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Atoms and Peridynamic Continua

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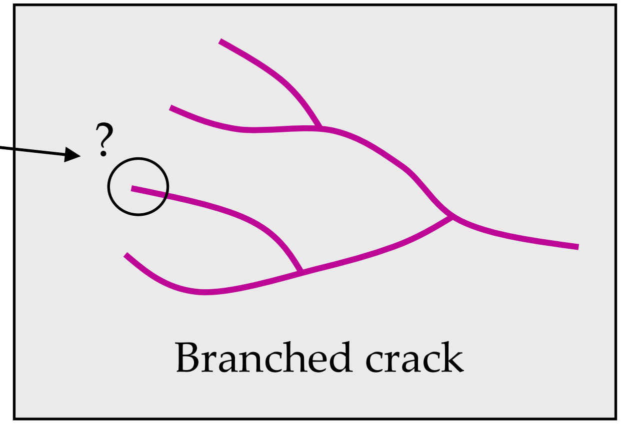
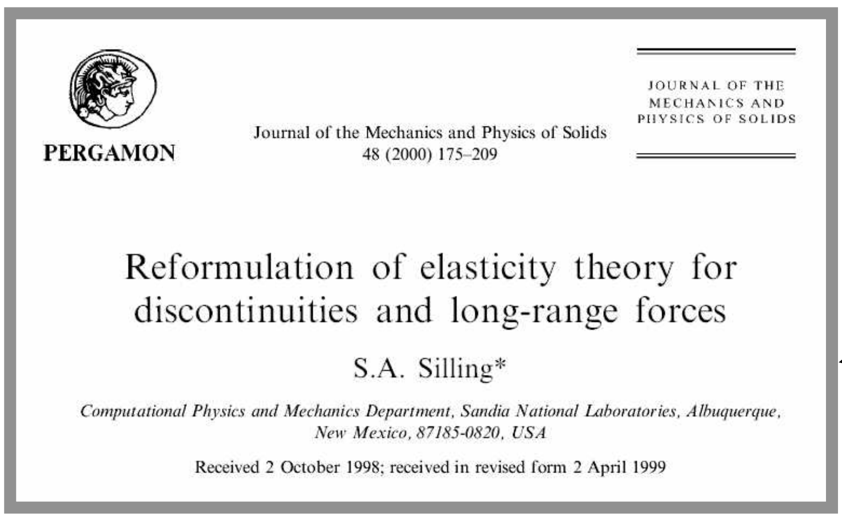
Peridynamics background: Alternative to traditional fracture mechanics

- Fracture mechanics has some troublesome aspects.
  - Requires supplemental equations to tell a crack what to do.
  - Treats fracture as a sort of pathology.
    - Need to keep redefining the body to avoid applying PDEs on a growing crack.





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Reformulation of elasticity theory for discontinuities and long-range forces

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- 1998 – Began looking for a new model of solid mechanics such that the same equations hold everywhere regardless of discontinuities.

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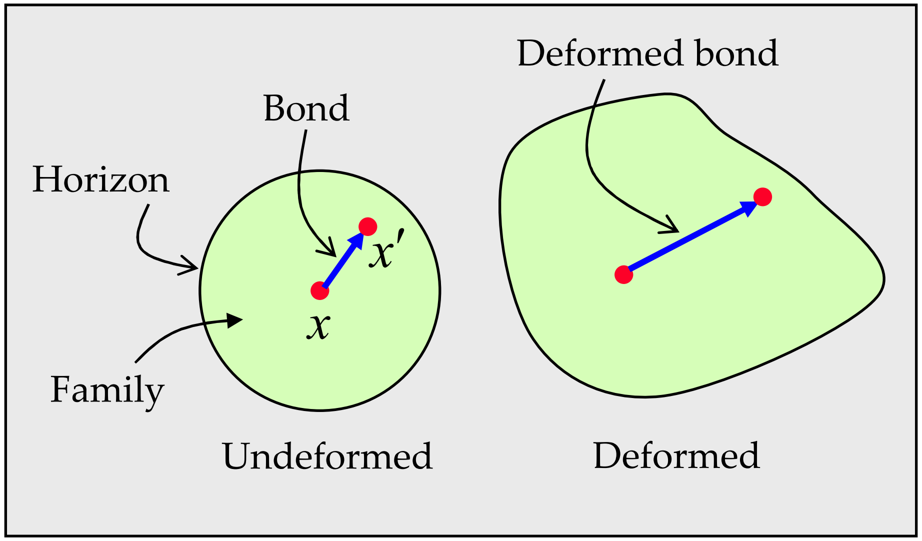
Peridynamics:
Horizon, family, and bonds

- Points $\boldsymbol{x}$ and $\boldsymbol{x}'$ can interact directly.
- Horizon δ :
  - Maximum interaction distance.
- Bond:
  - The vector connecting $\boldsymbol{x}$ to any $\boldsymbol{x}'$ within its horizon in the reference configuration.
- Family of $\boldsymbol{x}$:
  - The set of all bonds from $\boldsymbol{x}$ to any $\boldsymbol{x}'$ within its horizon.



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Vector states

- A vector state is a vector-valued function defined on a family *H*:

$$\underline{A}\langle\xi\rangle, \qquad \xi \in H$$

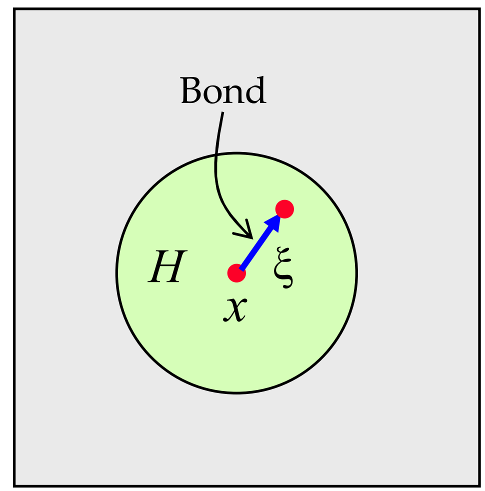
- Example:

$$\underline{A}\langle\xi\rangle = 3|\xi|^2\,\xi$$

- Define the <u>dot product</u> of 2 vector states by

$$\underline{A} \bullet \underline{B} = \int_H \underline{A}\langle\xi\rangle \cdot \underline{B}\langle\xi\rangle \, dV_\xi$$

Usual scalar product of 2 vectors

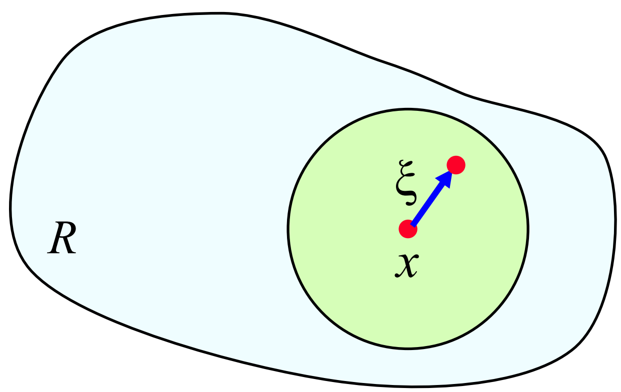


Can also have scalar states (scalar-valued functions of ξ).

Notation for vector state-valued fields

$\underline{A}[x,t]$ …a vector state at a point $\boldsymbol{x}$ in the body at time t

$\underline{A}[x,t]\langle\xi\rangle$ …the value (which is a vector) of $\underline{A[\boldsymbol{x},t]}$ evaluated at a bond ξ



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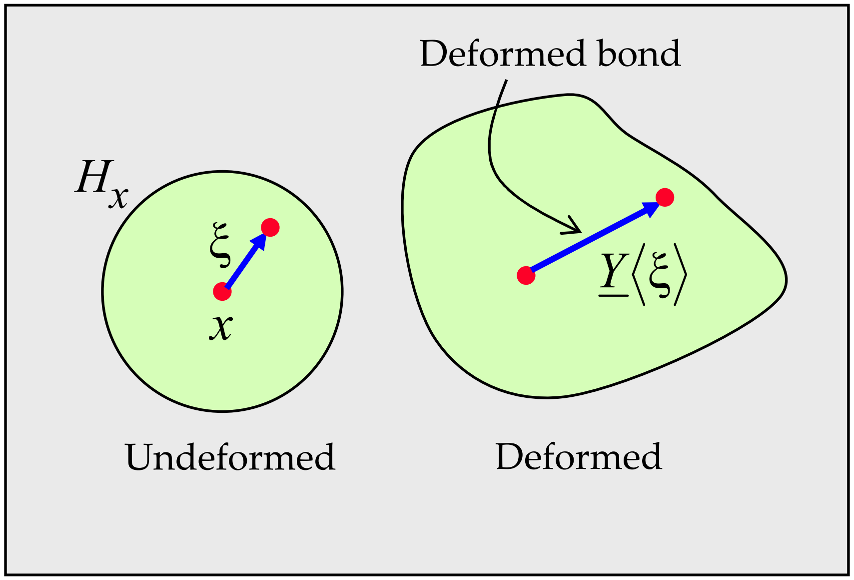
Deformation states

- Deformation:

$$y = \hat{y}(x,t)$$

- Deformation state maps a bond into its deformed image:



$$\underline{Y}[x,t]\langle\xi\rangle = \hat{y}(x+\xi,t) - \hat{y}(x,t), \qquad \xi \in H_x$$

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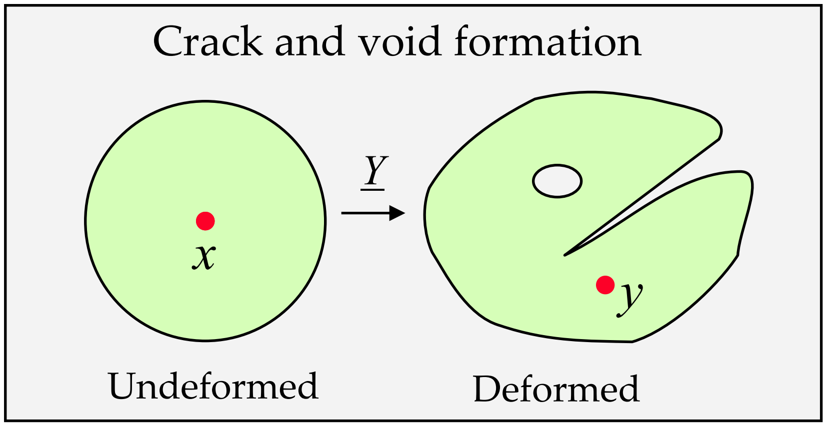
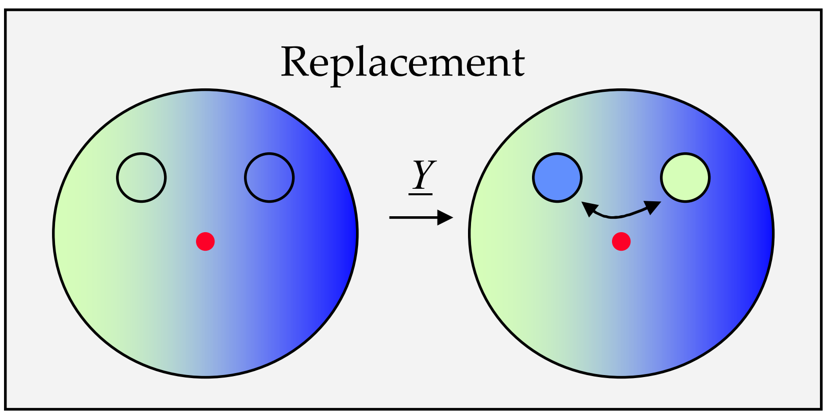
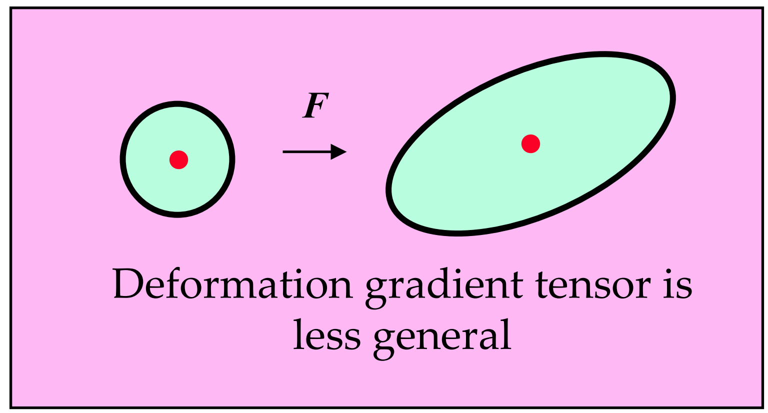
Deformation states can describe complex relative movements near *x*

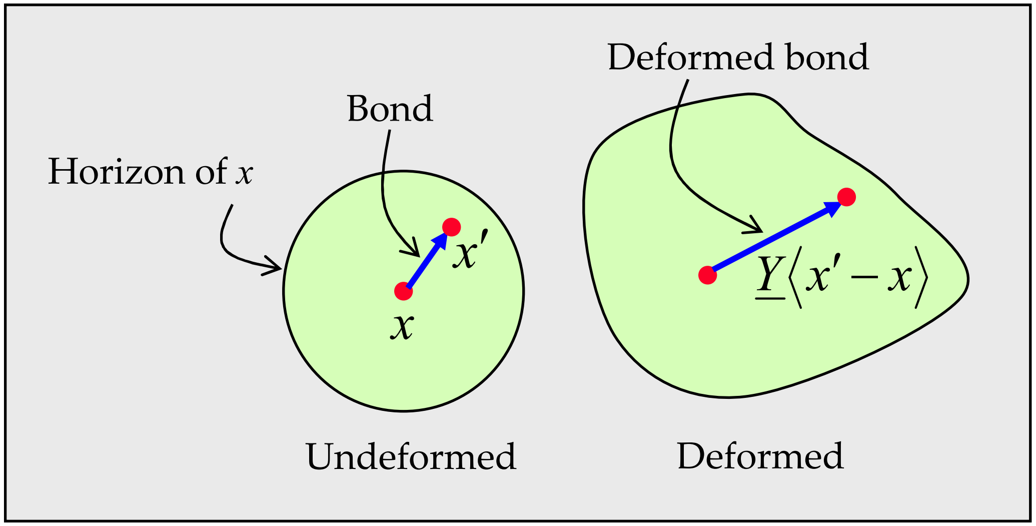






The basic assumption

- Strain energy density $W(\boldsymbol{x},t)$ depends only on $\underline{Y}[\boldsymbol{x},\mathrm{t}]$.



Peridynamic constitutive model

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

Energy depends on all the bonds collectively; it is not merely the sum of independent bond energies.

Strain energy and force states

If there is a vector state $\underline{T}$ such that if $\Delta\underline{Y}$ is any increment in the deformation state,

$$\Delta W = \hat{W}\left(\underline{Y} + \Delta\underline{Y}\right) - \hat{W}\left(\underline{Y}\right) = \underline{T} \bullet \Delta\underline{Y} + o\left(\Delta\underline{Y}\right)$$

then $\underline{T}$ is the <u>Frechet derivative</u> of W, and we write

$$\underline{T} = \nabla\hat{W}$$

(analogous to the tensor gradient in the classical theory)

Nonhomogeneous elastic bodies: include ***x*** explicitly in constitutive model:

$$\underline{T} = \hat{\underline{T}}\left(\underline{Y}, x\right) = \nabla\hat{W}\left(\underline{Y}, x\right)$$

$\underline{T}$ is called the <u>force state</u>. It is a vector state that associates every ξ with a force density.

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Equilibrium equation from stationary potential energy

Potential energy in a body:

$$\Phi = \int_R \hat{W}\left(\underline{Y}[x]\right) dV_x - \int_R b(x)\cdot u(x)\, dV_x$$

Take first variation:

$$\Delta\Phi = \int_R \underline{T} \bullet \Delta\underline{Y}\, dV_x - \int_R b\cdot\Delta u\, dV_x$$

$$= -\int_R \left(\int_R \left(\underline{T}[x]\langle x'-x\rangle - \underline{T}[x']\langle x-x'\rangle \right) dV_{x'} + b(x) \right) \cdot \Delta u(x)\, dV_x$$

So the Euler-Lagrange (equilibrium) equation is

$$\int_R \left(\underline{T}[x]\langle x'-x\rangle - \underline{T}[x']\langle x-x'\rangle \right) dV_{x'} + b(x) = 0$$

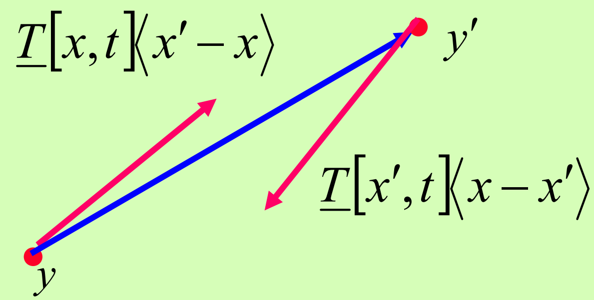
Internal forces

The force state $\underline{T}[\boldsymbol{x},t]$ associates a force density with each bond $\boldsymbol{x}'$-$\boldsymbol{x}$.

Peridynamic equation of motion:

$$\rho\ddot{u}(x,t)=\int_H \left\{\underline{T}[x,t]\langle x'-x\rangle-\underline{T}[x',t]\langle x-x'\rangle\right\}dV_{x'}+b(x,t)$$

Force states act together



Forces need not be parallel to each other or to the deformed bond.

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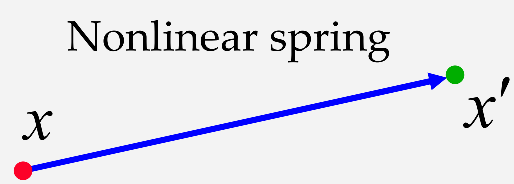
Special case:
Bonds independent of each other

Suppose the strain energy density function is

$$\hat{W}(\underline{Y}) = \frac{1}{2}\int_H w\left(\underline{e}\langle\xi\rangle, \xi\right) dV_\xi, \qquad \underline{e}\langle\xi\rangle = \left|\underline{Y}\langle\xi\rangle\right| - |\xi| \qquad \text{...extension state}$$

$$w\ldots \qquad \text{scalar-valued "micropotential" function}$$

- Magnitude of the bond force depends only on the deformed bond length.
- Bond force is parallel to the deformed bond.



Leads to the "bond-based" peridynamic model

$$\rho\ddot{u}(x,t) = \int_H f\left(\left|\hat{y}(x',t) - \hat{y}(x,t)\right|, x' - x\right) dV_{x'} + b(x,t)$$

$$f(\eta, \xi) = \frac{\partial w}{\partial \eta}(\eta, \xi)$$

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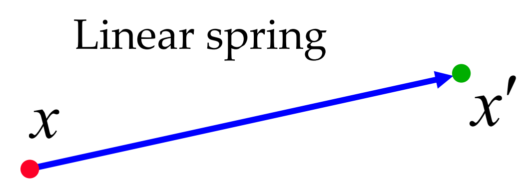
Further restriction of special case: Linearized bond-based model

- Magnitude of the bond force depends only on the bond extension (length change) .
- Bond force is parallel to the deformed bond.
- Bond force varies linearly with bond extension.
- Extension is evaluated by a linear approximation.

$$\rho\ddot{u}(x,t) = \int_H C(x'-x)\big(u(x',t)-u(x,t)\big)dV_{x'} + b(x,t)$$

$$C(\xi) = \frac{\partial f}{\partial \eta}(0,\xi)$$



I. A. Kunin's books *Elastic Media with Microstructure I & II* (1982, 1983) solve many important problems with this model.

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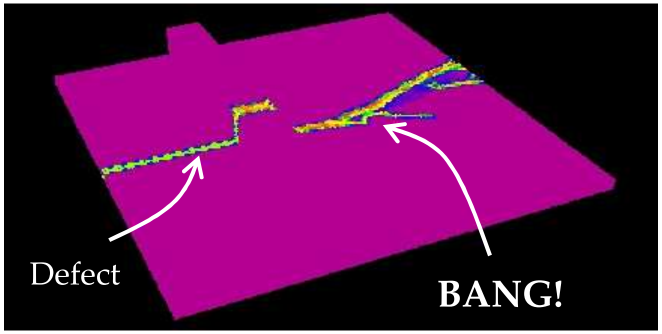
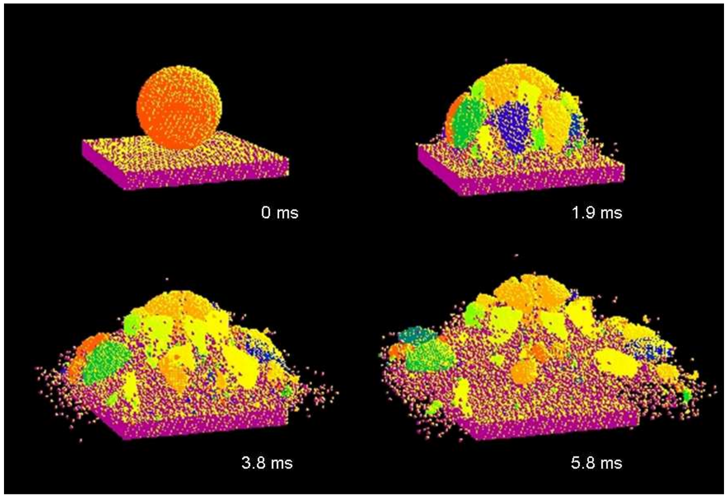
Some applications of the bond-based theory

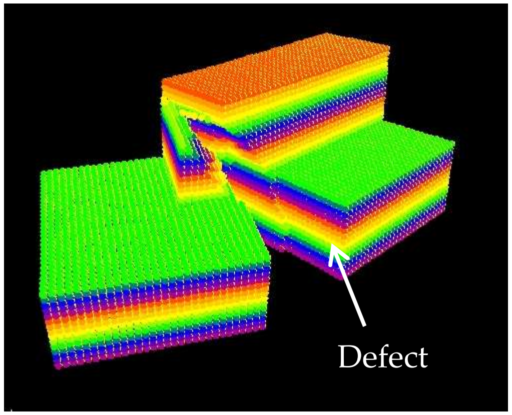
Results from the Emu computer code demonstrate the ability to model complex discontinuities



Transition to unstable crack growth



Impact and fragmentation



Crack turning in a 3D feature

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Back to full model: Global balances of conserved quantities

Linear momentum: Integrating the equation of motion over the body

$$\int_R \left(\int_R \left\{ \underline{T}[x,t]\langle x'-x\rangle - \underline{T}[x',t]\langle x-x'\rangle \right\} dV_{x'} + b(x,t) - \rho\ddot{u}(x,t) \right) dV_x = 0$$

$$\Rightarrow \int_R \left(b(x,t) - \rho\ddot{u}(x,t)\right) dV_x = 0$$

Angular momentum: The restriction on the constitutive model

$$\int_H \underline{Y}\langle\xi\rangle \times \underline{\hat{T}}(\underline{Y})\langle\xi\rangle dV_x = 0$$

$$\Rightarrow \int_R \hat{y}(x,t) \times \left(b(x,t) - \rho\ddot{u}(x,t)\right) dV_x = 0$$

Some properties of peridynamic constitutive models

Define the composition of two vector states by

$$\left(\underline{A} \circ \underline{B}\right)\langle \xi \rangle = \underline{A}\left\langle \underline{B}\langle \xi \rangle \right\rangle$$

Condition for material frame indifference (objectivity):

$$\underline{\hat{T}}\left(\underline{Q} \circ \underline{Y}\right) = \underline{Q} \circ \underline{\hat{T}}\left(\underline{Y}\right)$$

for all orthogonal states $\underline{Q}$

Orthogonal states rigidly rotate bonds

Condition for isotropy:

$$\underline{\hat{T}}\left(\underline{Y} \circ \underline{Q}\right) = \underline{\hat{T}}\left(\underline{Y}\right) \circ \underline{Q}$$

for all orthogonal states $\underline{Q}$

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What about stress?

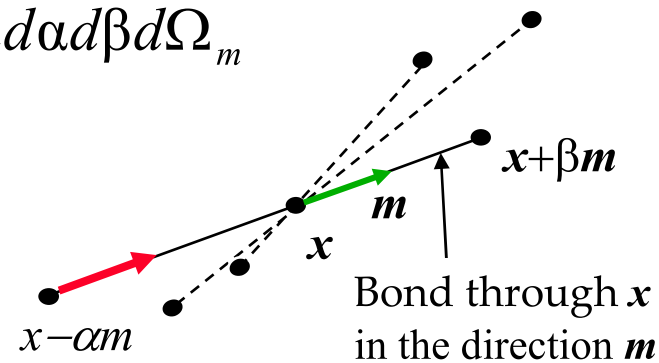
- How to eliminate stress from your life:

$$\rho\ddot{u}(x,t)=\int_H \left\{\underline{T}[x,t]\langle x'-x\rangle-\underline{T}[x',t]\langle x-x'\rangle\right\}dV_{x'}+b(x,t)$$

- But if you want stress in your life, define the <u>peridynamic stress tensor</u>:

$$\nu(x)=\int_S\int_0^\infty\int_0^\infty(\alpha+\beta)^2\,\underline{T}[x-\beta m]\langle(\alpha+\beta)m\rangle\otimes m\,d\alpha\, d\beta\, d\Omega_m$$

α,β ... scalars
$d\Omega_m$ ... differential solid angle in the direction of unit vector m
S ... unit sphere



Then:

$$\boxed{\nabla\cdot\nu=\int\left\{\underline{T}[x]\langle x'-x\rangle-\underline{T}[x']\langle x-x'\rangle\right\}dV_{x'}}$$

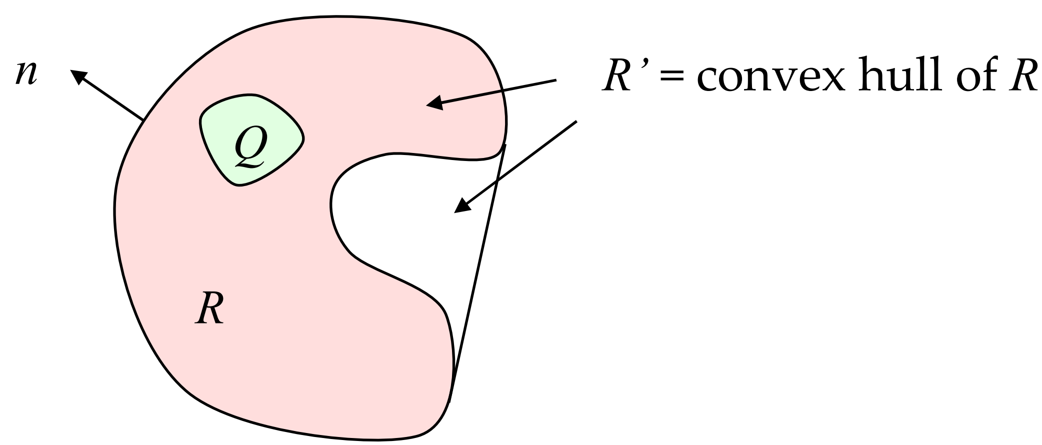
More about peridynamic stress

- Total force on subregion Q in R:

$$F = \int_{\partial Q} \nu n dA$$

- Stress satisfies the following boundary condition:

$$\nu n = 0 \qquad \text{on } \partial R'$$

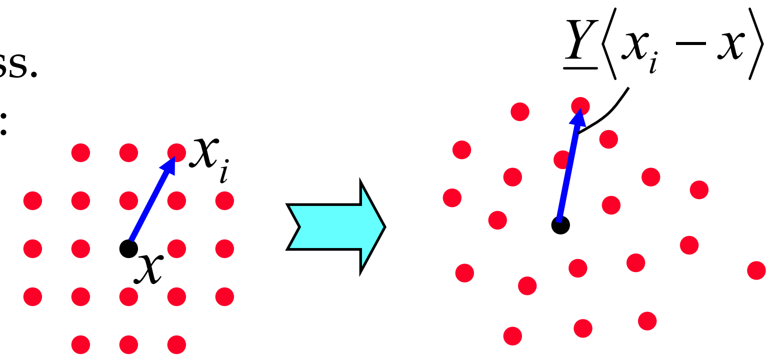


Atoms as a peridynamic continuum

Assume identical atoms for simplicity. M = mass.
Multibody interatomic potential of each atom k:

$$\psi\left(y_1 - y_k, y_2 - y_k, \ldots, y_N - y_k\right)$$

where y_i is the current position of atom i.



Undeformed Deformed

Description of this system as a nonhomogeneous peridynamic body:

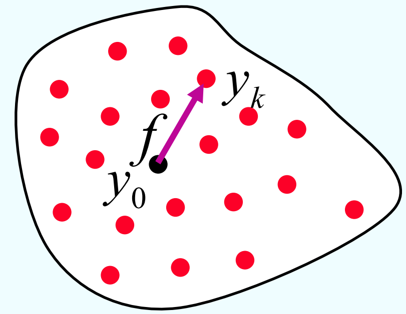
$$\rho(x) = M \sum_k \Delta(x - x_k)$$

Delta functions

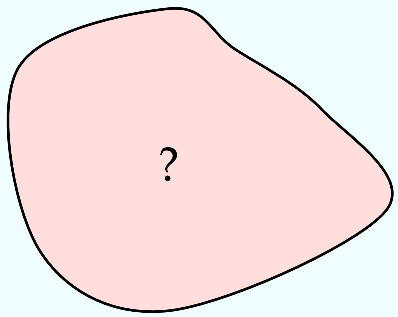
$$\hat{W}(\underline{Y}, x) = \sum_k \Delta(x - x_k)\psi\left(\underline{Y}\langle x_1 - x\rangle, \underline{Y}\langle x_2 - x\rangle, \ldots, \underline{Y}\langle x_N - x\rangle\right)$$

where x_i is the reference position of atom i.

Deformations:
A seeming paradox

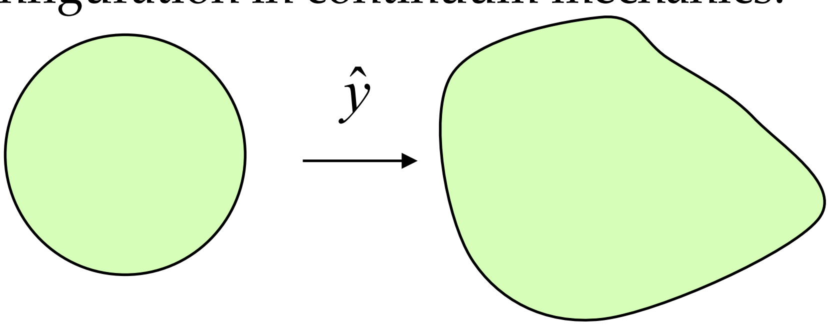


• If you have a finite set of atoms, you can determine the internal forces from their current configuration alone.



• But if you have a continuous body, you can't.

This is why we usually introduce a reference configuration in continuum mechanics.



Why not?
We lost something when went from a finite set into a continuous set: the spaces.

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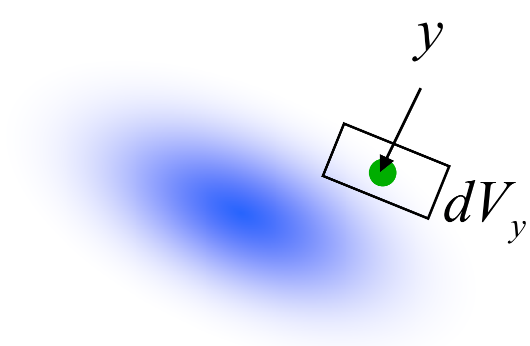
So, how should we define a deformation?
First, take a statistical view of atomic positions

- Suppose that the probability of finding atom k in a small volume dV_y at point y in the current configuration at time t is $p_k(y,t)dV_y$



Probability density p_k

- If atomic positions y_k are defined exactly, set $p_k(y,t) = \Delta(y-y_k)$.

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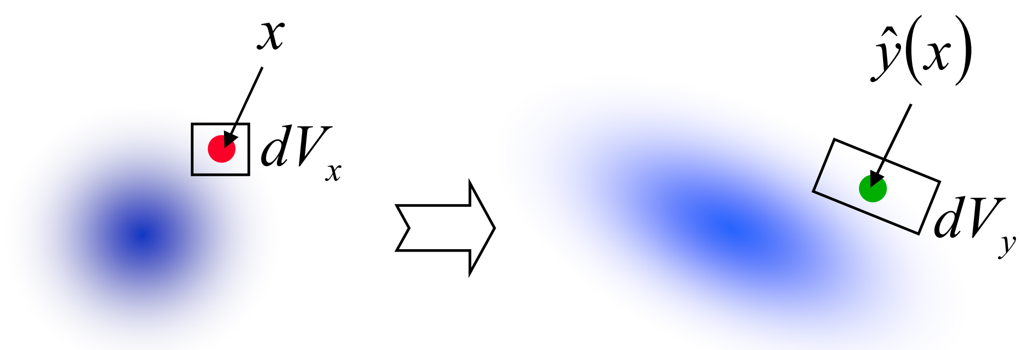
Statistical interpretation of a deformation



Undeformed probability density P_k

Deformed probability density p_k

Condition on the deformation:

$$p_k(\hat{y}(x,t),t)dV_y = P_k(x)dV_x \qquad \text{for all } x, t$$

Deformation "<u>conforms to</u>" the p_k

- This is the <u>only</u> condition we'll need on the deformation.
- In general, there is not a <u>unique</u> deformation that conforms to given p_k.

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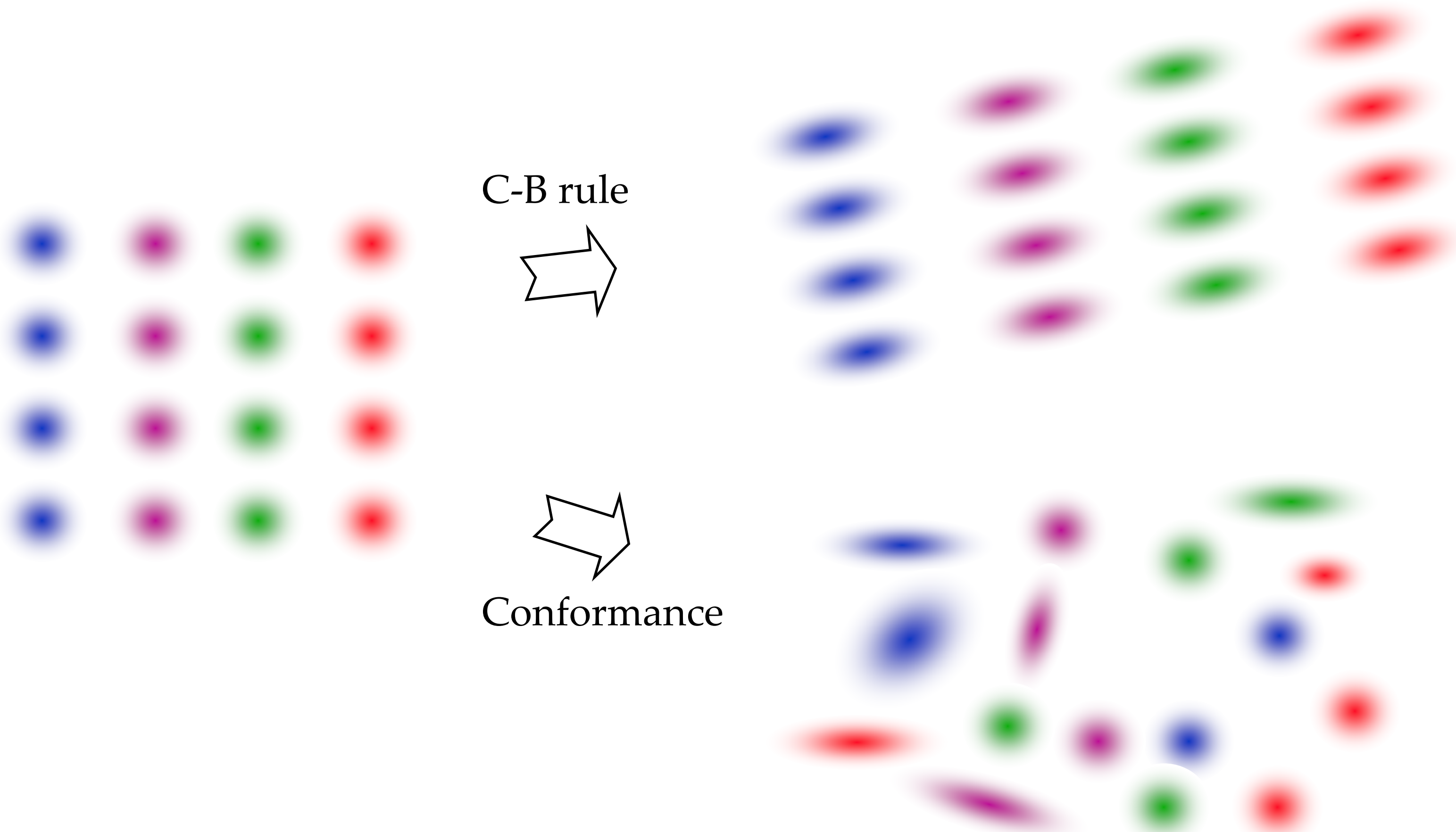
Resulting kinematics are less restrictive than the Cauchy-Born rule



Peridynamic representation of a statistical distribution of atoms

Define a nonhomogeneous peridynamic body by

$$\rho(x) = M \sum_k P_k(x)$$

$$\hat{W}(\underline{Y}, x) = \sum_k P_k(x) \iint \ldots \int \psi\left(\underline{Y}\langle \xi_1 \rangle, \underline{Y}\langle \xi_2 \rangle, \ldots, \underline{Y}\langle \xi_N \rangle\right)$$

$$P_1(\xi_1 + x) P_2(\xi_2 + x) \ldots P_N(\xi_N + x) dV_{\xi_1} dV_{\xi_2} \ldots dV_{\xi_N}$$

If the atomic positions are known exactly

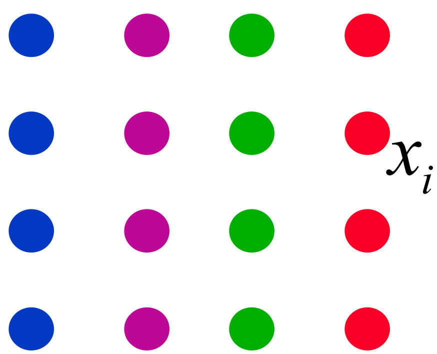
If the atomic positions $\boldsymbol{x}_i$ are known exactly:

$$\text{Set} \quad P_i(x) = \Delta(x - x_i) \quad \Rightarrow$$

$$\rho(x) = M \sum_k \Delta(x - x_i)$$

$$\hat{W}(\underline{Y}, x) = \sum_k \Delta(x - x_k)\psi\left(\underline{Y}\langle x_1 - x\rangle, \underline{Y}\langle x_2 - x\rangle, \ldots, \underline{Y}\langle x_N - x\rangle\right)$$

Same as before



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Total free energy in the statistical peridynamic body

$$
\begin{aligned}
U &= \int \hat{W}\left(\underline{Y}\right) dV_x \\
&= \int \sum_k P_k(x) \int\int \ldots \int \psi\left(\underline{Y}\langle \xi_1 \rangle, \underline{Y}\langle \xi_2 \rangle, \ldots, \underline{Y}\langle \xi_N \rangle\right) \\
&\qquad P_1(\xi_1 + x) P_2(\xi_2 + x) \ldots P_N(\xi_N + x) \, dV_{\xi_1} dV_{\xi_2} \ldots dV_{\xi_N} dV_x \\
&= \sum_k \int\int \ldots \int \psi\left(y_1 - y, y_2 - y, \ldots, y_N - y\right) \\
&\qquad p_1(y_1) p_2(y_2) \ldots p_k(y) \ldots p_N(y_N) \, dV_{y_1} dV_{y_2} \ldots dV_y \ldots dV_{y_N}
\end{aligned}
$$

Conformance

which is what a physicist would say is the expected value of total free energy in the *N*-atom system.

Homogenization:
Smooth out the spatial dependence of PD model

- Choose a scalar-valued weighting function $\varphi(q)$ where q is a vector;

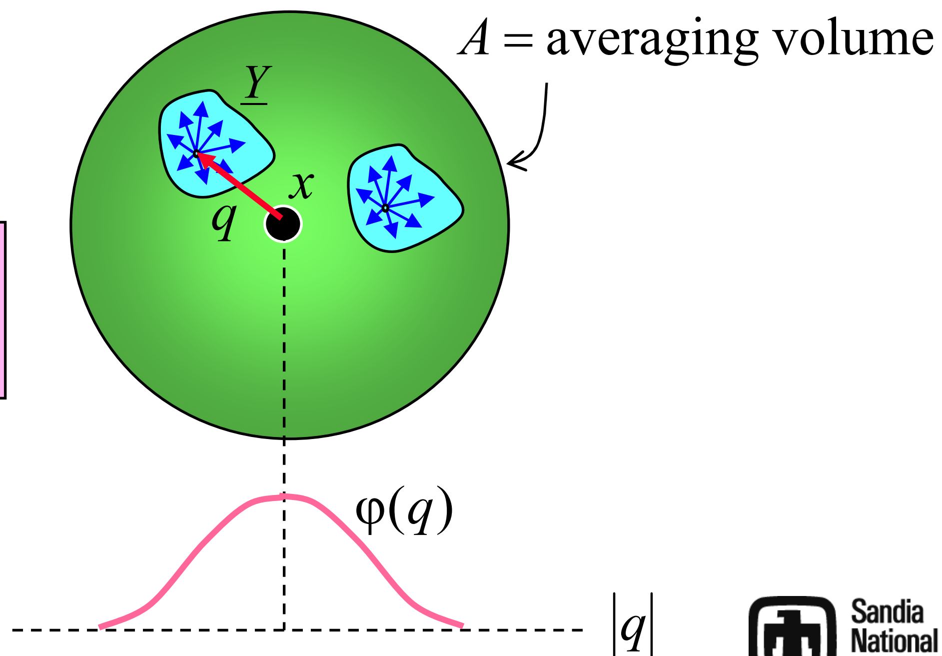
$$\int_A \varphi(q)\,dV_q = 1, \qquad \varphi(q) = \varphi(-q)$$

- Define a homogenized body by

$$\bar{\rho}(x) = \int_A \varphi(q)\rho(x+q)\,dV_q$$

$$\overline{W}(\underline{Y}, x) = \int_A \varphi(q)\hat{W}(\underline{Y}, x+q)\,dV_q$$

q moves around in A while $\underline{Y}$ is held fixed.



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Homogenization

- For a given homogeneous deformation, compute the total strain energy in the homogenized body:

$$
\begin{aligned}
\overline{U} &= \int_{R^3} \overline{W}\left(\underline{Y}, x\right) dV_x = \int_{R^3}\int_{R^3} \varphi(q)\hat{W}\left(\underline{Y}, x+q\right) dV_q dV_x \\
&= \int_{R^3} \varphi(q) dV_q \int_{R^3} \hat{W}\left(\underline{Y}, z\right) dV_z \\
&= \int_{R^3} \hat{W}\left(\underline{Y}, z\right) dV_z \\
&= U
\end{aligned}
$$

- Therefore the total strain energy is unchanged by homogenization.

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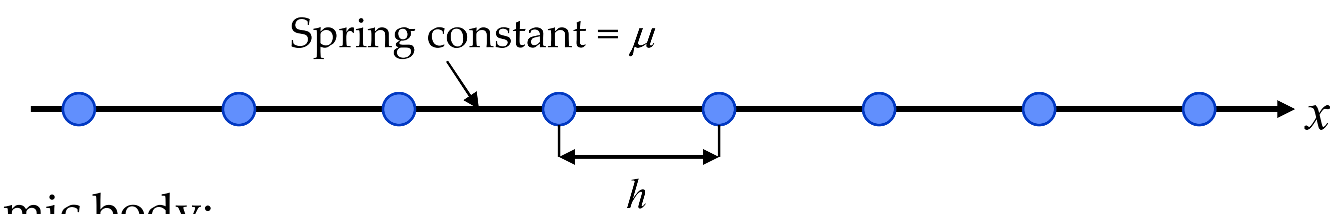
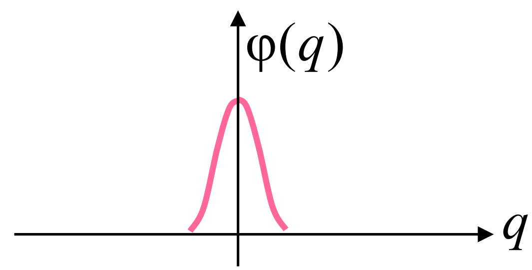
Homogenization example: 1D spring-mass system



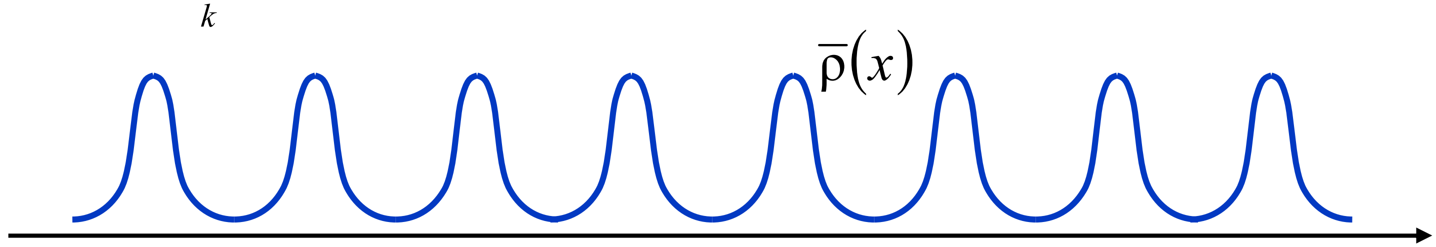
Peridynamic body:

$$\rho(x) = M \sum_k \Delta(x - hk)$$



Peridynamic body after homogenization:

$$\begin{aligned}\bar{\rho}(x) &= \int M \sum_k \Delta(x + q - hk)\varphi(q)\,dq \\ &= M \sum_k \varphi(x - hk)\end{aligned}$$



Homogenization example: 1D spring-mass system

Peridynamic body:

$$\hat{W}\left(\underline{Y},x\right)=\frac{\mu}{4}\sum_{k}\Delta\left(x-hk\right)\left\{\left(\underline{Y}\langle h\rangle-h\right)^{2}+\left(\underline{Y}\langle -h\rangle+h\right)^{2}\right\}$$

Peridynamic body after homogenization:

$$\begin{aligned}\overline{W}\left(\underline{Y},x\right)&=\frac{\mu}{4}\left(\int\sum_{k}\Delta\left(x+q-hk\right)\varphi\left(q\right)dq\right)\left\{\left(\underline{Y}\langle h\rangle-h\right)^{2}+\left(\underline{Y}\langle -h\rangle+h\right)^{2}\right\}\\&=\frac{\mu}{4}\sum_{k}\varphi\left(x-hk\right)\left\{\left(u\left(x+h\right)-u\left(x\right)\right)^{2}+\left(u\left(x-h\right)-u\left(x\right)\right)^{2}\right\}\end{aligned}$$

Homogenization example: 1D spring-mass system

Equation of motion after homogenization boils down to:

$$M\sum_k \varphi(x-hk)\ddot{u}(x,t)=\mu\sum_k \varphi(x-hk)\{u(x-h,t)-2u(x,t)+u(x+h,t)\}$$

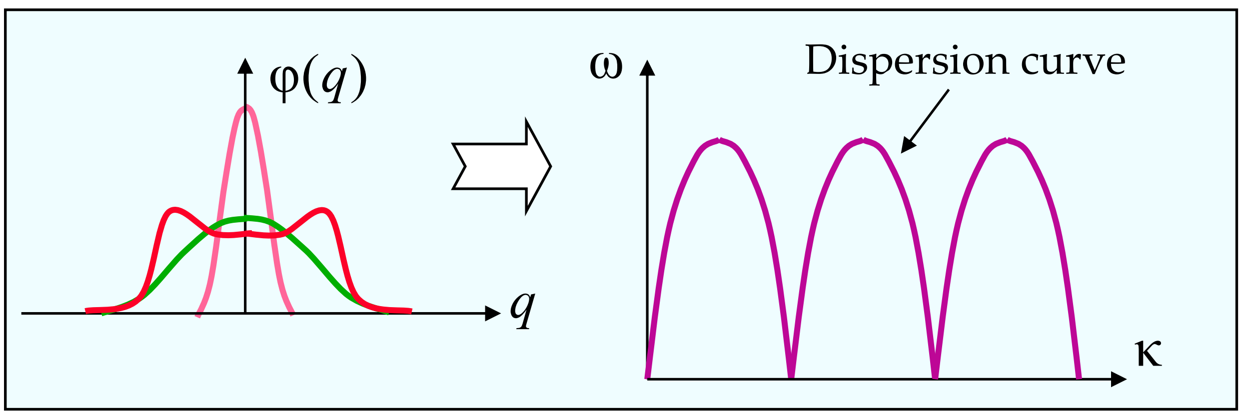
If we assume waves of the form

$$u(x,t)=e^{i(\kappa x-\omega t)}$$

This leads to the following dispersion relation:

$$\omega=\sqrt{\frac{2\mu(1-\cos\kappa h)}{M}}$$

same as for the original spring-mass system, regardless of φ

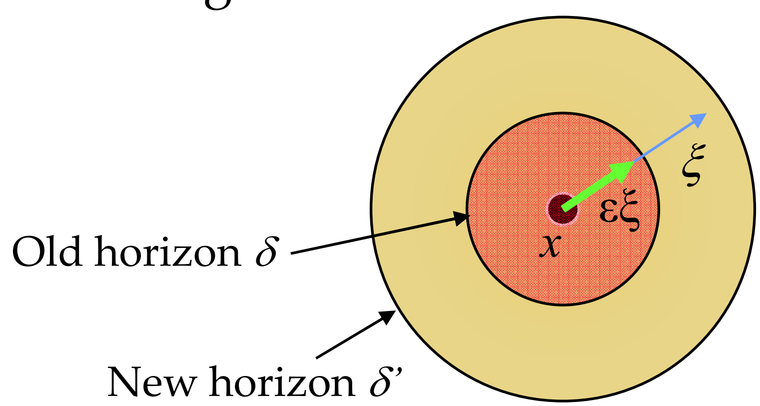


Rescaling:
Increase the length scale of a PD material model

- Take any strain energy density function and change its horizon from δ to δ'.
- Define:

$$\hat{W}_\varepsilon(\underline{Y}) = \hat{W}(\underline{E}(\underline{Y})), \qquad (\underline{E}(\underline{Y}))\langle\xi\rangle = \underline{Y}\langle\varepsilon\xi\rangle, \qquad \varepsilon = \delta/\delta'$$

- Can show the strain energy is invariant under rescaling if the deformation is homogeneous.



Discussion

- The peridynamic theory has a qualitative connection with molecular dyamics.
  - Our slogan: *"Nature integrates"*
- Possible strategy for coarse-graining includes
  - Representation of discrete atoms as a peridynamic continuum.
  - Continuum constitutive model IS the interatomic potential.
  - Homogenize.
  - Rescale.

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Some publications

- Peridynamic theory:
  - S. A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, *JMPS* (2000).
  - S.A. Silling, M. Zimmermann, and R. Abeyaratne, Deformation of a peridynamic bar, *J. Elast.* (2003).
  - O. Weckner and R. Abeyaratne, The effect of long-range forces on the dynamics of a bar, *JMPS* (2005).
  - M. Zimmermann, thesis (MIT, 2004).
  - R. B. Lehoucq and S. A. Silling, Force flux and the peridynamic stress tensor, *JMPS* (2007).
  - S. A. Silling et. al., Peridynamic states and constitutive modeling, *J. Elast.* (2007).
- Atomistics
  - R. B. Lehoucq and S. A. Silling, Statistical coarse-graining of atomistics into peridynamics, Sandia report (2007).
- Numerical method:
  - S.A. Silling and E. Askari, A meshfree method based on the peridynamic model of solid mechanics, *Computers and Structures* (2005).
  - E. Emmrich and O. Weckner, Analysis and numerical approximation of an integro-differential equation modelling non-local effects in linear elasticity, *Mathematics and Mechanics of Solids* (2005).
  - O. Weckner and E. Emmrich, Numerical simulation of the dynamics of a nonlocal, inhomogeneous, infinite bar, *J. Comp. Appl. Mech.* (2005).
  - E. Emmrich and O. Weckner, Energy conserving spatial discretisation methods for the peridynamic equation of motion in the non-local elasticity theory (to appear).
- Fracture and damage (mostly numerical):
  - S.A. Silling and E. Askari, Peridynamic modeling of impact damage, ASME PVP-Vol. 489 (2004).
  - S.A. Silling and F. Bobaru, Peridynamic modeling of membranes and fibers, *International Journal of Non-Linear Mechanics* (2005).
  - F. Bobaru and S.A. Silling, Peridynamic 3D models of nanofiber networks and carbon nanotube-reinforced composites, American Institute of Physics conference proceedings (2004).
- Phase boundaries:
  - K. Dayal and K. Bhattacharya, Kinetics of phase transformations in the peridynamic formulation of continuum mechanics, *JMPS* (2006).