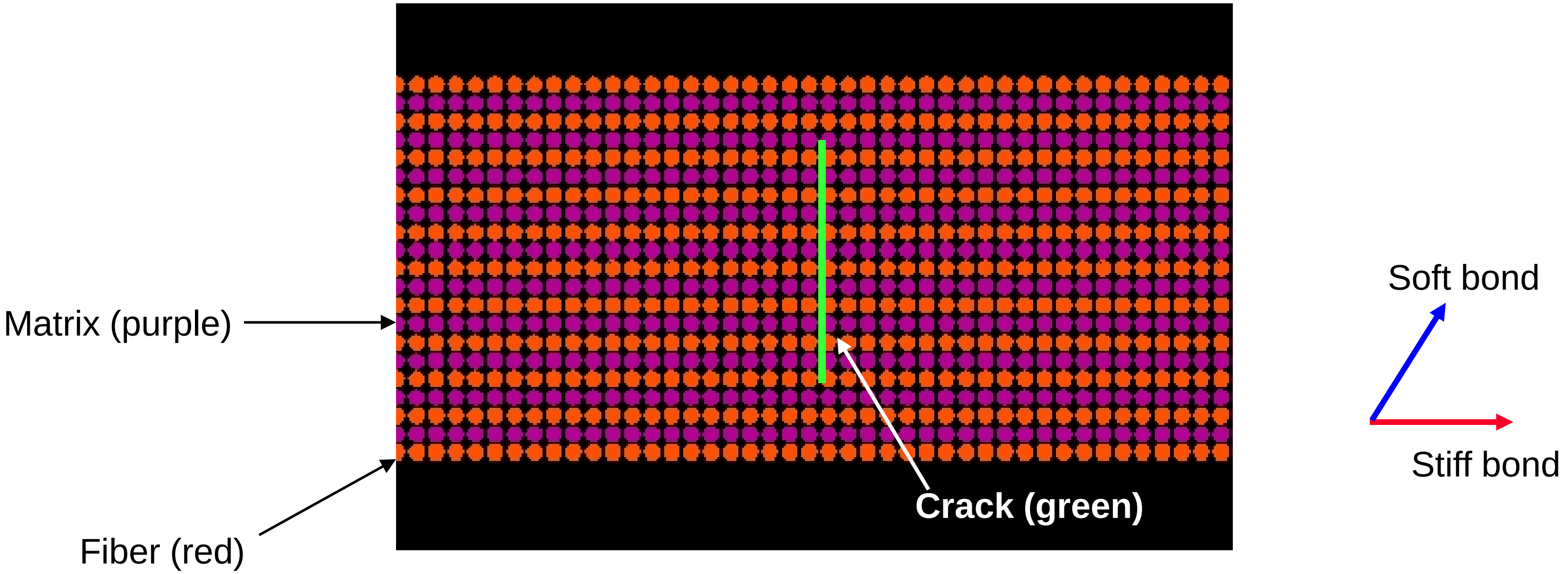
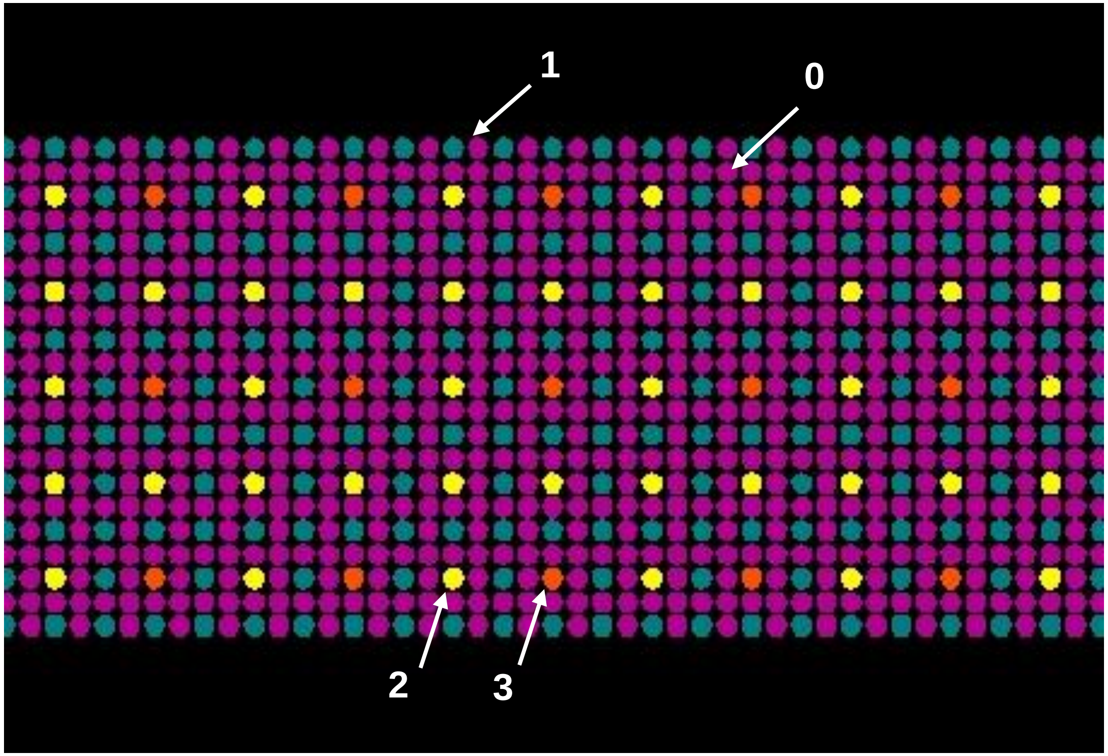
Example: Composite with a crack



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

3 levels of coarsening



- Purple: Level 0
- Green: Level 1
- Yellow: Level 2
- Red: Level 3
- Each level $m+1$ has $1/4$ as many nodes as level m.

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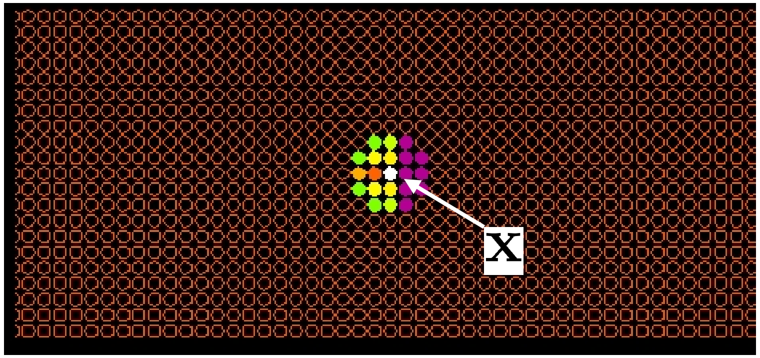
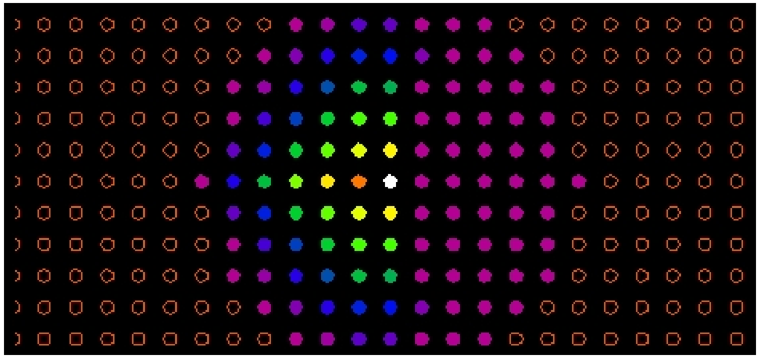
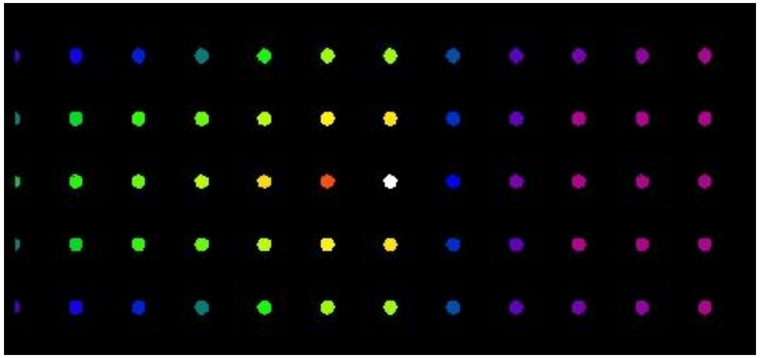
Composite bar with defect: Coarsened micromodulus



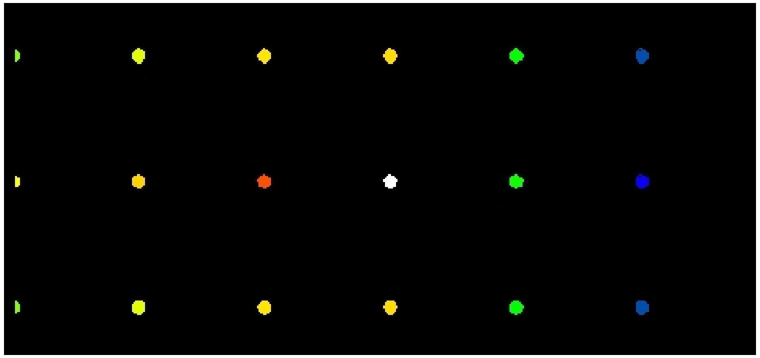
Level 0



Level 1



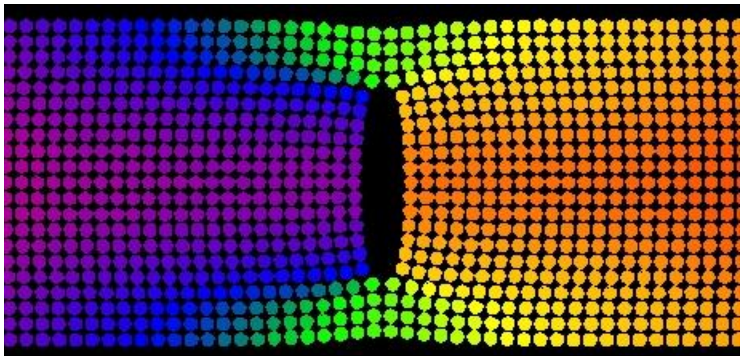
Level 2



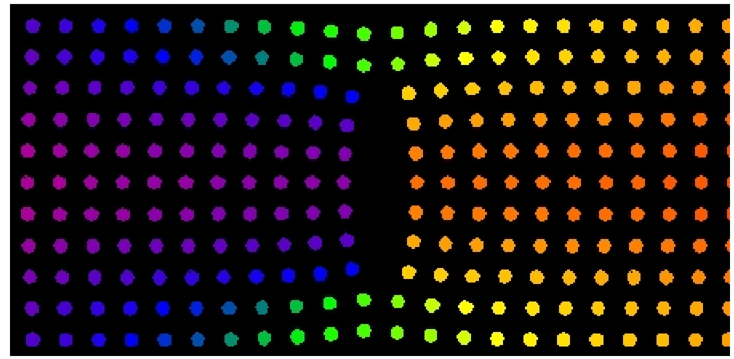
Level 3

- 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.

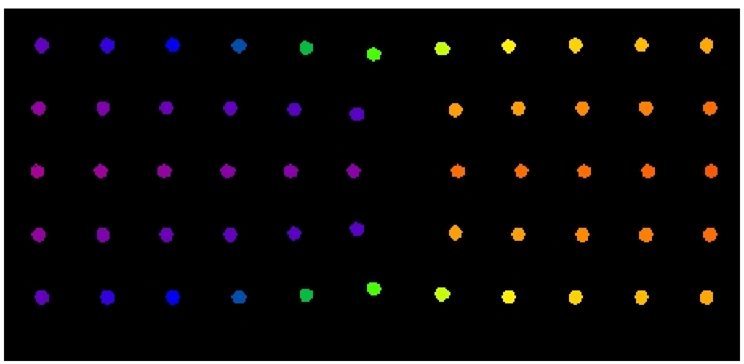
Composite bar with defect: Displacements



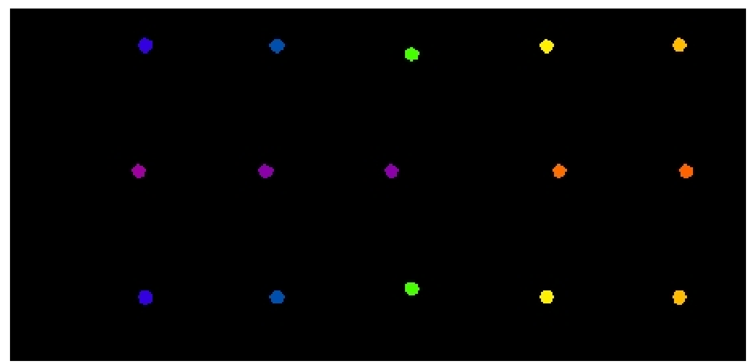
Level 0



Level 1



Level 2



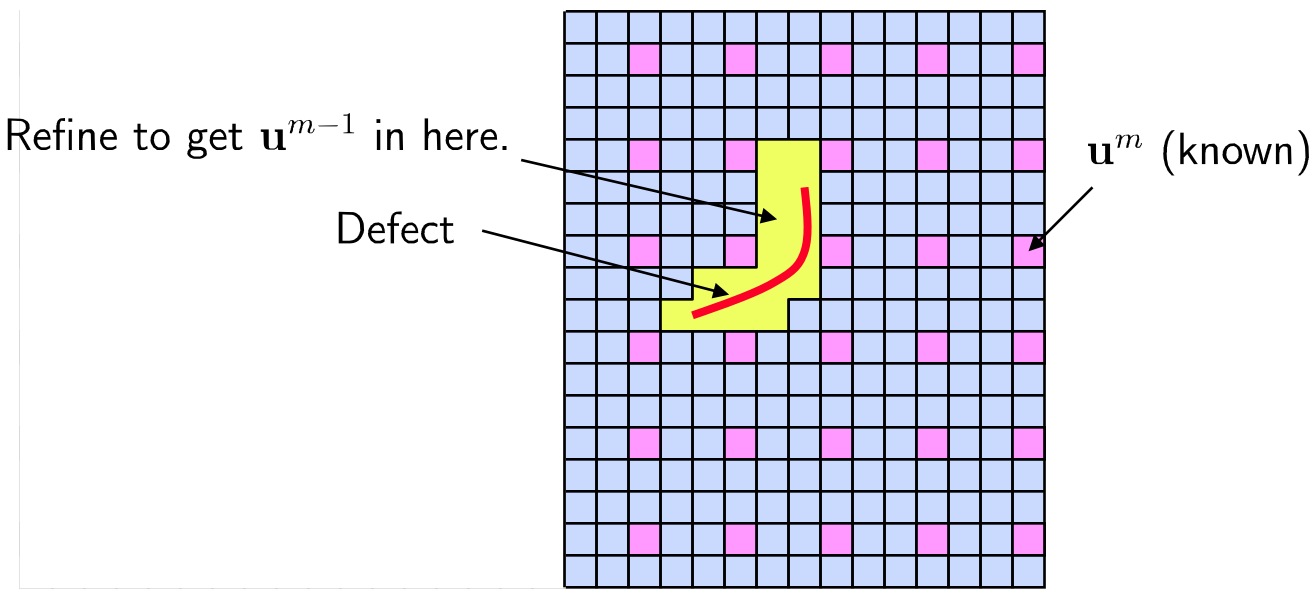
Level 3

- 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.

Remarks

- In practice, $\mathbf{S}^m$ has to be found numerically by discretizing the level $m-1$ equilibrium equation.
- We can *refine* in some region of interest by reversing the coarsening procedure.

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



Coarse graining in dynamics: Strong nonlocality in time

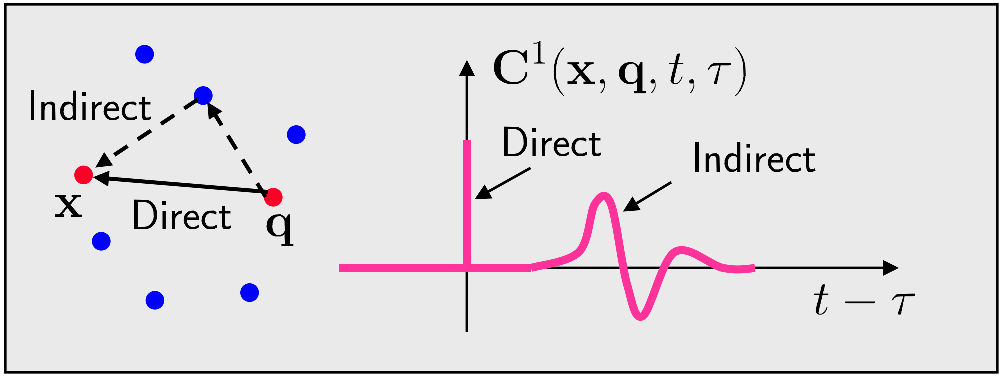
- Prescribe $\mathbf{u}^1$ over time as well as position.
- Solution operator in $\mathcal{B}^0$ is now time-dependent:

$$\mathbf{u}^0(\mathbf{x},t) = \int_{-\infty}^{\infty}\int_{\mathcal{B}^1} \mathbf{S}^{0,1}(\mathbf{x},\mathbf{q},t,\tau)\mathbf{u}^1(\mathbf{q},\tau)\,dV_{\mathbf{q}}\,d\tau.$$

- End up with time-dependent coarsened micromodulus:

$$\mathbf{L}^1(\mathbf{x},t) = \int_{-\infty}^{\infty}\int_{\mathcal{B}^1} \mathbf{C}^1(\mathbf{x},\mathbf{q},t,\tau)\big(\mathbf{u}^1(\mathbf{q},\tau) - \mathbf{u}^1(\mathbf{x},t)\big)\,dV_{\mathbf{q}}\,d\tau$$

$$\mathbf{C}^1(\mathbf{x},\mathbf{q},t,\tau) = \int_{-\infty}^{\infty}\int_{\mathcal{B}^0} \mathbf{C}^0(\mathbf{x},\mathbf{p},t,\sigma)\mathbf{S}^{0,1}(\mathbf{p},\mathbf{q},\sigma,\tau)\,dV_{\mathbf{p}}\,d\sigma$$



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Discussion

- Method accomplishes the following:
  - Two-way coupling between length scales (coarsening + refinement).
  - Forces on higher level DOFs exactly reproduce the original level 0 model.
  - Effects at smaller length scales are incorporated into larger length scales.

- Limitations:
  - Many issues remain regarding how to make the method efficient.
  - Need to re-linearize for evolving damage or other nonlinearities.

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

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