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Connecting Length Scales with Peridynamic Mechanics

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Peridynamic model of continuum mechanics: Purposes

- To apply the same field equations on or off of cracks.
- To treat discrete particles using the same equations as continua.
- To include long-range forces in a continuum model.

- Why do this?
  - Standard PDEs do not apply on cracks.
  - No natural way to couple atoms to standard PDEs.
  - Classical assumption of contact forces is not accurate at small length scales.

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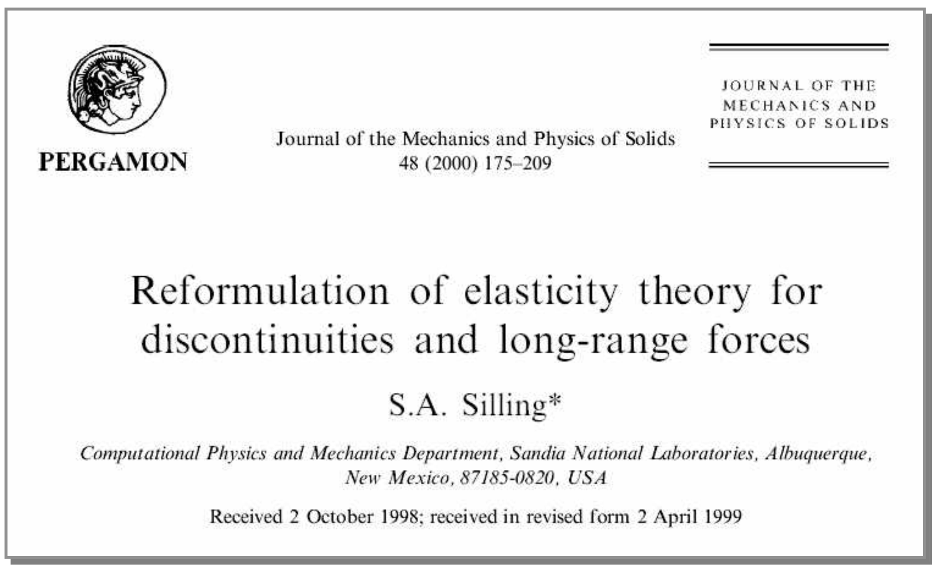
Strategy

Replace the standard PDEs with integral equations.

- The integral equations involve interaction between points separated by finite distances (nonlocality).
- These integral equations are not derivable from the PDEs.
    - But they converge to the PDEs in the limit of small length scales.



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Reformulation of elasticity theory for discontinuities and long-range forces

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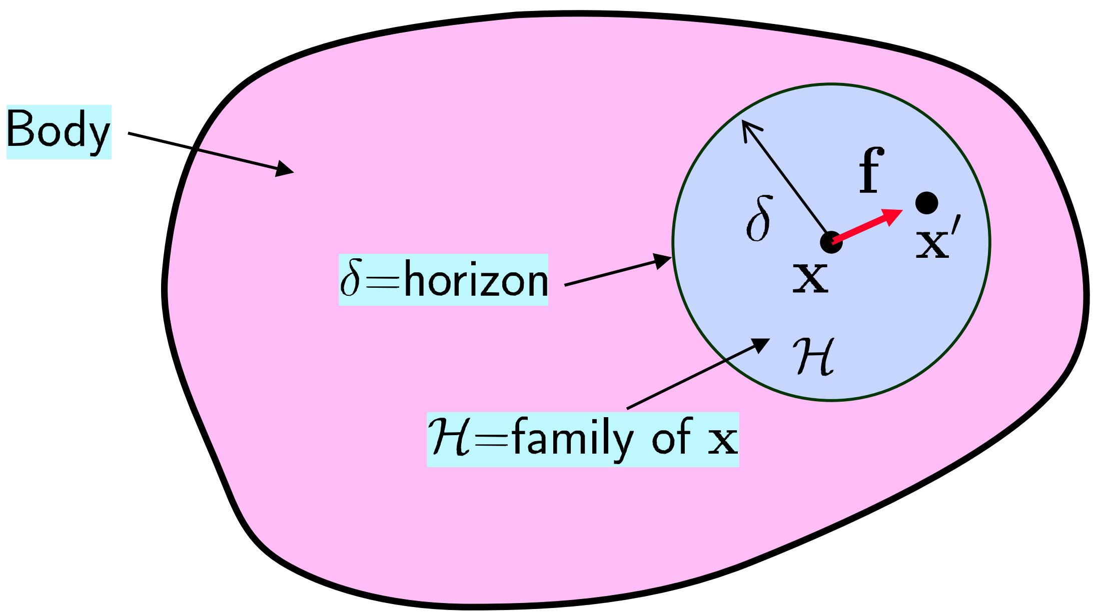
Peridynamic equation of motion

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t),$$

$\mathbf{y}$=motion, $\mathbf{b}$=body force density

$\mathbf{f}$=dual force density (force/volume^2)

The integral sums up the forces that all the $\mathbf{x}'$ exert on $\mathbf{x}$.



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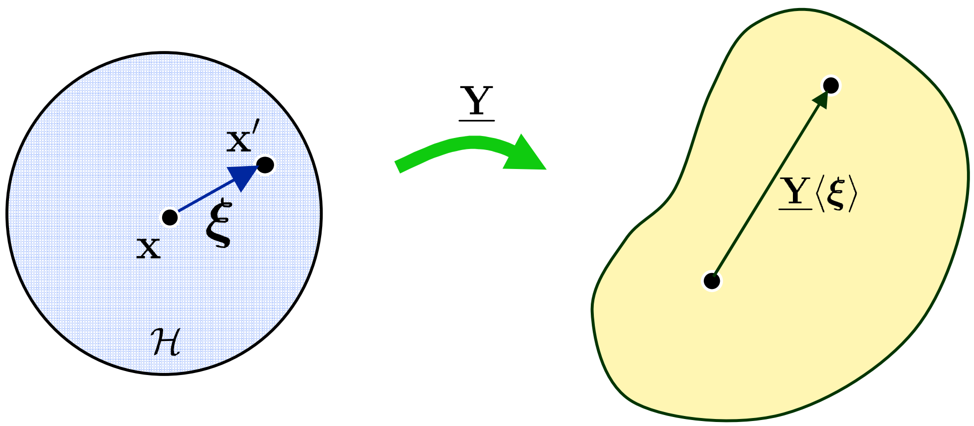
Determining f: Peridynamic states

Strain energy at $\mathbf{x}$ depends collectively on the deformation of the family of $\mathbf{x}$.



Undeformed family of $\mathbf{x}$

Deformed family of $\mathbf{x}$

Standard:	Peridynamic:
$\hat{W}\left(\dfrac{\partial \hat{\mathbf{y}}}{\partial \mathbf{x}}\right)$	$\hat{W}(\underline{\mathbf{Y}})$

Bond forces are found from the Frechet derivative of $\hat{W}$.

$$\mathbf{f}(\mathbf{x}', \mathbf{x}) = \nabla\hat{W}(\mathbf{x}, \mathbf{x}') - \nabla\hat{W}(\mathbf{x}', \mathbf{x})$$

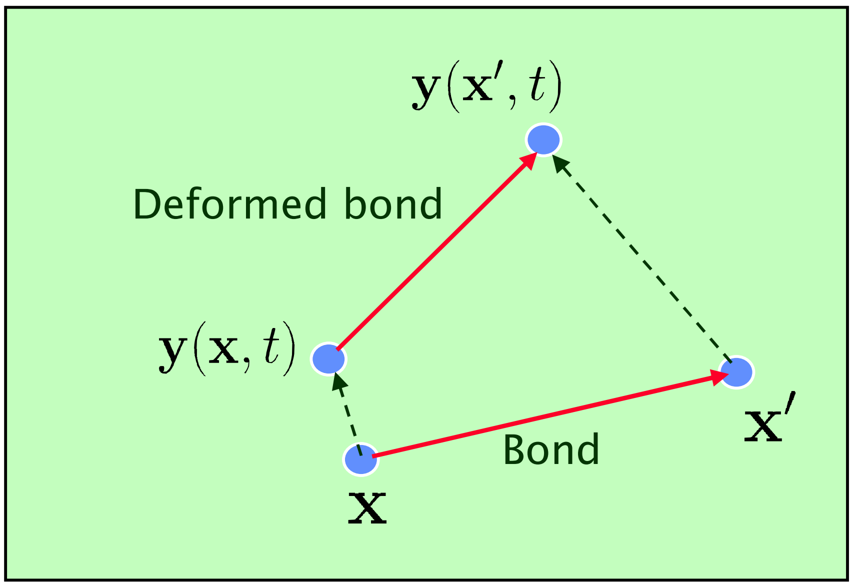
The Frechet derivative $\nabla\hat{W}$ is the work conjugate to $\underline{\mathbf{Y}}$.

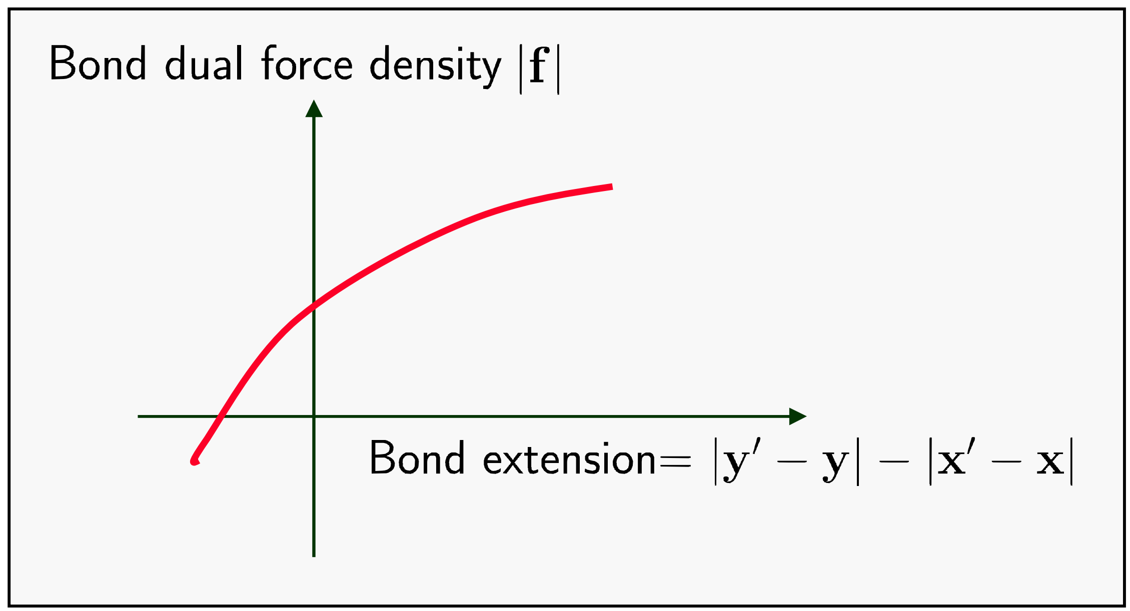
Bond–based materials

Special case: bonds respond independently of each other...

$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = \hat{\mathbf{f}}\Big(\mathbf{y}(\mathbf{x}', t) - \mathbf{y}(\mathbf{x}, t), \mathbf{x}', \mathbf{x}\Big)$$

$\hat{\mathbf{f}}$=pairwise force function (constitutive relation)





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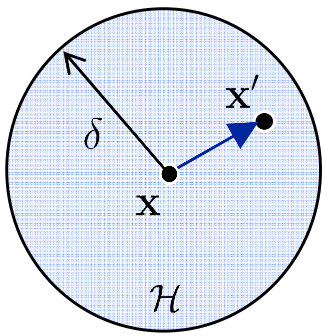
Simplest bond-based material

Linear microelastic material with constant micromodulus k:

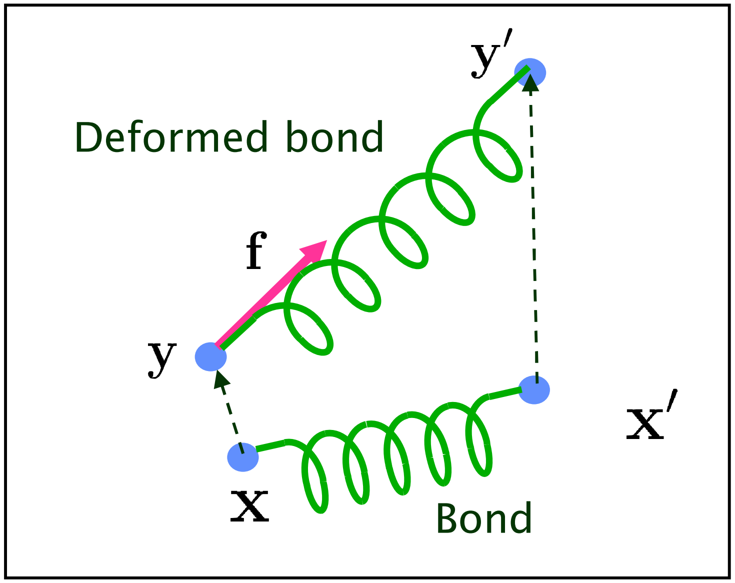
Bond extension

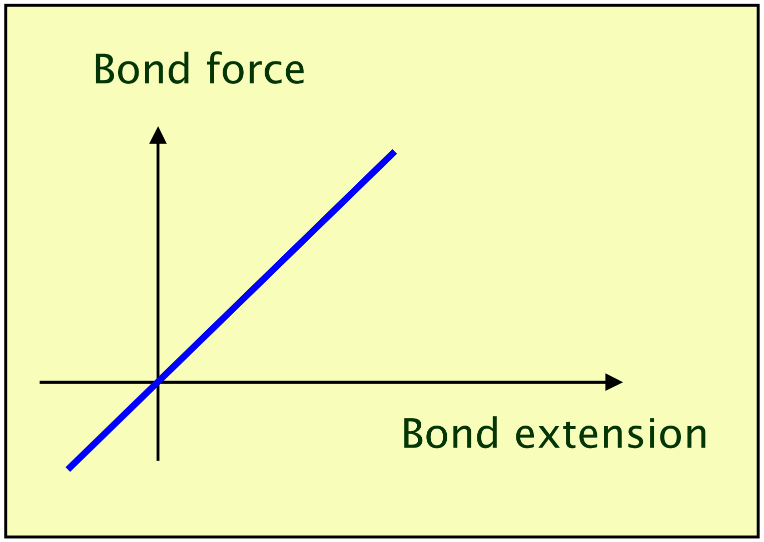
$$\mathbf{f}(\mathbf{x}',\mathbf{x},t)=\begin{cases} k\mathbf{M}\boxed{\Big(|\mathbf{y}'-\mathbf{y}|-|\mathbf{x}'-\mathbf{x}|\Big)}, & \text{if } |\mathbf{x}'-\mathbf{x}|<\delta, \\ 0 & \text{otherwise} \end{cases}$$



where the deformed bond direction is given by

$$\mathbf{M}=\frac{\mathbf{y}'-\mathbf{y}}{|\mathbf{y}'-\mathbf{y}|}$$





Length scale in the simplest material is the horizon

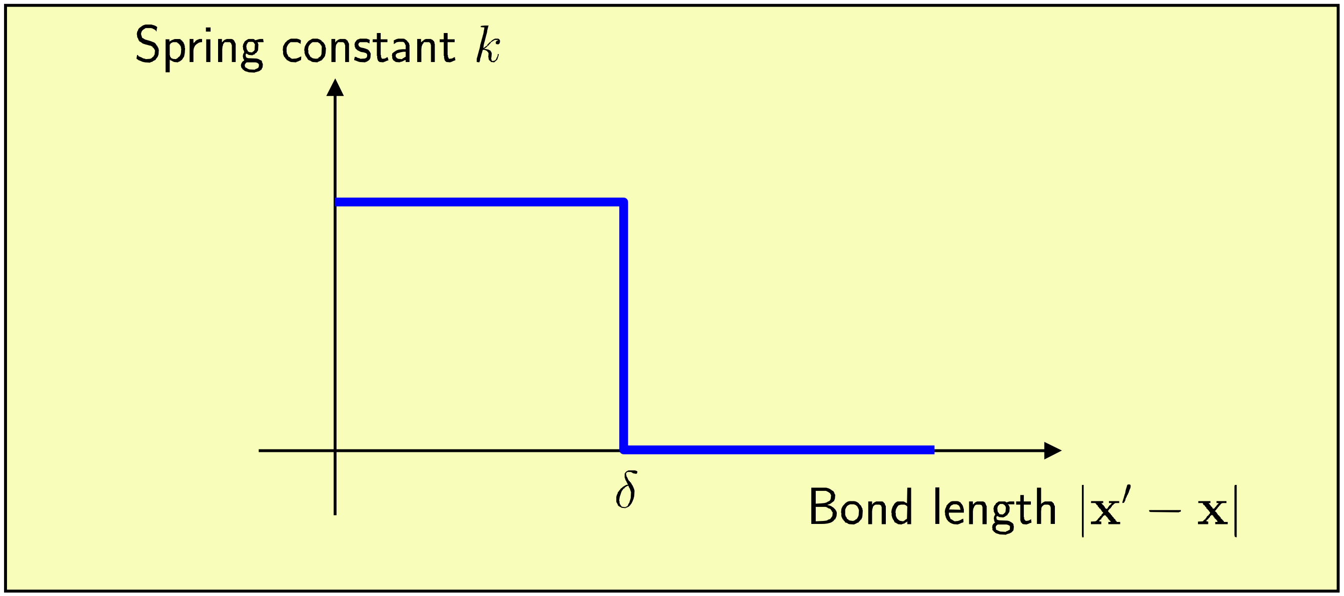
Microelastic material with constant micromodulus k:

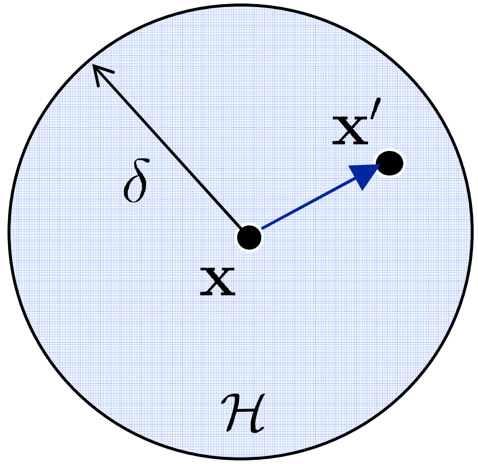
$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = \begin{cases} k\mathbf{M}\Big(|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|\Big), & \text{if } |\mathbf{x}' - \mathbf{x}| < \delta, \\ 0 & \text{otherwise} \end{cases}$$

Length scale

where the deformed bond direction is given by

$$\mathbf{M} = \frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|}$$

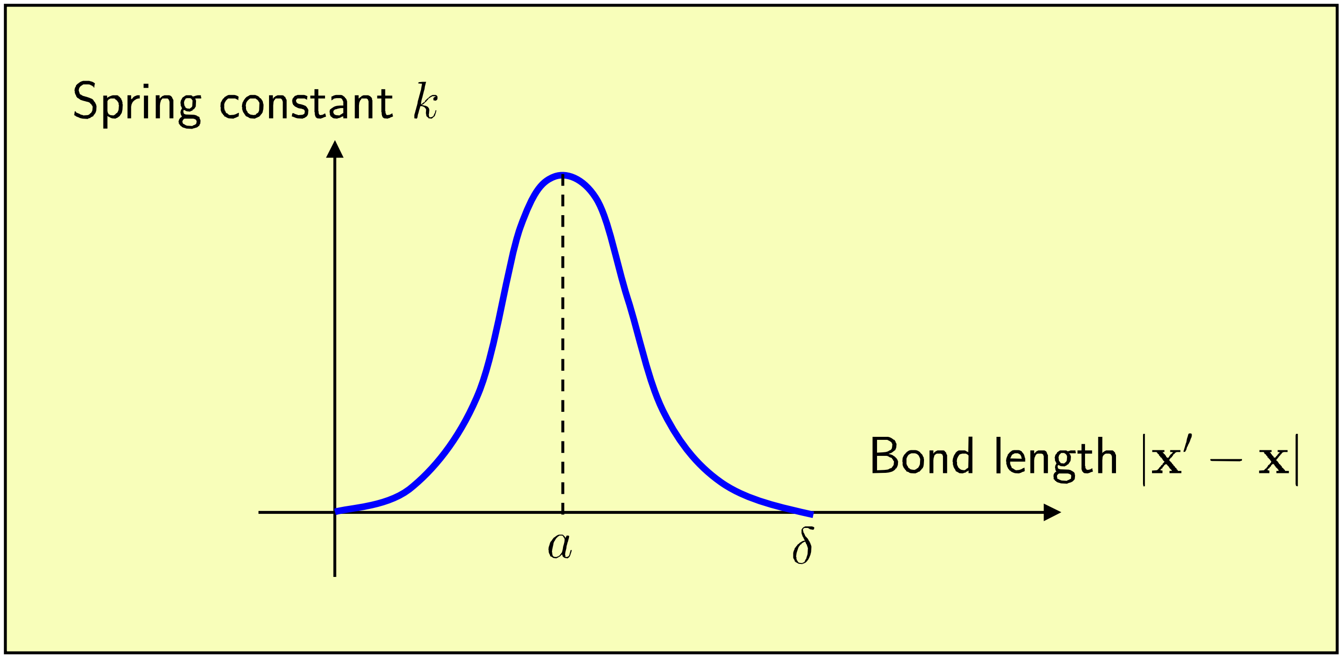


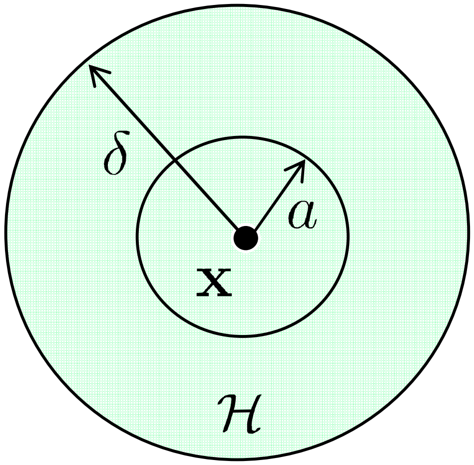


Length scales, ctd.

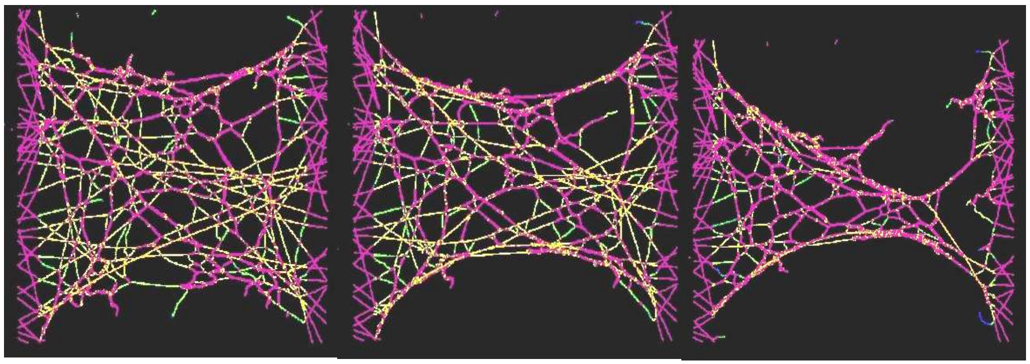
The spring constant can also depend on bond length, adding another length scale:

$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = k(|\mathbf{x}' - \mathbf{x}|)\mathbf{M}\big(|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|\big)$$

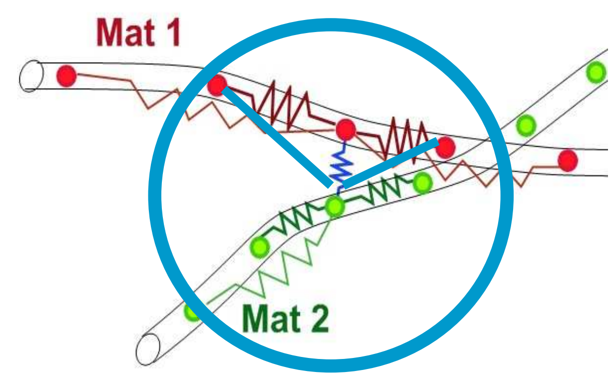




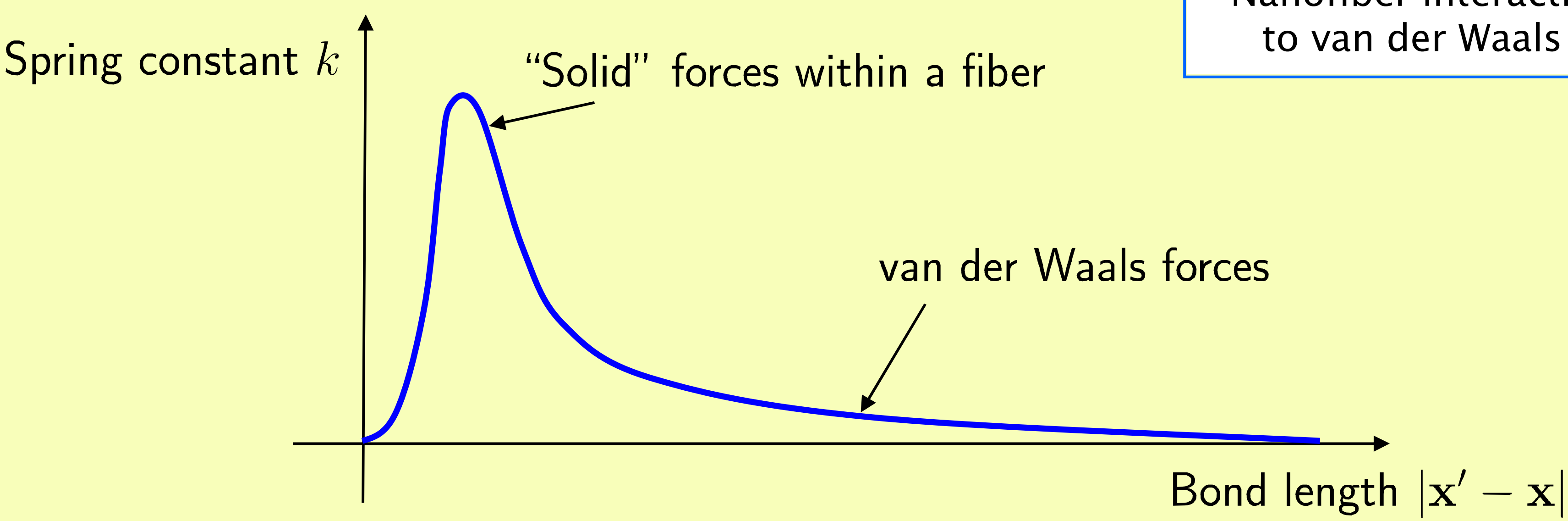
Example of multiple length scales: Nanofiber network



Nanofiber membrane (F. Bobaru, Univ. of Nebraska)



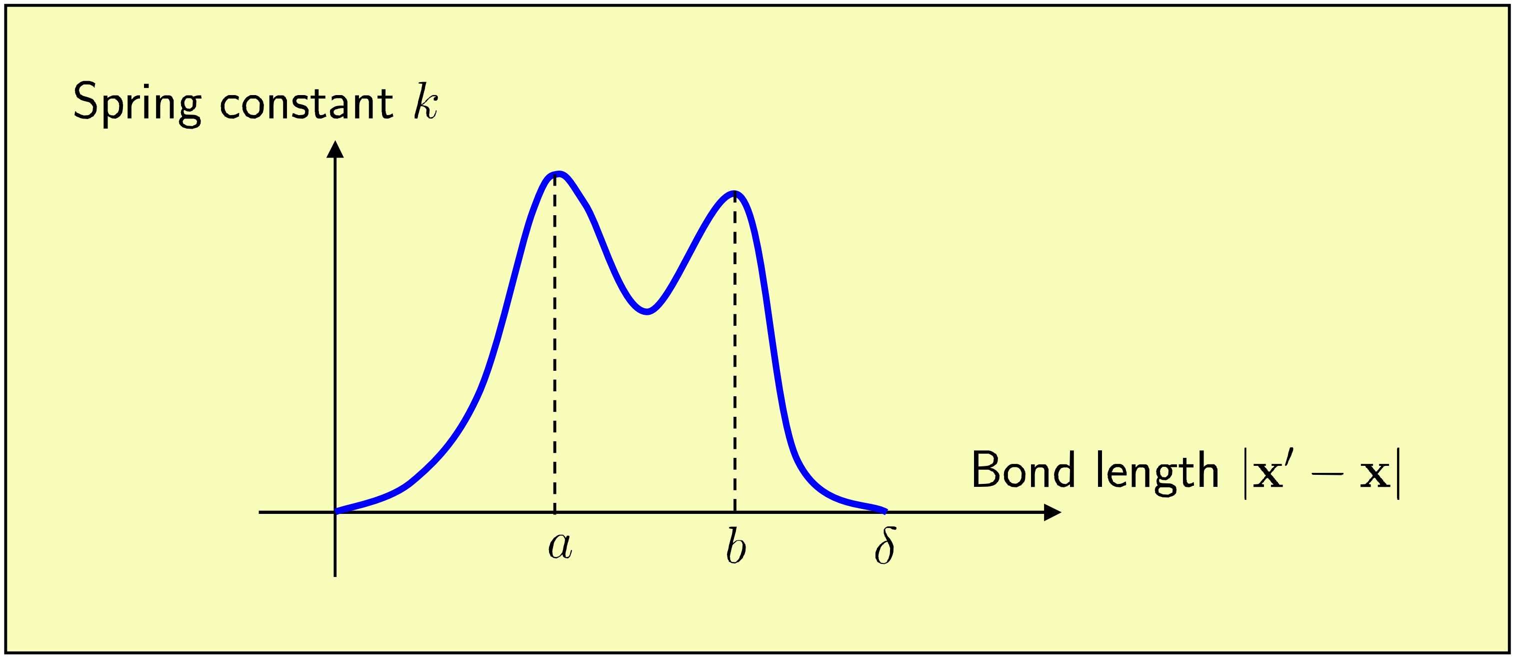
Nanofiber interactions due to van der Waals forces



Multiple length scales, ctd.

Microelastic material with 3 length scales: a, b, δ...

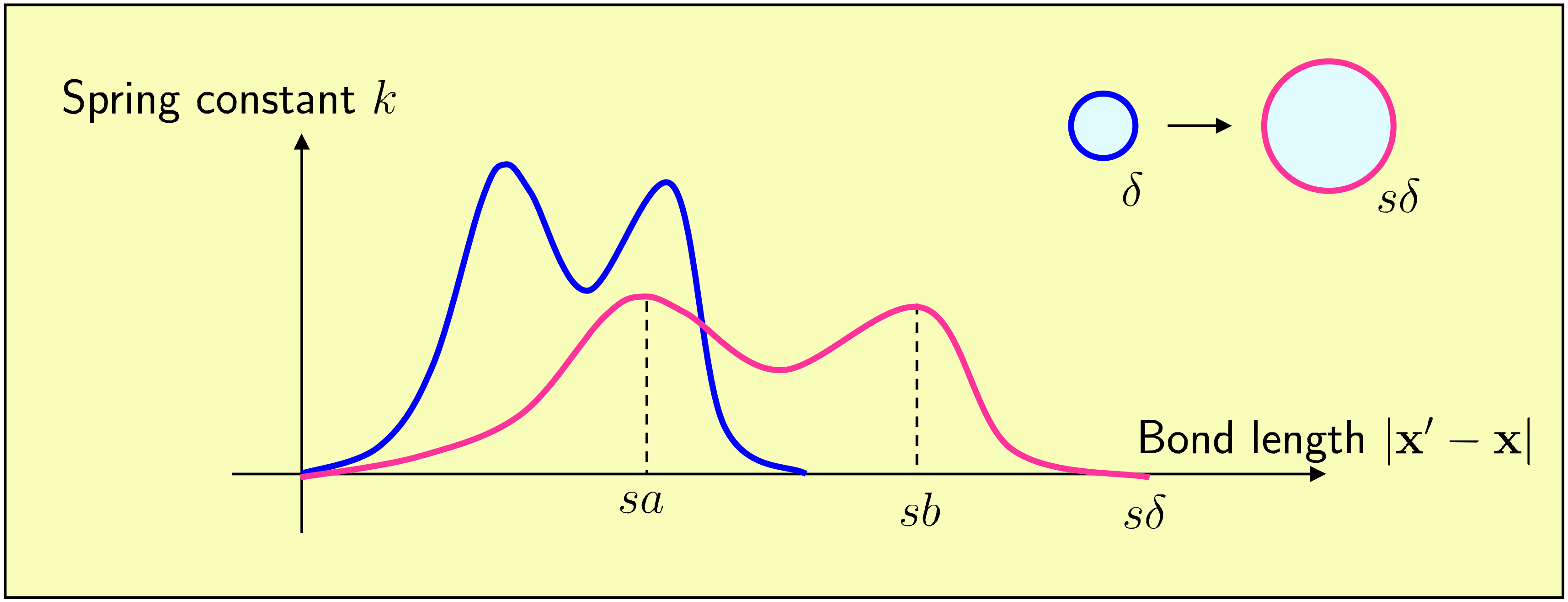
$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = k(|\mathbf{x}' - \mathbf{x}|)\Big(|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}|\Big)\mathbf{M}$$



Changing the length scale

Change length scales to sa, sb, $s\delta$, $s > 0$:

$$\mathbf{f}_s(\mathbf{x}', \mathbf{x}) = s^{-5} k \left(\frac{|\mathbf{x}' - \mathbf{x}|}{s} \right) \Big(|\mathbf{y}' - \mathbf{y}| - |\mathbf{x}' - \mathbf{x}| \Big) \mathbf{M}$$



Can show that under homogeneous deformation with this scaling, W is independent of s.

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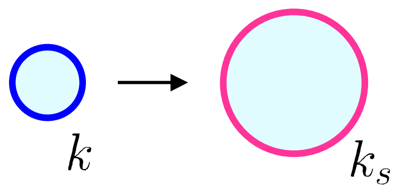
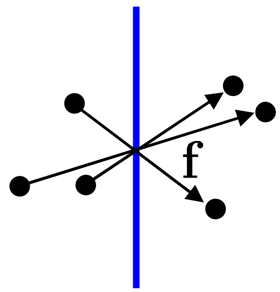
Changing the length scale, ctd.

In a linear microelastic model, this rescaling is equivalent to:

$$k_s(|\mathbf{x}' - \mathbf{x}|) = s^{-5} k \left(\frac{|\mathbf{x}' - \mathbf{x}|}{s} \right)$$



Can further show that under homogeneous deformation, force per unit area is independent of s.



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Discrete particle motion is a special case of peridynamics

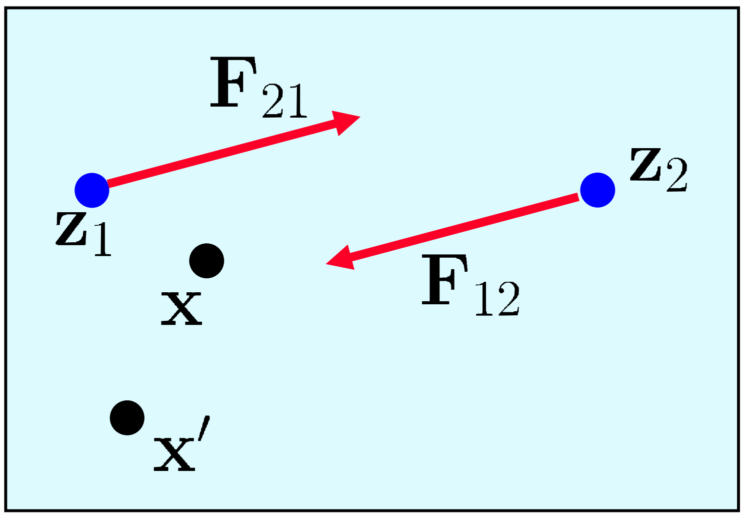
Example: Two atoms with reference locations $\mathbf{x}_1$ and $\mathbf{x}_2$:

Dirac delta

$$\rho(\mathbf{x}) = m\big(\Delta(\mathbf{x}-\mathbf{z}_1) + \Delta(\mathbf{x}-\mathbf{z}_2)\big)$$

$$\mathbf{f}(\mathbf{x}',\mathbf{x}) = \mathbf{F}_{21}\Delta(\mathbf{x}-\mathbf{z}_1)\Delta(\mathbf{x}'-\mathbf{z}_2) + \mathbf{F}_{12}\Delta(\mathbf{x}-\mathbf{z}_2)\Delta(\mathbf{x}'-\mathbf{z}_1)$$

where $\mathbf{F}$ is the 2-body force vector as a function of current atomic positions.



Easy to show that $\ddot{\mathbf{y}}(\mathbf{x}) = \int \mathbf{f}(\mathbf{x}',\mathbf{x})\, dV' \implies$

$$m\ddot{\mathbf{y}}(\mathbf{z}_1) = \mathbf{F}_{21}, \quad \text{and} \quad m\ddot{\mathbf{y}}(\mathbf{z}_2) = \mathbf{F}_{12}$$

which is Newton's 2nd law.

Works for multibody potentials too!

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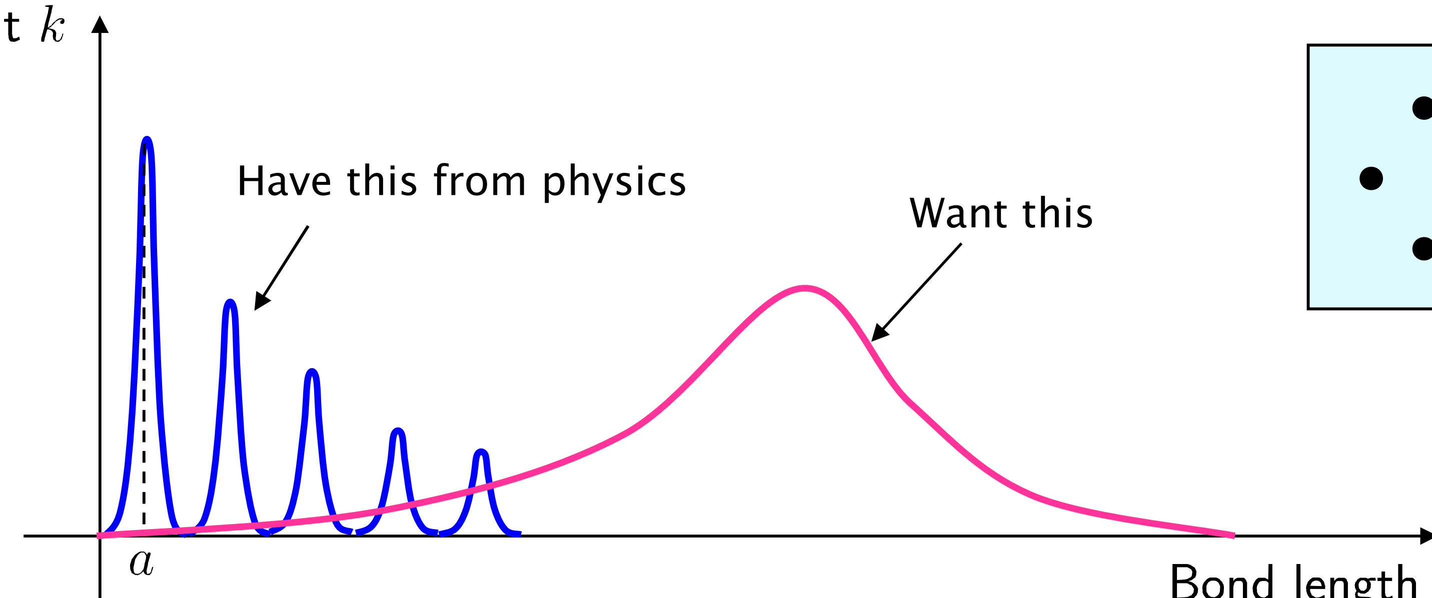
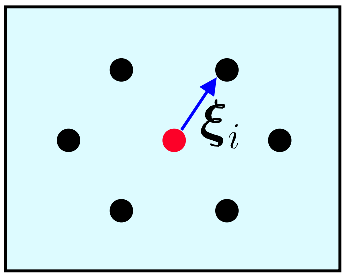
Homogenization: Removing length scales

- A model with small length scales is sometimes too hard to compute with…

$$\mathbf{f}(\mathbf{x}',\mathbf{x}) = c\mathbf{M}\sum_i \left[\left(\frac{a}{|\mathbf{y}'-\mathbf{y}|}\right)^6 - \left(\frac{a}{|\mathbf{y}'-\mathbf{y}|}\right)^{12}\right] \Delta(\mathbf{x}'-\mathbf{x}-\boldsymbol{\xi}_i)$$

Dirac delta





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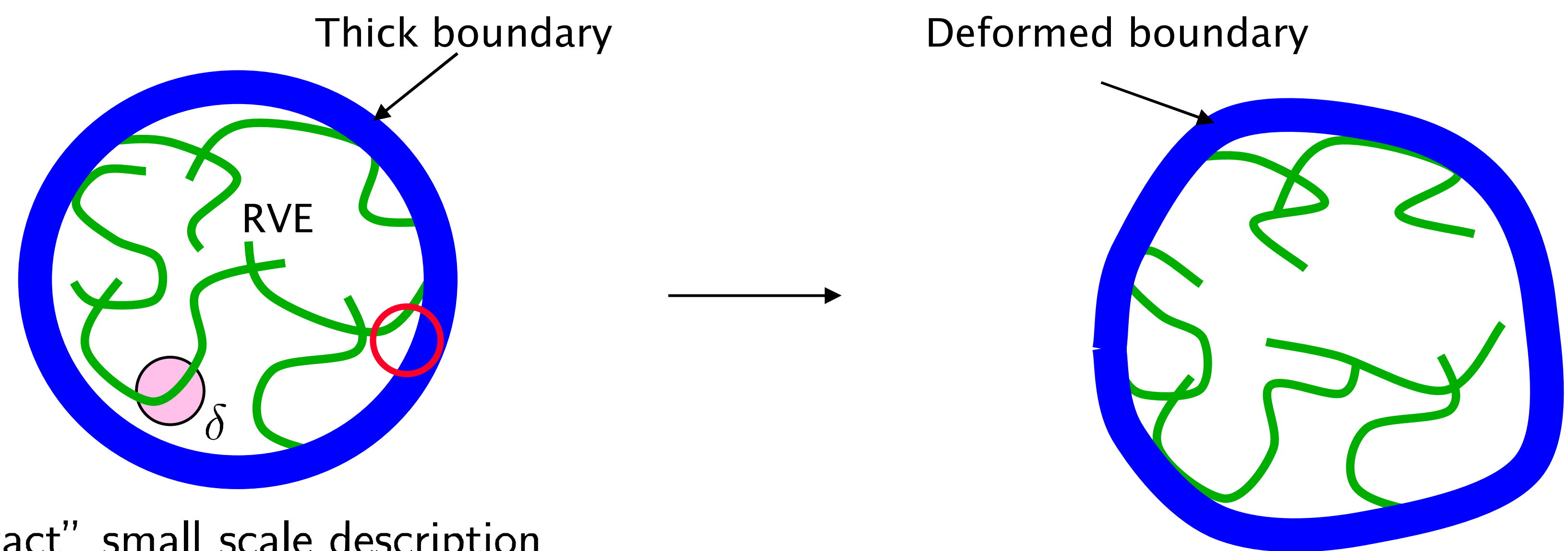
Homogenization method for peridynamics

- Set up a small scale model in a representative volume.
- Can express the change in total strain energy in the RVE in response to an arbitrary deformation of the boundary.



"Exact" small scale description

δ=horizon

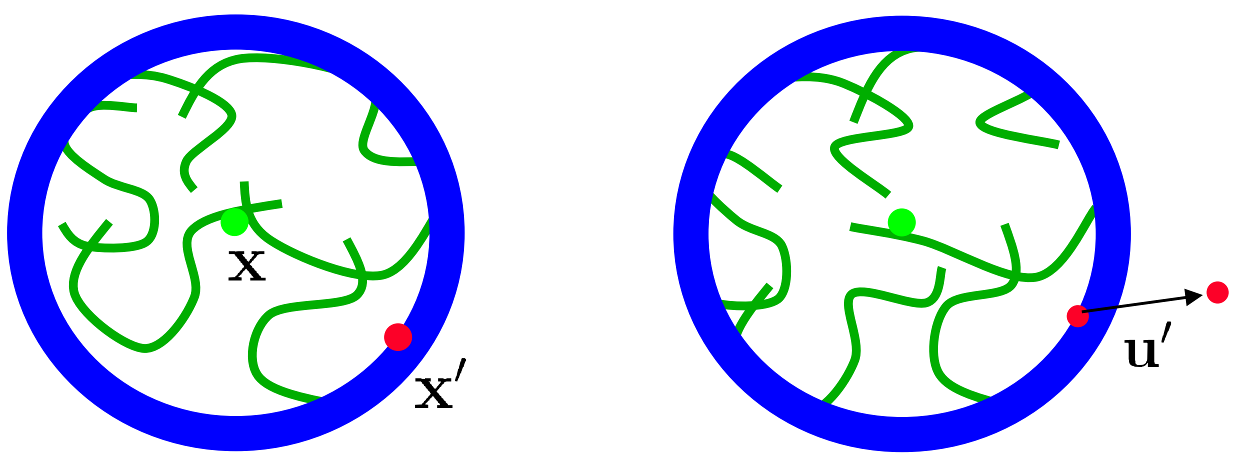
Φ=total energy in deformed RVE

Homogenization, ctd.

- Compute the change in mean energy in the RVE in response to a displacement of any point on the boundary.
- The homogenized micromodulus is defined by

$$\mathbf{k}_h(\mathbf{x}', \mathbf{x})\mathbf{u}' = \frac{1}{V}\frac{\partial \Phi}{\partial \mathbf{u}'}$$

V =RVE volume



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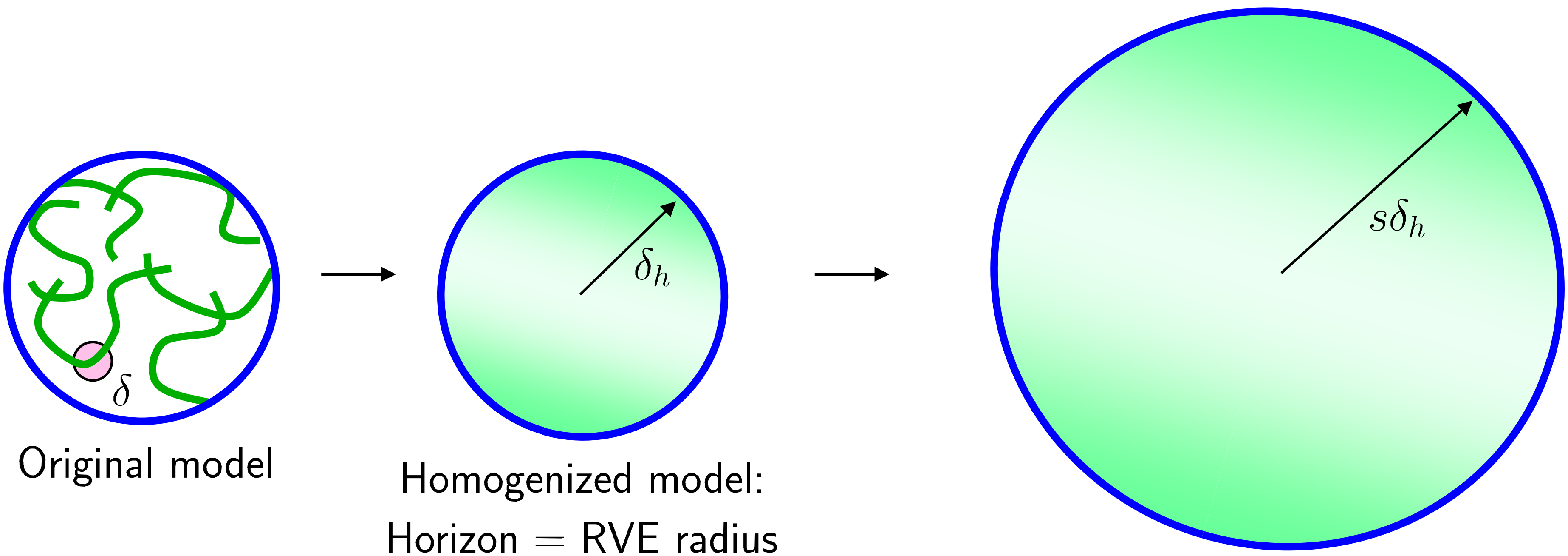
Properties of homogenization

- Incorporates small-scale deformation in computing the large-scale response.
    - But the small length scale does not appear explicitly.



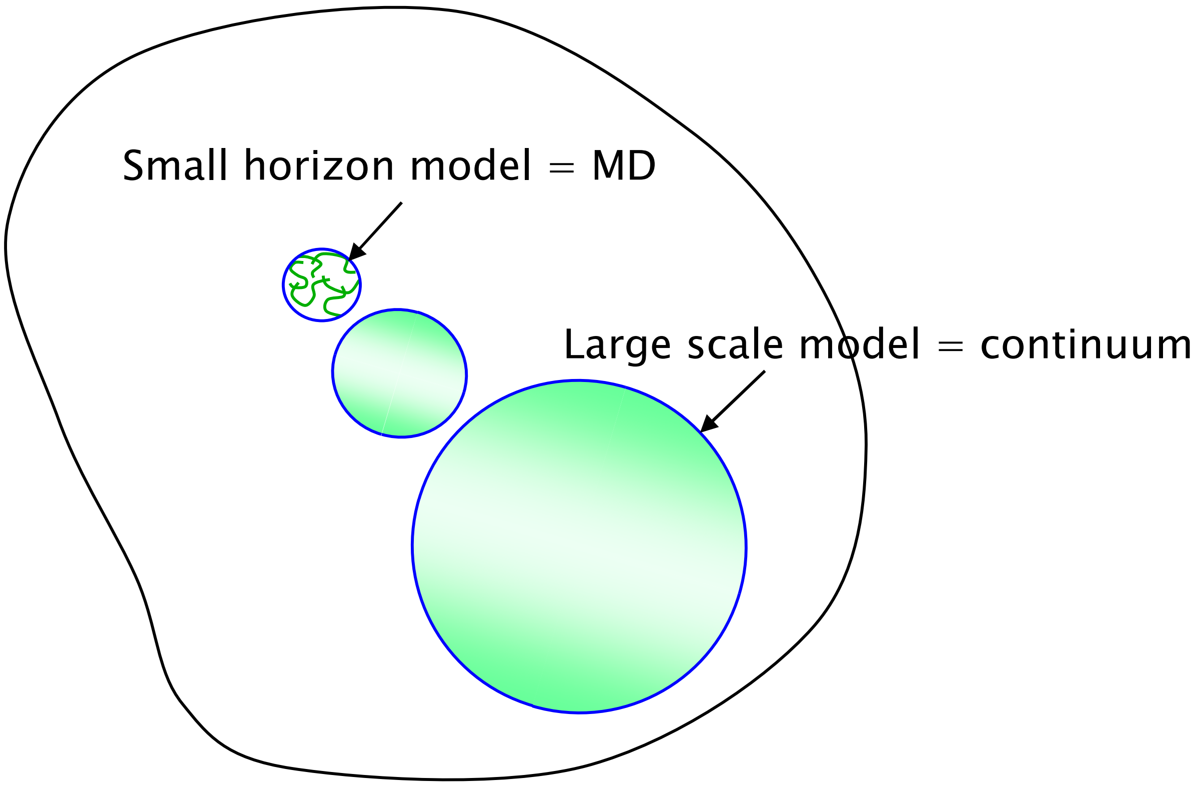
Original model

Homogenized model:
Horizon = RVE radius

Can get any desired horizon by rescaling

Variable length scales within a body

- Small scale peridynamic model is the same as molecular dynamics.
- Large scale peridynamic model is suitable for engineering calculations.
- The two are mathematically consistent: same field equations.



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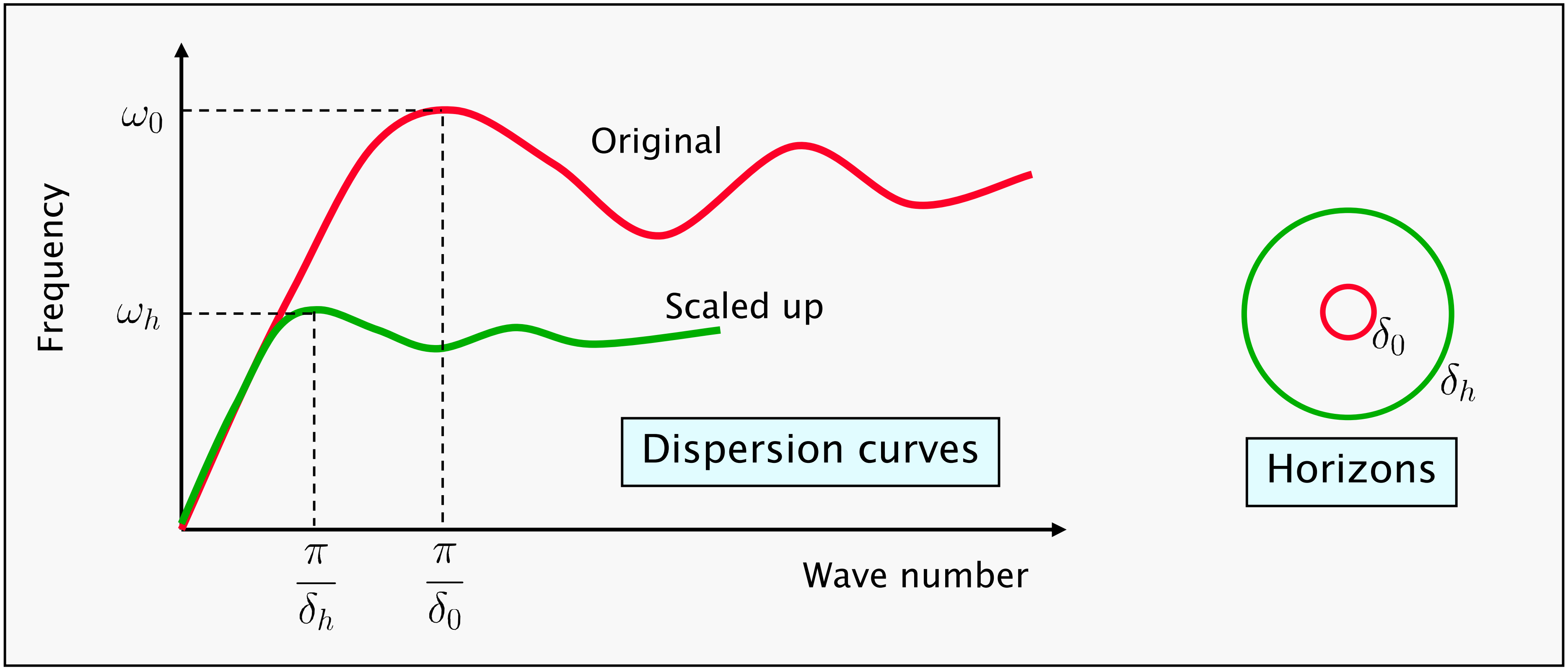
Changing the length scale also changes the time scale

- Removing the small length scale also removes the high frequencies that characterize that length scale.

$$\delta_h > \delta_0 \implies \omega_h < \omega_0$$



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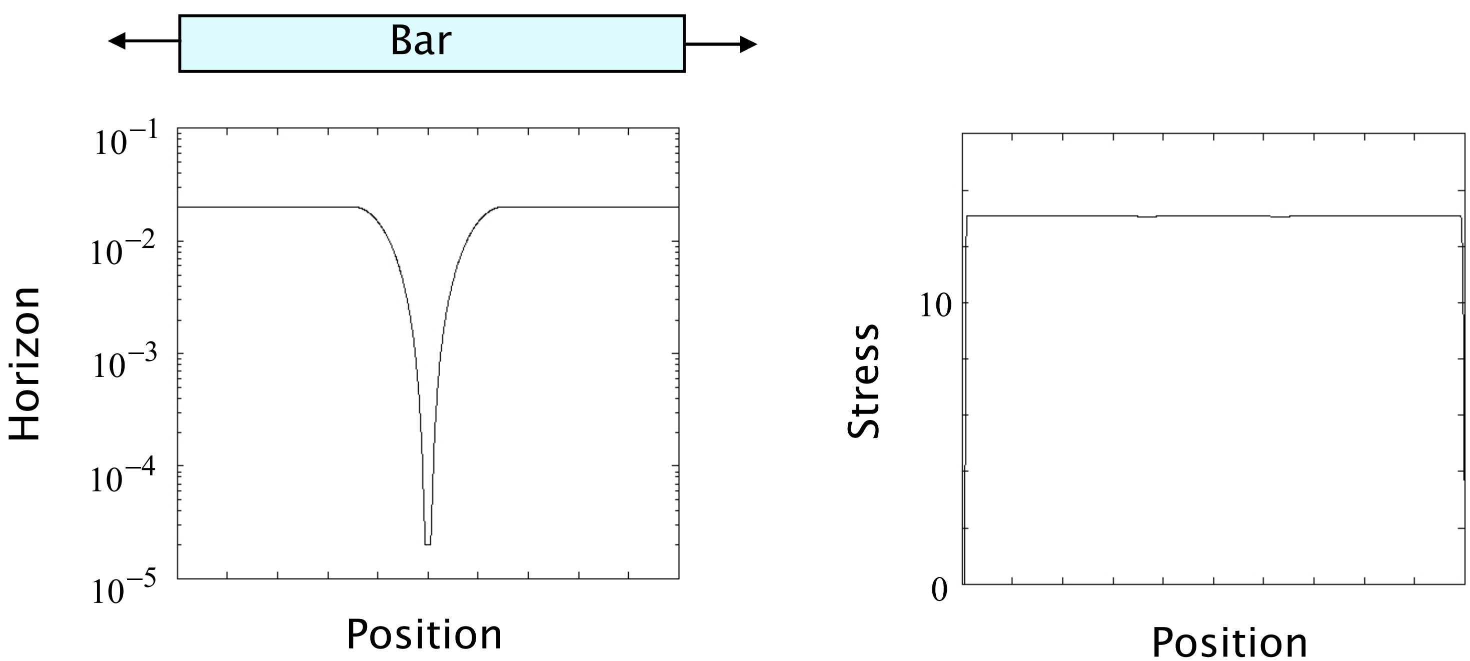
Conclusions

- Peridynamics offers mathematically consistent treatment across divergent length scales.
- Methods exist for
    - Homogenization (removing small length scales)
    - Rescaling (changing length scales)
    - These accomplish a type of coarse graining of MD into continuum.
- Regions with different length scales can communicate without coupling dissimilar methods and codes.

Variable length scales within a body: 1D example

- Homogeneous deformation (constant strain) is prescribed in a 1D bar.
- The horizon varies within the bar by 3 orders of magnitude.
- The resulting stress (force flux) is nearly constant.
- This demonstrates that a small scale model can coexist with large scale.



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Time-dependent homogenization

- So far we have assumed the RVE attains equilibrium immediately.
- Instead, could compute time-dependent RVE properties as the small-scale model adjusts to a sudden change in boundary displacement.

$$\mathbf{k}_h(\mathbf{x}', \mathbf{x}, t)\mathbf{u}' = \frac{1}{V}\frac{\partial \Phi(t)}{\partial \mathbf{u}'}$$